7 Polychlorinated Biphenyls (PCBs)

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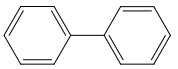
7.1 LIST OF CHEMICALS AND DATA COMPILATIONS

7.1.1 PCB CONGENERS

7.1.1.0 Biphenyl

(See also Chapter 4, Polynuclear Aromatic Hydrocarbons [PAHs] and Related Aromatic Hydrocarbons)



Common Name: Biphenyl
Synonym: diphenyl, phenylbenzene
Chemical Name: biphenyl
CAS Registry No: 92-52-4
Molecular Formula: $C_{12}H_{10}$
Molecular Weight: 154.207
Melting Point (°C):
68.93 (Lide 2003)
Boiling Point (°C):
256.1 (Lide 2003)
Density (g/cm^3 at 20°C):
0.866 (20°C, Weast 1982–1983)
1.04 (Lide 2003)
Molar Volume (cm^3/mol):
148.3 (20°C, calculated-density)
184.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18.58 (Parks & Huffman 1931)
18.66 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
51.05 (Miller et al. 1984)
54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.371 (mp at 68.93°C)
0.35 (Mackay et al. 1980,1983; Shiu & Mackay 1986; Shiu et al. 1987)
0.381 (calculated, ΔS_{fus} = 54 J/mol K, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
5.94 (shake flask-UV, Andrews & Keefer 1949)
7.48* (shake flask-UV, measured range 0.4–42.8°C, Bohon & Claussen 1951)
3.87 (shake flask-UV, Sahyun 1966)
7.08* (shake flask-UV, measured range 0–64.5°C, Wauchope & Getzen 1972)
$R \cdot \ln x = -4520/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 298.15]^2 - 20.8 + 0.0273 \cdot (T/K)$, temp range 24.6–73.4°C (shake flask-UV measurements, Wauchope & Getzen 1972)
7.45 (shake flask-GC, Eganhouse & Calder 1976)
7.0 (shake flask-fluorescence, Mackay & Shiu 1977)
8.50 (shake flask-nephelometry, Hollifield 1979)
7.51 (shake flask-LSC, Banerjee et al. 1980)
8.09 (TLC-RT correlation, Bruggeman et al. 1982)
6.71 (generator column-GC/ECD, Miller et al. 1984, 1985; quoted, Hawker 1989b)
7.09 (recommended, Pearlman et al. 1984)
7.05 (vapor saturation-UV, Akiyoshi et al. 1987)
6.5 (29°C, shake flask-GC/FID; Stucki & Alexander 1987)
7.20, 7.55 (generator column-HPLC/UV, Billington et al. 1988)

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9.96, 9.96, 9.96, 10.67 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.2* (recommended, IUPAC Solubility Data Series, Shaw 1989)
log [S_L/(mol/L)] = 1.872 –973.4/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln x = –1.5792 – 3669.26/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
5.37, 5.32 (generator column-GC/ECD, different flow rates, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
7933* (162.5°C, isoteniscope-manometer, measured range 162.5–255.2°C, Chipman & Peltier 1929)
104* (69.20°C, temp range 69.20–271.2°C, Cunningham 1930; quoted, Boublik et al. 1984)
133.3* (70.6°C, summary of literature data, temp range 70.6–254.0°C, Stull 1947)
1.30 (effusion method, measured range 4.0–34.5°C, Bright 1951)
log (P/mmHg) = 10.38 – 3799/(T/K); temp range: 4.0–34.5°C (Antoine eq., effusion, Bright 1951)
0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)
1.273* (effusion method, measured range 15.05–40.55°C, Bradley & Cleasby 1953)
log (P/cmHg) = 11.282 – 4263/(T/K); temp range 15.05–40.55°C (Antoine eq., Bradley & Cleasby 1953)
log (P/mmHg) = [– 0.2185 × 12910.0/(T/K)] + 8.218583; temp range 70.6–254.9°C (Antoine eq., Weast 1972–73)
1.41* (effusion method, interpolated-Antoine eq., measured range 24.9–50.33°C, Radchenko & Kitiagorodskii 1974)
log (P/mmHg) = 12.6789 – 4367.436/(T/K); temp range; 24.9–50.33°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)
2040* (123.0°C, pressure transducer, measured range 123.0–327.55°C, Nasir et al. 1980)
1.40 (HPLC-RT correlation, Swann et al. 1983)
log (P/atm) = [1 – 528.437/(T/K)] × 10^{0.821410 – 2.73337 × 10^{-4}·(T/K) + 1.02285 × 10^{-7}·$(T/K)^2$}; temp range: 342.35–673.15 K (Cox eq., Chao et al. 1983)
3.35, 3.41 (P_{GC} by GC-RT correlation, different GC columns, Bidleman 1984)
5.608 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
log (P/kPa) = 6.36895 – 1997.558/(202.608 + t/°C), temp range: 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1.15* (24.7°C, gas saturation-GC/FID, measured range 5.2–24.7°C, Burkhard et al. 1984)
log (P/Pa) = 14.840 – 4402.1/(T/K), temp range: 5.2–24.7°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)
2.03 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 7.24541 – 1998.725/(202.733 + t/°C), temp range: 69–271°C (Antoine eq., Dean 1985, 1992)
5.61; 6.62 (supercooled liquid P_L, quoted lit.; GC-RT correlation, Foreman & Bidleman 1985)
2.43; 6.90 (selected P_S; supercooled liq. P_L, Shiu & Mackay 1986; Shiu et al. 1987; Sklarew & Girvin 1987)
1.443; 1.23 (P_S, interpolated-Antoine equations; Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.71929 – 4143.054/(T/K); temp range 297–324 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 28.5175 – 21141.5/(374.85 + T/K); temp range: 283–342 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.37526 – 1794.8/(– 74.85 + T/K), temp range: 390–563 K, (Antoine eq.-III, Stephenson & Malanowski 1987)
5.10, 5.00 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
3.35 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)
0.422–2.54; 2.03–7.04(quoted range of lit. P_S values; lit. P_L values, Delle Site 1997)
5.31; 2.02 (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 11.05 – 3201/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 8.20 – 2228/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P/kPa) = 14.840 – 4402.1/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
3.63; 0.822 (supercooled liquid P_L, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
log (P_L/Pa) = – 3265/(T/K) + 11.51; ΔH_{vap}.= – 62.5 kJ·mol^{-1} (GC-RT correlation, Lei et al. 2002)

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Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

41.34 (batch stripping-GC, Mackay et al. 1979)
30.4 (batch stripping-GC, Mackay et al. 1980;)
11.55 (gas stripping-GC, Warner et al. 1987)
19.57 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
31.20 (gas stripping-GC, Shiu & Mackay 1997)
log [H/(Pa m^3/mol)] = 6.33 – 1255/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:

3.16 (shake flask-UV, Rogers & Cammarata 1969)
4.09 (shake flask, Leo et al. 1971; Hansch & Leo 1979)
4.04 (shake flask, Hansch et al. 1973)
4.17, 4.09, 3.16, 4.04 (Neely et al. 1974; Hansch & Leo 1979)
3.95 (HPLC-k′ correlation, Rekker & De Kort 1979)
3.75 (HPLC-RT correlation, Veith et al. 1979a)
4.04 (shake flask-HPLC, Banerjee et al. 1980)
3.88 (lit. average, Kenaga & Goring 1980)
4.10 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
4.08 (HPLC-k′ correlation, Hammers et al. 1982)
3.70 (HPLC-RT correlation, Woodburn 1982; Woodburn et al, 1984)
3.16–4.09, 3.91 (shake flask, range, average, Eadsforth & Moser, 1983)
3.91–4.15, 4.05 (HPLC, range, average, Eadsforth & Moser 1983)
4.03 (HPLC-k′ correlation, Hafkenscheid & Tomlinson 1983)
3.93 (HPLC correlation; Harnisch et al. 1983)
3.76 (generator column-GC/ECD, Miller et al. 1984,1985)
3.89 (generator column-HPLC, Woodburn et al. 1984)
3.79 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.11–4.13 (HPLC-RV correlation, quoted exptl., Garst 1984)
4.10 (HPLC-RV correlation, Garst & Wilson 1984)
4.05 (HPLC-RT correlation, Eadsforth 1986)
3.81 (shake flask-GC, Menges & Armstrong 1986)
4.13 (HPLC-RT correlation, Wang et al. 1991)
3.63 (HPLC-k′ correlation; De Kock & Lord 1987)
3.89 (generator column-GC, Doucette & Andren 1987,1988)
4.14, 4.06, 4.00, 3.94 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.69 (HPLC-RT correlation, Doucette & Andren 1988)
3.75 (HPLC-RT correlation, Sherblom & Eganhouse 1988)
4.008; 4.10 (slow stirring-GC; calculated-π const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
3.98 (recommended, Sangster 1989, 1993)
4.29 (dual-mode centrifugal partition chromatography, Gluck & Martin 1990)
4.26 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

6.92, 6.09; 6.09 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
6.15 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

2.64 (trout, calculated-k_1/k_2, Neely et al. 1974)
3.12 (rainbow trout, Veith et al. 1979; Veith & Kosian 1983)
2.53 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
2.73, 2.45, 3.41 (algae, fish, activated sludge, Freitag et al. 1985)

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Sorption Partition Coefficient, log K_{OC}:

3.15 (soil, Kenaga 1980)

3.0, 3.27 (Aldrich humic acid, reversed phase separation, Landrum et al. 1984)

3.57, 3.77 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/L DOC, Landrum et al. 1984)

5.58, 4.04 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)

5.68, 5.34, 5.23, 3.57 (humic materials in natural water: Huron River 6.7% DOC spring, Grand River 10.7% DOC spring, Lake Michigan 4.7% DOC spring, Lake Erie 9.6% DOC spring, RP-HPLC separation method, Landrum et al. 1984)

3.52, 2.94 (Apison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium, Southworth & Keller 1986)

3.40 (calculated, soil, Chou & Griffin 1986)

3.04, 3.32, 3.26, 3.04, 3.08 (5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)

4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

3.03, 3.12 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average values, Delle Site 2001)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization/Evaporation: $t_{½}$ = 7.52 d evaporation from water depth of 1 m (Mackay & Leinonen 1975)
rate of volatilization k = 0.92 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis: k = 5.1×10^{-4} h^{-1} to 7.4×10^{-3} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988);
photodegradation k = 5.1×10^{-4} min^{-1} and $t_{½}$ = 22.61 h in methanol-water (3:7, v/v) with initial concentration of 16.2 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = (8.06 \pm 0.77) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with an estimated lifetime of ~3 d, and $k_{O3} < 2.0 \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} at 294 ± 1 K (relative rate method, Atkinson et al. 1984)
$k_{OH} = (8.5 \pm 0.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1985)
$k_{OH} = (7 \pm 2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1985)
k_{OH}(calc) = 7.9×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = $(5.8 – 8.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)
k_{OH}(calc) = 7.1×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 7.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (SAR structure-activity relationship, Atkinson 1987b)
$k_{O3} < 2 \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1}; $k_{OH} = 7.0 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}; $k_{N2O5} < 2.0 \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} for reaction with N_2O_5 at room temp (Atkinson & Aschmann 1988)
k_{OH}* = 7.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH}(calc) = 6.44×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)
k_{OH}(exptl) = 7.2×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 6.7×10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 2.0 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 100% degraded by activated sludge in 47 h cycle (Monsanto Co. 1972)
k = 109 yr^{-1} in the water column and k = 1090 yr^{-1} in the sediment, microbial degradation pseudo first-order rate constant (Wong & Kaiser 1975; selected, Neely 1981)
k = 9.3–9.8 nmol L^{-1} d^{-1} with an initial biphenyl concentration of 4.4–4.7 µmol/L, and k = 3.2 nmol L^{-1} d^{-1} with initial concentration of 2.9 µmol/L, rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)
$t_{½}$ = 1.5 d, estimated by using water die-away test (Bailey et al. 1983)
$t_{½}$(aq. aerobic) = 36–168 h, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)
$t_{½}$(aq. anaerobic) = 144–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

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removal rate of 5.3 and 0.52 mg (g of volatile suspended solid d)$^{-1}$, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

k_1 = 6.79 h^{-1}; k_2 = 0.0155 h^{-1} (trout muscle, Neely et al. 1974; Neely 1979)

k_1 = 6.8 h^{-1}; $1/k_2$ = 65 h (trout, quoted, Hawker & Connell 1985)

log k_1 = 2.21 d^{-1}; log $1/k_2$ = 0.43 d (fish, Connell & Hawker 1988)

log k_2 = – 0.43 d^{-1} (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air: calculated lifetime of ~3 d due to reaction with OH radical, assuming an average daytime atmospheric OH radical concn of ~1 × 10^6 molecule/cm^3 (Atkinson et al. 1984);

estimated atmospheric lifetime of ~2.7 d due to reaction with the OH radical for a 24-h average OH radical concn of 5 × 10^5 cm^{-3} (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 9 d due to the rate constants of gas-phase reaction with OH radical (Atkinson 1987);

$t_{½}$ = 7.8–110 h, based on photooxidation half-life in air (Howard et al. 1991);

tropospheric lifetime of 2.0 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for biphenyl (Kwok et al. 1995).

Surface water: $t_{½}$ ~1.5 d in river water (Bailey et al. 1983);

$t_{½}$ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

photolysis $t_{½}$ = 19.18 min in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{½}$ = 72–336 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{½}$ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota: estimated $t_{½}$ = 29 h from fish in simulated ecosystem (Neely 1980).

TABLE 7.1.1.0.1
Reported aqueous solubilities of biphenyl at various temperatures:

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
			experimental		smoothed		
0.40	2.83	24.6	7.13	0	2.64	0	2.72
2.4	2.97	24.6	7.29	24.6	6.96	10	4.1
5.2	3.38	24.6	7.35	25	7.08	20	6.3
7.6	3.64	29.9	8.77	29.9	8.73	25	7.2
10	4.06	29.9	8.64	30.3	8.88	30	9.1
12.6	4.58	29.9	895	38.4	12.7	40	14.4
14.9	5.11	30.3	8.55	40.1	13.8	50	22
15.9	5.27	30.3	8.54	47.5	19.5	69	37
25	7.48	30.3	8.48	50	22.0		
25.6	7.78	38.4	13.2	50.1	22.1		
30.1	9.64	38.4	13.3	50.2	22.2		
30.4	9.58	38.4	13.5	54.7	27.7		
33.3	11.0	40.1	13.1	59.2	34.8		
34.9	11.9	40.1	13.4	60.5	37.2		
36	12.5	40.1	13.4	64.5	45.9		
42.8	17.2	47.5	18.8				
		47.5	19.0	temp dependence eq. 1			

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TABLE 7.1.1.0.1 (*Continued*)

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
for supercooled liquid:		47.5	18.7	ln *x*	mole fraction		
ΔH_{sol}/(kJ mol^{-1}) =		50.1	20.6	ΔH_{fus}	18.9 ± 0.50		
at 275 K	7.03	50.1	21.6	10^2·b	2.73 ± 0.12		
280 K	10.13	50.1	21.8	c	20.8 ± 0.4		
285 K	11.25	50.2	20.7				
290 K	12.55	50.2	21.8				
295 K	13.43	54.7	28.3				
300 K	15.02	54.7	28.8				
305 K	18.58	59.2	36.4				
310 K	21.42	59.2	36.3				
315 K	21.09.	59.2	36.0				
		60.5	40.4				
		64.5	43.7, 44.7				
		64.5	46.5				
		ΔH_{fus}/(kJ mol^{-1}) = 18.91					

Empirical temperature dependence equations:

Wauchope & Getzen (1972): $R \cdot \ln x = -[H_{fus}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K)$ (1)

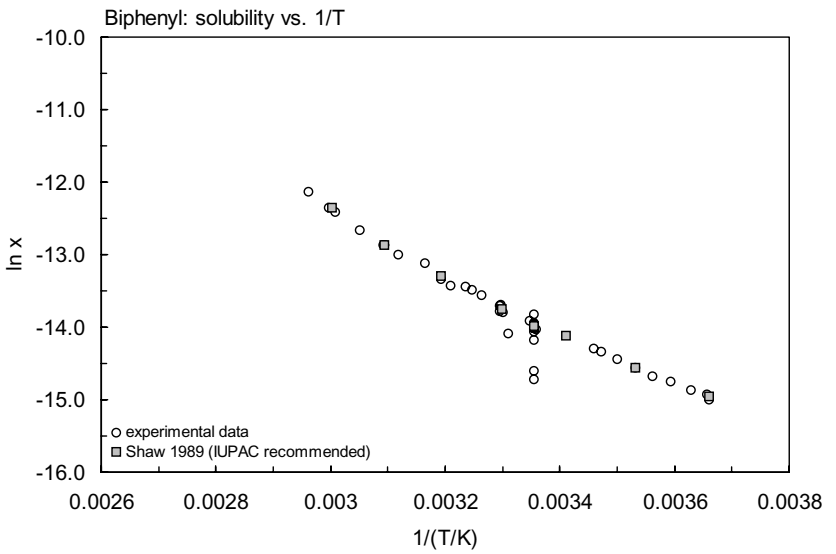

FIGURE 7.1.1.0.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for biphenyl.

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TABLE 7.1.1.0.2
Reported vapor pressures of biphenyl at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C/(T/K)^2$	(5)		

1.

Chipman & Peltier 1929		Stull 1947		Bright 1951		Bradley & Cleasby 1953	
isoteniscope-manometer		summary of literature data		effusion		effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
162.5	7933	70.6	133.3	Data presented in graph		15.05	0.416
172.3	10959	101.8	666.6	25	0.579	20.7	0.7786
177.7	12799	117.0	1333		(interpolated)	24.7	1.2252
183.5	15705	134.2	2666	eq. 1	P/mmHg	24.0	1.1825
191.6	19972	152.5	5333	A	10.38	24.1	1.184
198.75	24691	165.2	7999	B	3799	27.05	1.600
293.8	28504	180.7	13332	temp range 4.9–34.5°C		29.15	2.053
211.25	34677	204.2	26664			32.45	2.973
220.05	43756	229.4	53329	$\Delta H_{subl}/(kJ\ mol^{-1}) = 72.80$		35.05	3.866
229.8	56329	254.0	101325			37.9	5.160
238.2	68901					40.55	6.693
247.7	85580	mp/°C	69.5			23.05	1.027
253.7	98019					36.5	1.533
255.2	101178					31.25	2.546
						35.9	4.133
bp/°C	266.25						
$\Delta H_V/(kJ\ mol^{-1}) = 44.99$ at bp						eq. 1	P/mmHg
						A	11.282
						B	4262
eq. 5	P/mmHg					temp range 15–41°C	
A	7.0220						
B	1723						
C	245700						
temp range 162–322°C							

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TABLE 7.1.1.0.2 *(Continued)*

2.

Radchenko& K. 1974		Nasir et al. 1980		Burkhard et al. 1984		Cunningham 1930	
Knudsen effusion		pressure transducer		gas saturation-GC		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.9	1.433	123.0	2040	5.2	0.106	69.20	104
31.75	2.976	143.81	4773	14.9	0.361	93.3	413
33.7	3.734	164.69	9962	24.7	1.15	148.7	4833
35.5	4.538	181.28	16447			160.0	7239
37.6	5.726	200.87	28599	eq. 1	P/Pa	171.1	10548
39.57	6.913	223.66	51518	A	14.840	182.2	15031
41.52	8.26	245.65	86254	B	4402.1	193.3	21098
43.48	10.26	257.91	111343			204.4	28958
45.45	12.35	274.09	154493			215.6	39093
47.4	15.49	296.14	235345			226.7	51986
50.0	19.46	315.19	329300			237.8	68051
		327.55	400175			248.9	88252
eq. 1	P/mmHg					255.3	101353
A	12.6789	data fitted to				260.0	112384
B	4367.436	Chebyshev polynomial				271.2	142032
for temp range 24.9–50°C							
						eq. 2	P/kPa
						A	6.36895
Sharma & Palmer 1974						B	1997.558
gas saturation-GC						C	202.608
t/°C	P/Pa					bp/°C	255.208
53.05	16.0						
61.05	34.66						
71.95	92.0						
81.05	220.0						

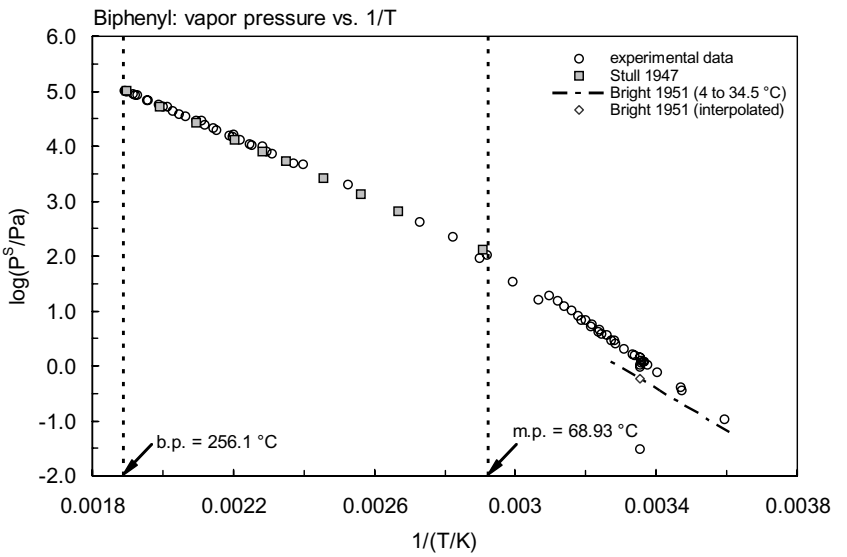

FIGURE 7.1.1.0.2 Logarithm of vapor pressure versus reciprocal temperature for biphenyl.

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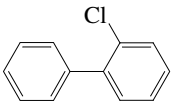
7.1.1.1 2-Chlorobiphenyl (PCB-1)



Common Name: 2-Chlorobiphenyl
Synonym: PCB-1, *o*-chlorobiphenyl, 2-chloro-1,1′-biphenyl
Chemical Name: 2-chlorobiphenyl
CAS Registry No: 2051-60-7
Molecular Formula: $C_{12}H_9Cl$
Molecular Weight: 188.652
Melting Point (°C):
34 (Beaven et al. 1961; Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
274 (Weast 1972–73, 1082–83; Lide 2003)
Density (g/cm^3 at 20°C): 0.9837
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
57.8 (Geidarov et al. 1975)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
72.3 (Geidarov et al. 1975)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
14.52 (Geidarov et al. 1975)
15.3 (differential scanning calorimetry, Miller et al. 1984)
14.54 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
47.66 (Geidarov et al. 1975)
50.21 (Miller et al. 1984)
Fugacity Ratio at 25°C, F (assuming ΔS_{fus} = 56 J/mol K), F: 0.816 (mp at 34°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1.60 (Webb 1970)
0.90 (Hoover 1971)
5.90 (shake flask-GC/ECD, Wallnöfer et al. 1973)
4.13 (generator column-GC/ECD, Weil et al. 1974)
5.08 (supercooled liquid S_L, shake flask-GC/ECD, Chiou et al. 1983)
5.06 (generator column-GC/ECD, Miller et al. 1984,1985)
4.13, 4.74, 14.0, 4.13 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (89.3°C, summary of literature data, temp range 89.3–267.5°C, Stull 1947)
log (P/mmHg) = (8.306 ± 0.087) – (3018 ± 45)/(T/K), temp range: 410–510 K (static method-quartz manometer measurements, Geidarov et al. 1975)
1.84 (supercooled liquid P_L, extrapolated Antoine eq., Weast 1976–77)
1.12 (Neely 1981,1983)
0.605; 0.159; 0.367* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from exptl. derived Antoine eq., measured range 33–110°C, Ferro et al. 1983)

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log (P_L/kPa) = – 3893/(T/K) + 9.99; temp range: 33–77°C (Knudsen effusion data, Ferro et al. 1983)
log (P_L/kPa) = – 4406/(T/K) + 10.98; temp range: 64–110°C (torsion effusion data, liquid, Ferro et al. 1983)
log (P_L/kPa) = – (4149 ± 230)/(T/K) + (10.48 ± 0.50); temp range: 33–110°C (torsion-Knudsen effusion data, Ferro et al. 1983)
1.096, 1.456 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
1.892, 2.56 (supercooled liquid P_L from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.755 (GC-RI correlation, Burkhard et al. 1985a)
0.926 (GC-RI correlation, supercooled liquid P_L, Burkhard et al. 1985b)
2.20 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
1.096 (P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
log (P_L/Pa) = – 3366/(T/K) + 11.57 (GC-RT correlation, Falconer & Bidleman 1994)
0.27–2.70; 0.367–2.56 (literature P_S range; literature supercooled liquid P_L range, Delle Site 1997)
log (P/kPa) = 9.99 – 3893/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

28.9 (calculated-P/C, Burkhard et al. 1985b)
70.1 (calculated-P/C, Shiu & Mackay 1986)
74.6 (Dow Chemical, Neely 1982)
30.18 (calculated-QSPR, Dunnivant et al. 1992)
5.13, 8.32, 13.17, 20.43 ± 0.52, 29.3 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[– (42.7/kJ·mol^{-1})/ RT] + (0.104/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
22.0 (gas stripping-GC, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 43 ± 6 kJ/mol, ΔS_H = 0.10 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:

4.54 (shake flask-GC, Tulp & Hutzinger 1978)
4.80 (Hansch & Leo 1979)
4.35 (HPLC-RT correlation, Veith et al. 1979)
4.10 (HPLC-RT correlation, McDuffie 1981)
4.59 ± 0.1; 4.56(shake flask-GC; RP-TLC-k′ correlation, Bruggeman et al. 1982)
3.75 (HPLC-RT correlation, Woodburn 1982)
4.51 (shake flask-GC, Chiou et al. 1983)
4.50 (generator column-GC, Miller et al. 1984,1985)
4.38 (generator column-HPLC, Woodburn et al. 1984)
3.90, 4.60 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.44 (HPLC-RP/MS correlation, Burkhard & Kuehl 1986)
4.38 (generator column-GC/ECD, Doucette & Andren 1987)
4.33, 4.39, 4.53, 4.43 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.92 (HPLC-RT correlation, Doucette & Andren 1988)
4.531 ± 0.029(shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
4.52 (recommended, Sangster 1989, 1993)
4.68 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated:

7.54, 6.65 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
6.04 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

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Sorption Partition Coefficient, log K_{OC}:

3.50 (Woodburn silt loam soil, batch equilibrium isotherm-GC/ECD, Chiou et al. 1983)
4.35 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.47 (calculated, soil, Chou & Griffin 1986)
2.59 (Borden soil 0.29% OC, Hu et al. 1995)

Sorption Partition Coefficient, log K_{OM}:

3.23 (soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

k(calc) = 3.7×10^{-4} d^{-1} and with $t_{½}$ = 18 yr, calculated sunlight photolysis rate constant in surface water at 40°N in summer (Dulin et al. 1986)

k(calc) = 3.0 h^{-1} maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)

$t_{½}$ = 31 d under sunlight in water (Mansour & Feicht 1994)

k = 0.081 min^{-1} at pH 3, k = 0.045 min^{-1} at pH 7 and k = 0.035 min^{-1} at pH 10 with half-lives of 9, 15 and 20 min, respectively, in aqueous solutions when irradiated by UVA-340 light tubes in the presence of 25 µg/mL of TiO_2;

k = (0.043–0.045) min^{-1} with $t_{½}$ = 15–16 min, k = (0.082–0.091) min^{-1} with $t_{½}$ = 8 min, and k = (0.21–0.29) min^{-1} with $t_{½}$ = 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively;

k = (0.043–0.044) min^{-1} with $t_{½}$ = 15–16 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2;

k = (0.030–0.055) min^{-1} with $t_{½}$ = 13–22 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.9 \pm 0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K with estimated atmospheric lifetime of ~8 d (relative rate method, Atkinson & Aschmann 1985)

$k_{OH} = 1.6 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to the C_6H_4Cl ring (ring B), $k_{OH} = 1.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to ring A, and $k_{OH} = 2.8 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)

k_{OH}(calc) = $(2.8 – 5.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = $(3.1 – 4.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)

$k_{OH} = 2.82 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1989)

k_{OH}(exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = $(3.2 – 4.6) \times 10^{-12}$ cm^3 $molecule^{-1} \cdot s^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{½}$ = 100 h biodegradation by bacteria (Wong & Kaiser 1975);

within 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

k = 63 yr^{-1} microbial degradation pseudo first-order rate constant of in the water column and k = 630 yr^{-1} in the sediment (Wong & Kaiser 1975; quoted, Neely 1981);

k = 4.1 nmol L^{-1} d^{-1} biodegradation rate in water from Port Valdez with an initial concn of 1.5 µmol/L (data of Aug. 1977, Reichardt et al. 1981) and k = 1.2 nmol L^{-1} d^{-1} with initial concn of 4.5 µmol/L (data of Aug. 1978, Reichardt et al. 1981); and $t_{½}$ = 2–3.5 d, an initial concn of 1–100 µg/L by river dieaway test (Bailey et al. 1983)

k = 1.10 µg mL^{-1} d^{-1}, the degradation rate at 30 µg mL^{-1}, under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Sayler 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

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Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~8 d due to reaction with the OH radical for a 24-h average OH radical concn of 5×10^5 cm^{-3} (Atkinson & Aschmann 1985);
calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);
photolysis $t_{½}$ ~10–25 h for noontime summer sunshine, or more realistically, several days (Bunce et. 1989);
tropospheric lifetime of 3 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);
tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 1.4 d in Lake Michigan (Neely 1983);
photolysis $t_{½}$ = 18 yr in surface water at 40° L in summer (Dulin et al. 1986);
photolysis $t_{½}$ = 31 d under sunlight (Mansour & Feicht 1994);
half-lives in aqueous solutions with initial concn of 265 ng/mL, $t_{½}$ = 9 min at pH 3, $t_{½}$ = 15 min at pH 7 and $t_{½}$ = 20 min at pH 10 when irradiated by UVA-340 light tubes (simulated sun light) in the presence of 25 µg/mL TiO_2, half-lives of 15–16 min, 8 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; half-lives of 15–16 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{½}$ = 13–22 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:
Sediment:
Soil:
Biota:

TABLE 7.1.1.1.1
Reported vapor pressures of 2-chlorobiphenyl (PCB-1) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log (P/mmHg) = A - B/(C + t/°C)$ (2)
$\log (P/Pa) = A - B/(C + T/K)$ (3)
$\log (P/mmHg) = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		Geidarov et al. 1975		Ferro et al. 1983			
compiled literature data		static-quartz manometer		torsion effusion		Knudsen	average
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	P/Pa	P/Pa
				cell C			
89.3	133.3	exptl data presented as eq. 1		50	10.3	17.3	13.8
109.8	666.7	eq 1	P/mmHg	54	10.9	19.2	10.0
134.7	1333	A	8.306	59	16.2	24.8	20.5
151.2	2666	B	3018	63	25.6	36.9	32.2
169.9	5333	range: 137–267°C		cell C			
182.1	7999			50	8.1	12.8	10.4
197.0	13333	mp/°C	31.61	59	15.8	22.9	20.6
219.6	26664	bp/°C	24	69	34.1	51.1	46.1
243.8	53329			73	44.3	65.5	59.0
267.5	101325	ΔH_v/(kJ mol^{-1}) = 57.78		77	63.3	85.8	78.0
		ΔH_{fus}/(kJ mol^{-1}) = 14.52		81	83.5	115	99.2

(*Continued*)

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TABLE 7.1.1.1.1 (*Continued*)

Stull 1947		Geidarov et al. 1975		Ferro et al. 1983			
compiled literature data		static-quartz manometer		torsion effusion		Knudsen	average
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	P/Pa	P/Pa
mp/°C	34.0	ΔS_{fus}/(J mol^{-1}K^{-1}) = 47.66		86	120	163	142
		ΔH_{subl}/(kJ mol^{-1}) = 72.30		cell B			
				28	0.762	1.50	1.13
				33	1.52	2.36	1.93
				37	2.30	3.42	2.85
				40	3.05	4.13	3.59
				46	3.81	5.17	4.50
				50	4.57	6.10	5.34
				54	6.10	9.69	7.90
				eq. 1	P/mmHg	P/mmHg	P/mmHg
				A	10.98	9.99	10.48
				B	4406	3898	4149
				temp range: 64–110°C		33–86°C	
				ΔH_v/(kJ mol^{-1}) = 79.4			

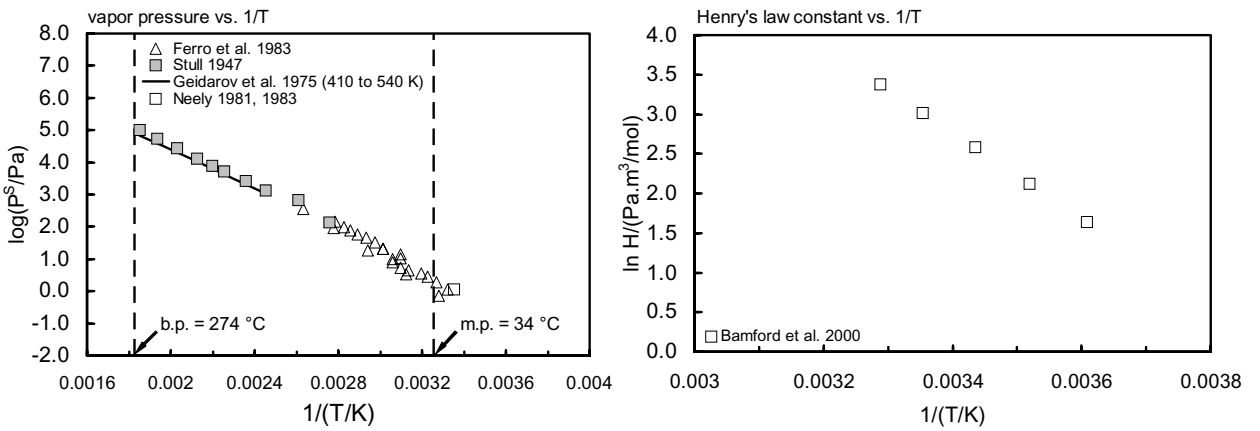

FIGURE 7.1.1.1.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for 2-chlorobiphenyl (PCB-1).

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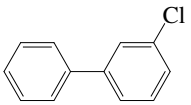
7.1.1.2 3-Chlorobiphenyl (PCB-2)



Common Name: 3-Chlorobiphenyl
Synonym: PCB-2, *m*-chlorobiphenyl, 3-chloro-1,1′-biphenyl
Chemical Name: 3-chlorobiphenyl
CAS Registry No: 2051-61-8
Molecular Formula: $C_{12}H_9Cl$
Molecular Weight: 188.652
Melting Point (°C):
16 (Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
284.5 (Lide 2003)
Density (g/cm^3 at 20°C): 0.9837
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
15.31 (Miller et al. 1984)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0 (mp at 16°C)

Water Solubility (g/m^3 or mg/L at 25°C):
3.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
1.30 (generator column-GC/ECD, Weil et al. 1974)
0.56, 0.82, 0.88, 0.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.63 (generator column-HPLC/UV, Billington et al. 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.723 (extrapolated P_L, Antoine eq., Weast 1972–73)
0.711; 4.01; 0.362* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from exptl. derived Antoine eq., measured range 37–129°C, Ferro et al. 1983)
$\log (P_L/kPa) = -3458/(T/K) + 8.45$; temp range: 37–86°C (Knudsen effusion data, liquid, Ferro et al. 1983)
$\log (P_L/kPa) = -3371/(T/K) + 8.91$; temp range: 68–129°C (torsion effusion data, liquid, Ferro et al. 1983)
$\log (P_L/kPa) = -(3614 \pm 188)/(T/K) + (8.68 \pm 0.47)$; temp range: 37–129°C (torsion-Knudsen effusion data, Ferro et al. 1983)
0.98, 1.01 (supercooled P_L, GC-RT correlation with different stationary phases, Bidleman 1984)
0.366 (GC-RI correlation, Burkhard et al. 1985a)
0.362 (liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.997 (liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -3476/(T/K) + 11.65$ liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.220–1.01 (quoted lit. range, Delle Site 1997)
$\log (P/Pa) = 11.64178 - 3514.98/(T/K)$ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C):
14.49 (calculated-P/C, Burkhard et al. 1985b)
75.55 (calculated-P/C, Shiu & Mackay 1986)
62.11 (Dow Chemical, Neely 1982)
27.78 (calculated-QSAR, Dunnivant et al. 1992)

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20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.54 (shake flask-GC/ECD, Tulp & Hutzinger 1978)
4.35 (HPLC-RT correlation, Veith et al. 1979)
4.80 (Hansch & Leo 1979)
4.71 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)
4.72 (RP-TLC-retention time correlation, Bruggeman et al. 1982)
4.35 (HPLC-RT correlation, Woodburn 1982)
4.58 (generator column-HPLC, Woodburn et al. 1984)
3.75 (HPLC-RT correlation, Woodburn et al. 1984)
4.60 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.60 (selected, Shiu & Mackay 1986)
4.58 (generator column.-GC/ECD, Doucette & Andren 1987)
4.65 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
4.58 (recommended, Sangster 1989, 1993)
4.72 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.58 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
7.86, 6.99 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
6.88 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
4.42 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.62 (calculated-S, soil, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
$t_{½}$ = 45 d under sunlight in water (Mansour & Feicht 1994)
k(calc) = 0.5 h^{-1}, maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)
k = (0.036–0.045) min^{-1} with $t_{½}$ = 15–19 min, k = (0.069–0.085) min^{-1} with $t_{½}$ = 8–10 min, and k = (0.18–0.23) min^{-1} with $t_{½}$ = 3–4 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively;
rate constant of k = (0.027–0.042) min^{-1} with $t_{½}$ = 16–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2;
k = (0.033–0.036) min^{-1} with $t_{½}$ = 19–21 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = (5.4 \pm 0.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 ± 1 K, with an estimated atmospheric lifetime of ~4 d (relative rate method, Atkinson & Aschmann 1985)
$k_{OH} = 2.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to the C_6H_4Cl ring (ring B), $k_{OH} = 1.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to ring A, and $k_{OH} = 5.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)
k_{OH}(calc) = $(2.8 - 5.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = $(3.1 - 4.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)
$k_{OH} = 5.28 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1989)

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k_{OH}(exptl) = (2.8 – 5.3) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = (3.2 – 4.6) × 10^{-12} cm^3 $molecule^{-1}$·s^{-1}, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegradation $t_{½}$ ≈ 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumara 1976; selected, Pal et al. 1980);

biodegradation rate k ~ 2.6 nmol L^{-1} d^{-1} with an initial concentration of 3.6 µmol L^{-1} in water from Port Valdez estimated to be (data of August 1977, Reichardt et al. 1981);

biodegradation $t_{½}$ ~ 3–4 d for 50% initial concentration of 1–100 µg L^{-1} by river dieaway test (Bailey et al. 1983);

degradation rate k = 1.6 µg mL^{-1} d^{-1} at 30 µg mL^{-1} under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Sayler 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 0.29 d^{-1}, 0.13 d^{-1}, 0.11 d^{-1}, 0.11 d^{-1} (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~ 4 d due to reaction with the OH radical for a 24-h average OH radical concn of 5 × 10^5 cm^{-3} (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 5–11 based on the calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 2 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);

tropospheric lifetime of 2.7–5.1 d based on both the experimentally determined and calculated rate constant for reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{½}$ = 45 d under sunlight in water (Mansour & Feicht 1994);

$t_{½}$ = 15–19 min, 8–10 min and 3–4 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; $t_{½}$ = 16–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{½}$ = 19–21 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 7.1.1.2.1
Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		

Ferro et al. 1983

torsion effusion		Knudsen	average
T/K	**P/Pa**	**P/Pa**	**P/Pa**
cell B			
310	1.52	2.43	1.97
313	2.29	3.62	2.96
319	3.05	4.12	3.58

(Continued)

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TABLE 7.1.1.2.1 (*Continued*)
Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and the coefficients for the vapor pressure equations

Ferro et al. 1983			
torsion effusion		Knudsen	average
T/K	P/Pa	P/Pa	P/Pa
323	3.81	6.23	5.02
327	8.33	8.53	6.93
332	8.38	12.9	10.6
336	11.4	18.0	14.7
341	14.5	22.5	15.4
346	19.8	30.0	24.9
350	28.2	43.2	35.7
cell C			
332	13.6	19.1	16.3
336	15.8	22.3	19.0
341	23.4	29.0	26.2
346	27.5	35.6	31.5
350	33.7	46.2	40.0
354	47.3	63.6	55.4
359	63.2	84.9	74.0
eq. 1	P/mmHg	P/mmHg	P/mmHg
	torsion	Knudsen	average
A	8.91	8.45	8.68
B	3771	3458	3614
range, K	341–402	310–359	

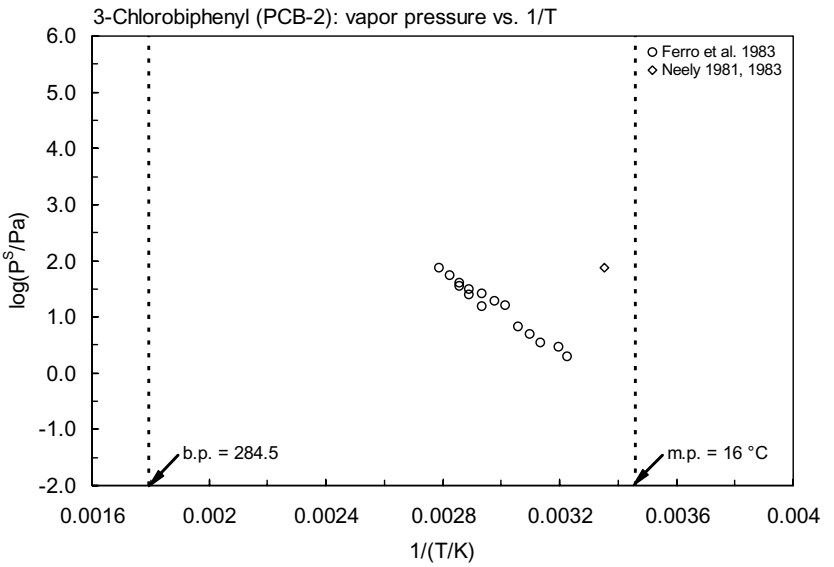

FIGURE 7.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chlorobiphenyl (PCB-2).

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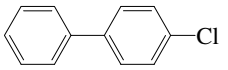
7.1.1.3 4-Chlorobiphenyl (PCB-3)



Common Name: 4-Chlorobiphenyl
Synonym: PCB-3, *p*-chlorobiphenyl, 4-chloro-1,1′-biphenyl
Chemical Name: 4-chlorobiphenyl
CAS Registry No: 2051-62-9
Molecular Formula: $C_{12}H_9Cl$
Molecular Weight: 188.652
Melting Point (°C):
78.8 (Lide 2003)
Boiling Point (°C):
292.9 (Lide 2003)
Density (g/cm^3 at 20°C): 0.9837
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
172.9 (Ruelle & Kesselring 1997)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
65.94 (Geidarov et al. 1975)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
79.24 (Geidarov et al. 1975)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
13.32 (Geidarov et al. 1975; quoted, Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.297 (mp at 78.8°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.0 (Webb 1970)
0.40 (Hoover, 1971)
1.19 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.90 (generator column-GC/ECD, Weil et al. 1974)
1.65 (Branson 1977)
0.0151 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
1.478* (generator column-GC/ECD, measured range 4–32°C, Stolzenburg & Andren 1983)
ln x = – 3428/(T/K) – 4.2786, ΔH_{ss} = 28.5 kJ/mol (regression eq. given by Dickhut et al. 1986, based on exptl data of Stolzenburg & Andren 1983)
log x = – 1486/(T/K) – 1.850; ΔH_{ss} = 28.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983); or
S/(mol/L) = 2.94×10^{-8} exp(0.041·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983)
1.20 (selected, Shiu & Mackay 1986)
1.30, 1.38 (generator column-HPLC/UV, Billington et al. 1988)
0.82, 0.88, 0.84, 0.95 (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.207 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.81 (shake flask-LSC, [^{14}C] 4-monoCB, Eadie et al. 1990)
1.34 (shake flask-GC/ECD, Li et al. 1992; Li & Andren 1994)
1.32 (shake flask-GC/ECD, Li & Doucette 1993)
1.37* ± 0.042 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
ln x = – 5.9137 – 2926.22/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
3.23, 3.81 (supercooled liquid: LDV literature-derived value, FAV final-adjusted value, Li et al. 2003)

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log S_L/(mol m^{-3}) = – 631/(T/K) + 0.35 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log S_L/(mol m^{-3}) = – 963/(T/K) + 1.53 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (96.4°C, summary of literature data, temp range 96.4–292.9°C, Stull 1947)
1.41 (supercooled liq. P_L, Weast 1972–1973)
log (P/mmHg) = (9.037 ± 0.635) – (3445 ± 18)/(T/K), temp range: 452–536 K (static method-quartz manometer measurements, Geidarov et al. 1975)
0.61 (Neely 1981,1983)
0.339*; 0.253 (P_S- Knudsen effusion; P_L-torsion effusion, extrapolated from exptl. derived from Antoine eq., Ferro et al. 1983)
log (P_S/kPa) = – (3849 ± 200)/(T/K) + (9.44 ± 0.63); temp range 33–73°C (Knudsen effusion data, solid, Ferro et al. 1983)
log (P_L/kPa) = – (3541 ± 250)/(T/K) + (8.28 ± 0.55); temp range 75–136°C (torsion effusion data, liquid, Ferro et al. 1983)
1.41 (supercooled liquid P_L, converted from literature P_S, Bidleman 1984)
0.951, 0.567 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.92, 0.942 (supercooled liquid P_L from P_{GC}, GC-RT correlation, different GC columns, Bidleman 1984)
0.175* (gas saturation-GC, measured range 5.2–24.9°C, Burkhard et al. 1984; Burkhard et al. 1985a)
log (P_S/Pa) = – 4754.1/(T/K) + 15.188; temp range: 5.2–24.9°C (gas saturation-GC, Clapeyron eq. Burkhard et al. 1984)
0.0979 (GC-RI correlation, Burkhard et al. 1985a)
0.320 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.907 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
0.270, 0.90 (selected P_S, supercooled P_L, Shiu & Mackay 1986)
0.593 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)
0.275 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 3488/(T/K) + 11.67 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
0.0677* (20°C, as saturation-GC/ECD, Wania et al. 1994)
log (P_S/Pa) = – 4493/(T/K) + 14.15; temp range: – 20 to 30°C (gas saturation-GC, Wania et al. 1994)
0.087–0.339; 0.253–0.942 (quoted literature P_S range; literature P_L range, Delle Site 1997)
log P/kPa = 15.188 – 4751.1/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.468, 0.479 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 3737/(T/K) + 12.21 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log P_L/Pa = – 3627/(T/K) + 11.84 (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
58.06 (batch stripping, Atlas et al. 1982; Dow Chemical, Neely 1982))
42.56 (calculated-P/C, Shiu & Mackay 1986)
34.14 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
24.39 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
23.30 (wetted-wall column-GC, Brunner et al. 1990)
5.84 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
18.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = – $\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 56 ± 27 kJ/mol, ΔS_H = 0.15 ± 0.10 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
36.3, 23.44 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2664/(T/K) + 10.31 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
4.90 (Branson 1977)
4.26 (Sugiura et al. 1978)
4.80 (Hansch & Leo 1979)
4.61 ± 0.1 (shake flask-GC, Bruggeman et al. 1982)

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4.69 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
4.34 (HPLC-RT correlation, Woodburn 1982)
4.49 (generator column-HPLC, Woodburn et al. 1984)
4.34 (HPLC-RT correlation, Woodburn et al. 1984)
4.40 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.49 (generator column-GC/ECD, Doucette & Andren 1987,1988)
4.55, 4.73, 4.64, 4.59 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.53, 4.27 (RP-HPLC-k′ correlation, different stationary phases, Sherbolm & Eganhouse 1988)
4.61 (recommended, Sangster 1989, 1993)
4.72 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.37 (generator column-HPLC, Li & Doucette 1993)
4.61 (recommended, Hansch et al. 1995)
4.49, 4.65 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.01* (generator column-GC; measured range – 10 to 30°C, Harner & Mackay 1995)
log K_{OA} = – 6.50 + 3962/(T/K); temp range –10 to 20°C, (generator column-GC, Harner & Mackay 1995)
7.01* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = – 4.82 + 3470/(T/K); temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
7.86, 6.99; 6.99 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
6.80; 6.93 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
6.82, 6.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 3520/(T/K) – 4.97 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.08 (killifish, Goto et al. 1978)
2.68 (NAS 1979)
2.77 (estimated, fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
2.67 (calculated-solubility, Kenaga 1980)
3.88 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
2.77, 4.07 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

3.52 (calculated, Kenaga 1980)
4.43 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.90 (soil, calculated-S, Chou & Griffin 1986)
4.71 (Great Lake suspended matter, phase partitioning-reversed phase chromatography by Sep Pak, Eadie et al. 1990)
4.70 (Green Bay suspended matter, reversed phase separation, Eadie et al. 1992)
3.49 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Sorption Partition Coefficient, log K_{OM}:

4.02 (Great Lakes DOC, reversed phase separation, Eadie et al. 1990)
4.61 (Green Bay DOC, reversed phase separation, Eadie et al. 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:

$k = 2.3 \times 10^{-4}$ d^{-1} with $t_{½}$ = 8.2 yr in surface water at 40°N in summer sunlight is (Dulin et al. 1986)
$t_{½}$ = 45 d in water (Mansour & Feicht 1994)

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k(calc) = 13.5 h^{-1}, maximum summer photolysis rate calculated under midday clear skies, experimental k(exptl) ~1.0×10^{-8} mol s^{-1}, irradiated with a low-pressure mercury lamp (Bunce et al. 1989)

k = (0.036–0.045) min^{-1} with $t_{½}$ = 15–19 min, k = (0.048–0.082) min^{-1} with $t_{½}$ = 8–14 min and k = (0.13–0.30) min^{-1} with $t_{½}$ = 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively;

k = (0.027–0.046) min^{-1} with $t_{½}$ = 15–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2;

k = (0.022–0.038) min^{-1} with $t_{½}$ = 18–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (3.9 \pm 0.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 ± 1 K, with an estimated atmospheric lifetime of ~6 d (relative rate method, Atkinson & Aschmann 1985)

$k_{OH} = 2.6 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to the C_6H_4Cl ring (ring B), $k_{OH} = 1.2 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} to ring A, and $k_{OH} = 3.8 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)

k_{OH}(calc) = $(2.8 – 5.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(exptl) = $(3.1 – 4.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)

$k_{OH} = 5.28 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (Atkinson 1989)

k_{OH}(exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = $(3.2 – 4.6) \times 10^{-12}$ cm^3 $molecule^{-1} \cdot s^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{½}$ = 175 h biodegradation by bacteria (Wong & Kaiser 1975; quoted, Pal et al. 1980);

within 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980)

k = 38 yr^{-1} in the water column, and k = 380 yr^{-1} in the sediment, pseudo first-order rate constant for microbial degradation (Wong & Kaiser 1975; quoted, Neely 1981)

k = 3.1 nmol L^{-1} d^{-1} with an initial concentration of 2.9 µmol/L, degradation rate in water from Port Valdez(data of Aug. 1977, Reichardt et al. 1981); $t_{½}$ = 2–5 d, time for 50% degradation of an initial concentration of 1–100 µg L^{-1} by river dieaway test (Bailey et al. 1983)

k = 2.0 µg mL^{-1} d^{-1} at 30 µg mL^{-1}, under culture conditions include river water as supportive medium and mixed bacteria cultures obtained from river sediments (Kong & Sayler 1983)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.01 d^{-1} with $t_{½}$ = 67 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~6 d due to reaction with the OH radical for a 24-h average OH radical concn of 5×10^5 cm^{-3} (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);

photolysis $t_{½}$ ~10–25 h for noontime summer sunshine, or more realistically, several days (Bunce et. 1989);

tropospheric lifetime of 3 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);

tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 4.9 d in Lake Michigan (Neely 1983);

photolysis $t_{½}$ = 8.2 yr in summer sunlight at 40°L in surface waters (Dulin et al. 1986);

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photolysis $t_{½}$ = 45 d, sunlight days in water (Mansour & Feicht 1994)

$t_{½}$ = 15–19 min, 8–14 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2 respectively; $t_{½}$ = 15–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{½}$ = 18–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 88 d for high-dose treatment, $t_{½}$ = 67 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.3.1
Reported aqueous solubilities and octanol-air partition coefficients of 4-chlorobiphenyl (PCB-3) at various temperatures

Aqueous solubility				log K_{OA}			
Stolzenburg & Andren 1983		Shiu et al. 1997		Harner & Mackay 1995		Harner & Bidleman 1996	
generator column-GC/ECD		generator column-GC/ECD		generator column-GC		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	log K_{OA}	t/°C	log K_{OA}
4	0.661	5	0.822	–10	8.65	–10	8.34
20	1.206	15	1.07	0	8	0	7.91
25	1.478	25	1.37	10	7.48	10	7.43
32	2.128	35	2.17	20	7.01	20	7.01
		45	3.04	25	6.76	30	6.62
ΔH_{sol}/(kJ mol^{-1}) = 28.5 for 5–45°C		ΔH_{sol}/(kJ mol^{-1}) = 24.5 for 5–45°C		ΔH_{OA}/(kJ mol^{-1}) = 75.9		ΔH_{OA}/(kJ mol^{-1}) = 75.86	
				log K_{OA} = A + B/T		log K_{OA} = A + B/T	
				A	–6.52	A	–4.82
				B	3962.2	B	3470

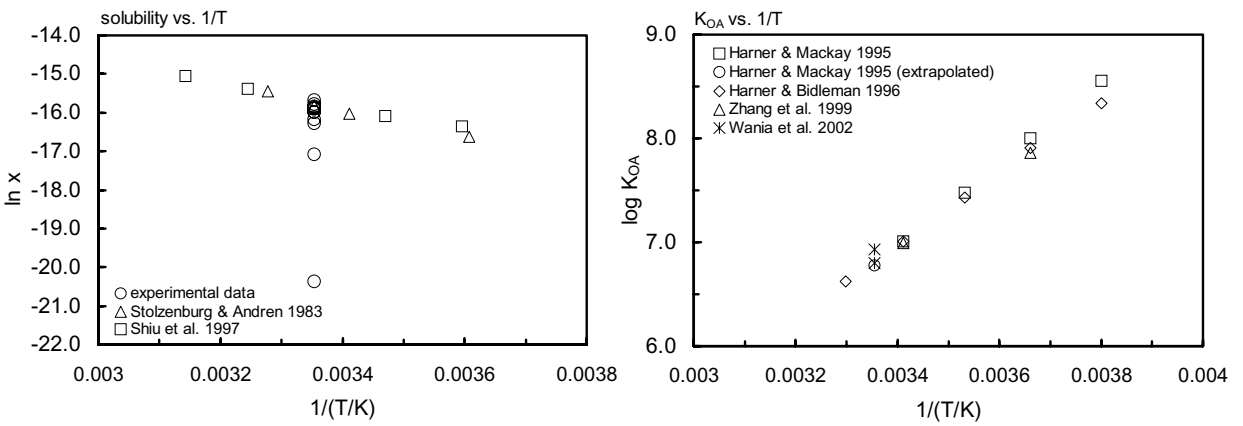

FIGURE 7.1.1.3.1 Logarithm of mole fraction solubility and K_{OA} versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).

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TABLE 7.1.1.3.2
Reported vapor pressures of 4-chlorobiphenyl (PCB-3) at various temperatures and the coefficients for the vapor pressure equations:

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		

1.

Stull 1947		Geidarov et al. 1975		Ferro et al. 1983			
compiled literature data		static-quartz manometer		torsion-effusion		Knudsen	average
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	P/Pa	P/Pa
				cell B			
96.4	133.3	data presented in graph and		33	0.762	0.697	0.729
129.8	666.7			37	1.52	0.902	1.21
146.0	1333	eq 1	P/mmHg	50	3.05	3.57	3.31
164.0	2666	A	9.037	54	3.81	4.90	4.38
183.8	5333	B	3445	59	6.10	7.41	6.75
196.0	7999	range: 179–263°C		63	9.14	10.4	9.77
212.6	13333			73	21.3	18.3	19.8
237.8	26664	mp/°C	74.75	cell B			
284.5	53329	bp/°C	287	35	0.762	0.917	0.840
292.9	101325			41	1.62	1.41	1.47
		ΔH_V/(kJ mol^{-1}) = 65.94		44	2.29	1.72	2.00
mp/°C	75.5	ΔH_{fus}/(kJ mol^{-1}) = 13.32		50	3.05	2.85	2.95
		ΔS_{fus}/(J mol^{-1} K^{-1}) = 38.3		52	3.81	4.44	4.12
		ΔH_{subl}/(kJ mol^{-1}) = 79.24		57	5.33	6.04	5.69
				61	7.62	8.43	8.03
				62	8.38	10.9	9.66
				65	10.7	10.8	10.8
				67	12.9	11.9	12.4
				68	13.7	12.9	13.3
				69	15.2	13.9	14.6
				73	21.1	18.6	15.3
				eq. 1	P/mmHg	P/mmHg	
				A	8.28	9.44	
				B	3541	3849	
				range, °C	75–136(liq.)	33–73(solid)	
				ΔH_V/(kJ mol^{-1}) = 67.8			

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TABLE 7.1.1.3.2 *(Continued)*

2.

Burkhard et al. 1984		Wania et al. 1994	
gas saturation-GC		gas saturation-GC	
t/°C	**P/Pa**	**t/°C**	**P/Pa**
4.2	0.0111	–20	2.446×10^{-4}
15.0	0.0493	–10	1.297×10^{-3}
24.9	0.172	0	4.889×10^{-3}
25.0	0.175	10	1.883×10^{-2}
		20	6.771×10^{-2}
		30	0.2233
eq. 1	P/Pa		
A	15.188	eq. 1	P/Pa
B	4754.1	A	14.15
range: 4.2–25°C		B	4493
		temp range –20 to30°C	
		ΔH_{subl}/(kJ mol^{-1}) = 86.0	

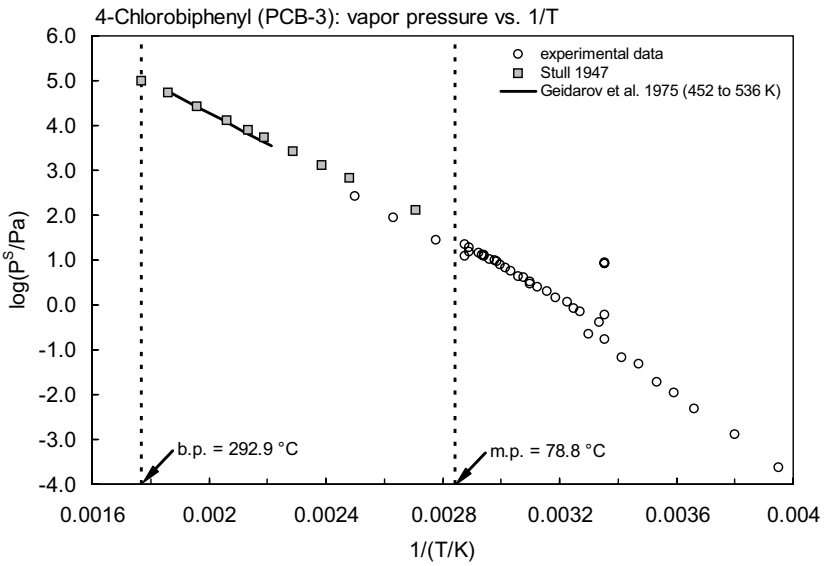

FIGURE 7.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).

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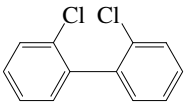
7.1.1.4 2,2′-Dichlorobiphenyl (PCB-4)



Common Name: 2,2′-Dichlorobiphenyl
Synonym: PCB-4, 2,2-dichloro-1,1′-biphenyl
Chemical Name: 2,2′-dichlorobiphenyl
CAS Registry No: 13029-08-8
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
60.5 (Hutzinger et al. 1974)
Boiling Point (°C):
312 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.448 (mp at 60.5°C)
0.442 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
1.0 (Webb 1970)
0.90 (Hoover 1971)
1.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.79 (generator column-GC/ECD, Weil et al. 1974)
0.0212 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
1.86 (20°C, supercooled liquid, shake flask-GC/ECD, Chiou et al. 1982,1983; Chiou 1985)
1.124 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.511, 0.322, 0.362, 0.511 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.207 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.133 (Knudsen-effusion technique, extrapolated from 37–54.92°C, Smith et al. 1964)
0.36 (quoted, Neely 1981)
0.82 (P_L calculated from P_S using F, Neely 1981)
0.189 (GC-RI correlation, Burkhard et al. 1985a)
0.424 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985a)
0.326, 0.335 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.134 (extrapolated-Antoine eq., solid, Stephenson & Malanowski 1987)
log (P_S/kPa) = – 5019/(T/K) + 12.962; temp range 37–55°C (Antoine eq., Stephenson & Malanowski 1987)
0.152 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.275, 0.363 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3462/T + 11.73 (supercooled liquid P_L, GC-RT, Falconer & Bidleman 1994)
0.0603–0.315; 0.280–0.424 (quoted literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
30.2 (20°C, calculated-P/C, Murphy et al. 1987)
34.14 (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
23.3 (wetted-wall column-GC, Brunner et al. 1990)

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8.02 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
23.0(from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 50 \pm 25$ kJ/mol, $\Delta S_H = 0.13 \pm 0.09$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

4.04 (HPLC-RT correlation, Sugiura et al. 1978)
5.70 (HPLC-RT correlation, Sugiura et al. 1979)
5.51 (Hansch & Leo 1979)
4.00 (HPLC-k′ correlation, McDuffie 1981)
5.00 ± 0.1 (shake flask-GC, Bruggeman et al. 1982)
3.02 (RP-TLC-retention correlation, Bruggeman et al. 1982)
3.55 (HPLC-RT correlation, Woodburn 1982)
4.80 (shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
4.90; 3.55 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
3.63; 4.89 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
4.90 (generator column-GC/ECD, Doucette & Andren 1987,1988)
4.25, 4.86, 4.65, 4.94(RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.965 ± 0.013(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.09 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
4.73 (recommended, Sangster 1993)
4.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

7.18; 6.56 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -4.84 + 3590/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
7.66, 6.86 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
6.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

2.04 (killifish, Goto et al. 1978)
3.72, 2.95, 3.60, 3.26 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
– 1.40, – 1.30, – 1.35 (adipose tissue of male, female Albino rats, rodents, Geyer et al. 1980)
2.05, 2.45 (fish: flowing water, microcosm condition Garten & Trabalka 1983)
3.43, 2.90 (algae, calculated, Geyer et al. 1984)
3.43, 3.38, 3.80(algae, fish, activated sludge, Freitag et al. 1984,1985)
3.85 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
3.38; 3.413, 3.715(quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

3.68 (Woodburn silt loam soil, soil organic matter, sorption isotherm-GC, Chiou et al. 1983)
4.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.84 (soil, calculated-S, Chou & Griffin 1986)
3.92 (soil, calculated-MCI, Sabljic et al. 1995)
3.96; 3.92 (soil, calculated-Characteristic Root Index CRI; quoted lit., Saçan & Balcioğlu 1996)
4.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.90; 3.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Sorption Partition Coefficient, log K_{OM} at 25°C or as indicated:

3.68 (20°C, Wood burn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
3.68, 4.18 (quoted, calculated-MCI χ, Sabljic 1984)

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Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½}$ ~ 3.1 h of evaporation with an initial concentration of 0.1 ppm from 4.5 cm depth of water solution in a glass dish at 24°C is 3.1 h and $t_{½}$ = 0.4 h with stirring of the solution; the experimental $t_{½}$ = 3.9 h and 0.9 h of evaporation under same condition with stirring of the solution (Chiou et al. 1979).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

k_{OH}(calc) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH} = (2.0 \pm 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, $k_{O3} < 2.0 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} at 297 ± 2 K (relative rate method, Kwok et al. 1995)

tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: Biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

microbial degradation with pseudo first-order k = 0.65 yr^{-1} in the water column and k = 6.5 yr^{-1} in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.027 d^{-1} (10°C, sandworm, Goerke & Erst 1977; quoted, Waid 1986)

k_1 = 0.29 d^{-1}, 0.13 d^{-1}, 0.11 d^{-1}, 0.11 d^{-1} (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

k_2 = 0.017 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

k_1 = 122 d^{-1}; k_2 = 0.014 d^{-1} (rainbow trout, calculated, Gobas & Mackay 1987)

k_2 = 0.004 d^{-1} with $t_{½}$ = 183 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 93 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 34.5 d in Lake Michigan (Neely 1983)

Groundwater:

Sediment:

Soil:

Biota: $t_{½}$ = 40 d in rainbow trout, and $t_{½}$ = 20 d in its muscle (Niimi & Oliver 1983).

Depuration $t_{½}$ = 183 d for high-dose treatment, $t_{½}$ = 93 d for high-dose + enzyme treatment (juvenile rainbow trout, Buckman et al. 2004)

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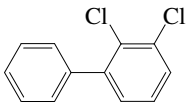
7.1.1.5 2,3-Dichlorobiphenyl (PCB-5)



Common Name: 2,3-Dichlorobiphenyl
Synonym: PCB-5, 2,3-dichloro-1,1′-biphenyl
Chemical Name: 2,3-dichlorobiphenyl
CAS Registry No: 16605-91-7
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C): 28.0
27.8–28.2 (Erickson 1985)
Boiling Point (°C):
172 (at 4000 Pa, Erickson 1986)
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.934 (mp at 28°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1.70 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
1.31, 1.23, 0.756, 0.829 (quoted lit.; RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.00, 0.658 (quoted average of Brodsky & Ballschmiter 1988, calculated-MCI χ, Patil 1991)
1.36 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.147, 0.144, 0.114(calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.151 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
0.162 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -3769/(T/K) + 11.81$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
19.56 (calculated-P/C, Burkhard et al. 1985b)
28.57 (calculated-MCI χ, Sabljic & Güsten 1989)
23.30 (wetted-wall column-GC, Brunner et al. 1990)
24.19 (calculated-QSPR, Dunnivant et al. 1992)
8.97 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
24.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 48 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.20 (RP-TLC-RT correlation, Bruggeman et al. 1982)
4.82, 4.92, 5.17, 5.05 (RP-PLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.99 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
7.40; 6.98 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -5.41 + 3820/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)

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8.55, 7.59 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.08 (oyster, Vreeland 1974)
3.45–4.11 mean 4.11 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.41; 4.11 (rainbow trout, 15°C, kinetic BCF k_1/k_2, steady-state BCF C_F/C_W, Oliver & Niimi 1985)
4.11, 5.25; 3.388, 3.895 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
3.08, 5.33 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.11, 5.20 (rainbow trout: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

4.76 (suspended particulate matter, Burkhard 1984)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constant k = (0.031–0.036) min^{-1} with $t_{½}$ = 19–23 min, k = (0.054–0.067) min^{-1} with $t_{½}$ = 10–13 min and k = (0.22–0.25) min^{-1} with $t_{½}$ = 3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA–340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; k = (0.022–0.028) min^{-1} with $t_{½}$ = 25–32 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; k = (0.022–0.024) min^{-1} with $t_{½}$ = 29–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

k_{OH}(aq.) = 7.9×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.011 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 300 d^{-1}; k_2 = 0.011 d^{-1} (rainbow trout, Oliver & Niimi 1985)
log $1/k_2$ = 2.0, 2.2 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

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$t_{½}$ = 19–23 min, 10–13 min and 3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 16–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{½}$ = 29–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: $t_{½}$ = 61 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{½}$ = 26 d in its muscle (Niimi & Oliver 1983).

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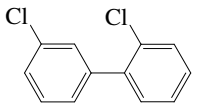
7.1.1.6 2,3′-Dichlorobiphenyl (PCB-6)



Common Name: 2,3′-Dichlorobiphenyl
Synonym: PCB-6
Chemical Name: 2,3′-dichlorobiphenyl
CAS Registry No: 25569-80-6
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
36 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.605 (supercooled liquid S_L, Burkhard et al. 1985a)
0.580 (20°C, supercooled liquid S_L, Murphy et al. 1987)
1.226 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.928 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.165 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.157, 0.169, 0.0754 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.173, 1.208 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0799 (20°C, supercooled liquid, Murphy et al. 1987)
0.141, 0.178 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -3769/(T/K) + 11.88$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
27.76 (calculated-P/C, Burkhard et al. 1985a)
30.0 (20°C, calculated-P/C, Murphy et al. 1987)
39.42 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
25.33 (wetted-wall column-GC, Brunner et al. 1990)
33.09 (calculated-QSPR, Dunnivant et al. 1992)
4.016, 11.74 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
9.14 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
24.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.03 (calculated-TSA, Burkhard 1984)
5.02 (quoted and selected, Brownwell & Farrington 1985)
4.84 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

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5.06 (calculated-TSA, Hawker & Connell 1988a)
5.02 (recommended, Hansch et al. 1995)
5.044 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

8.51; 7.55 (0; 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

4.83 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: k = (0.018–0.052) min^{-1} with $t_{½}$ = 13–38 min, irradiated by sunlight in the presence of 100 µg/mL TiO_2 of diCBs in St. Lawrence River water containing 3 ng/mL of total PCB (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 2.1×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyl at room temp. (Atkinson 1987)

k_{OH}(aq.) = 8.0×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

tropospheric lifetime τ(calc) = 3.4–7.2 d, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.012 d^{-1} with $t_{½}$ = 56 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.013 d^{-1} with $t_{½}$ = 53 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

$t_{½}$ = 13–38 min for dichlorobiphenyl in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996)

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 56 d for high-dose treatment, $t_{½}$ = 53 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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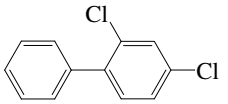
7.1.1.7 2,4-Dichlorobiphenyl (PCB-7)



Common Name: 2,4-Dichlorobiphenyl
Synonym: PCB-7, 2,4-dichloro-1,1′-biphenyl
Chemical Name: 2,4-dichlorobiphenyl
CAS Registry No: 33284-50-3
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
24.1–24.4 (Dickerman & Weiss 1957; Weingarten 1961; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
1.0 (calculated, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1.40 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.637 (shake flask-GC/ECD, Haque & Schmedding 1975)
1.13 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
0.587, 0.535, 0.689, 0.659 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.148 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C):
0.184, 0.321 (supercooled liquid P_L, GC-RT correlation, different GC columns, Bidleman 1984)
0.175 (supercooled liquid P_L, Burkhard et al. 1984)
0.179 (GC-RI correlation, Burkhard et al. 1985a)
0.175 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.210, 0.216 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.170, 0.195 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)

Henry's Law Constant (Pa m^3/mol at 25°C):
96.66 (gas stripping-GC, Atlas et al. 1982)
35.26 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
28.37 (wetted-wall column.-GC/ECD, Brunner et al. 1990)
24.78 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
11.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
28.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 43 \pm 22$ kJ/mol, $\Delta S_H = 0.11 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.15 (RP-TLC-RT correlation, Bruggeman et al. 1982)
4.67 (HPLC-RT correlation, Rapaport & Eisenreich 1984)

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5.09, 5.21, 5.20, 5.10 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.13 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.16 (recommended, Sangster 1993)
5.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

8.37, 7.39; 7.25(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
6.98 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

4.83 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half Lives, $t_{½}$:

Volatilization:

Photolysis: calculated sunlight $k < 2 \times 10^{-8}$ s^{-1} and 5.7×10^{-11} s^{-1}, with $t_{½} > 400$ d at 40°N latitude in winter (Dulin et al. 1986);

k = (0.30–0.036) min^{-1} with $t_{½}$ = 19–23 min, k = (0.054–0.067) min^{-1} with $t_{½}$ = 10–13 min and k = (0.13–0.21) min^{-1} with $t_{½}$ = 3–5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constants k = (0.015–0.043) min^{-1} with $t_{½}$ = 36–29 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; rate constants k = (0.018–0.022) min^{-1} with $t_{½}$ = 31–38 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

k_{OH}-(aq.) = 7.1×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 from lake sediments but small amount residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.004 d^{-1} with $t_{½}$ = 192 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 149 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

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Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH· oxidation (Sedlak & Andren 1991);
$t_{½}$ = 19–23 min, 10–13 min and 3–5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2 respectively; $t_{½}$ = 36–29 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{½}$ = 31–38 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 192 d for high-dose treatment, $t_{½}$ = 149 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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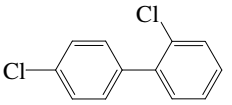
7.1.1.8 2,4′-Dichlorobiphenyl (PCB-8)



Common Name: 2,4′-Dichlorobiphenyl
Synonym: PCB-8, 2,4′-dichloro-1,1′-biphenyl
Chemical Name: 2,4′-dichlorobiphenyl
CAS Registry No: 34883-43-7
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
46 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.66 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.50 (Webb 1970; Hoover 1971)
1.88 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.637 (shake flask-GC, Haque & Schmedding 1975)
0.620 (generator column-GC/ECD, Weil et al. 1974)
0.139 (shake flask-GC/ECD from Aroclor 1242 mixture, Lee et al. 1979)
1.17 (20°C, supercooled liquid P_L, shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985)
0.974, 0.848, 0.643, 0.658 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.58, 1.45 (supercooled liquid S_L: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -1000/(T/K) + 1.17$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0998 (GC-RI correlation, Burkhard et al. 1985a)
0.147 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.157, 0.143 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P/\text{mmHg}) = 9.74 - 3840/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.129, 0.158 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -3769/(T/K) + 11.84$ (GC-RT correlation, Falconer & Bidleman 1994)
0.123, 0.148 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/\text{Pa} = -3818/(T/K) + 11.90$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log P_L/\text{Pa} = -3728/(T/K) + 11.68$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°Cor as indicated and reported temperature dependence equations):
96.7 (gas stripping-GC, Atlas et al. 1982)
23.30 (wetted wall column-GC/ECD, Brunner et al. 1990)
35.67 ± 2.7 (gas stripping-GC/ECD; Girvin et al. 1997)
6.01, 9.87, 15.85, 24.89* ± 0.29, 36.07 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 13.2307 - 5304.31/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(44.1/\text{kJ·mol}^{-1})/RT] + (0.110/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)

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25.7 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 44 \pm 3$ kJ/mol, $\Delta S_H = 0.11 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
26.3, 22.9 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log H/(Pa m^3/mol) = – 2428/(T/K) + 9.56 (LDV linear regression of literature data, Li et al. 2003)
log H/(Pa m^3/mol) = – 2728/(T/K) + 10.51 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

5.51 (Hansch & Leo 1979)
4.48 (HPLC-RT correlation, Woodburn 1982)
5.10 (shake flask-GC, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
5.10 ± 0.4 (selected, Shiu & Mackay 1986)
5.14 (generator column-GC/ECD, Woodburn et al. 1984)
4.47; 5.10 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
5.14 (generator column-GC/ECD, Doucette & Andren 1987,1988)
4.93, 5.05, 5.24, 5.15 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.13 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.27 (average value, generator column-GC, Larsen et al. 1992)
5.09 (recommended, Sangster 1993)
5.10 (recommended, Hansch et al. 1995)
5.09, 5.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

7.40 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
log K_{OA} = – 5.41 + 3820/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.58, 7.61 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 3785/(T/K) – 5.35 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

3.83, 3.55, 3.99(algae, fish, act. sludge, Freitag et al. 1984,1985)
2.60–4.08 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.12–5.33 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
3.83, 4.53 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)
3.57, 5.76 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

3.90 (soil/sediment, sorption isotherm, Haque & Schmedding 1976)
4.16 (Woodburn silt loam soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
4.83 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.90 (Lake Michigan water column, Swackhamer & Armstrong 1987)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
3.99; 4.13 (soil, calculated-Characteristic Root Index CRI; quoted lit., Saçan & Balcioğlu 1996)
4.54–4.56 (Catlin silt loam, f_{OC} = 0.0226, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.65–4.70 (Cloudland loam, f_{OC} = 0.0024, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997
4.61 (Kenoma silt loam, f_{OC} = 0.0153, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.38–4.39 (Kenoma silt loam, f_{OC} = 0.0092, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.57–4.73 (Kenoma silt loam, f_{OC} = 0.002, depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.52–4.54 (Norborne silt loam, f_{OC} = 0.0137, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.54–4.57 (Norborne silt loam, f_{OC} = 0.009, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
4.53–4.66 (Norborne silt loam, f_{OC} = 0.0057, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)

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4.23–4.53; 3.90–5.90 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

4.23; 3.93, 4.53, 4.46 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:

3.89 (soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: depletion rate constant k = 45 d^{-1} from aqueous solution in a 26-cm or 67-cm purge vessel, (Girvin et al. 1997).

Photolysis: photolysis rate k_P(exptl) < 2×10^{-8} d^{-1} with $t_{½}$ > 400 d; k_P(calc) < 2×10^{-8} d^{-1} in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Sorption-Desorption Rate Constants:

k_2 = 0.006 d^{-1} with $t_{½}$ = 109 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 104 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{½}$ > 400 d in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 109 d for high-dose treatment, $t_{½}$ = 104 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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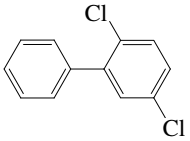
7.1.1.9 2,5-Dichlorobiphenyl (PCB-9)



Common Name: 2,5-Dichlorobiphenyl
Synonym: PCB-9, 2,5-dichloro-1,1′-biphenyl
Chemical Name: 2,5-dichlorobiphenyl
CAS Registry No: 34883-39-1
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
22–23 (Weingarten 1962)
Boiling Point (°C):
171 (15mm Hg, Erickson 1986))
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
1.0 (calculated, assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.58 (generator column-GC/ECD, Weil et al. 1974)
2.028 (shake flask-GC, Chiou et al. 1977)
0.190 (generator column-GC/ECD, Bruggeman et al. 1981)
1.940 (generator column-GC/ECD, Miller et al. 1984; 1985)
0.0739, 0.0739, 0.0722, 0.07055 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.115 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0775 (Augood et al. 1953)
0.184 (supercooled liquid P_L, Yalkowsky et al. 1983)
0.184 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.202 (GC-RI correlation, Burkhard et al. 1985a)
0.198 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.231, 0.232 (supercooled P_L, GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)
0.180 (selected, Shiu & Mackay 1986)
0.204 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -3862/(T/K) + 12.22$, (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.105–0.232 (quoted lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations
39.31 (batch stripping-GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
28.37 (wetted wall column-GC/ECD, Brunner et al. 1990)
16.1, 29.6, 58.2, 82.2, 123, 165.4 (10.4, 20, 30.1, 34.9, 42.1, 47.9°C, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)
30.95 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 6.055 - 2331/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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29.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.18 (RP-TLC-k′ correlation, Bruggeman et al. 1982; Bruggeman et al. 1984)
5.16 (generator column-GC/ECD, Miller et al. 1984,1985)
5.03 (calculated-TSA, Burkhard 1984)
4.67; 5.30 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
5.01, 5.10, 5.19, 5.10 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.13 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.10 (recommended, Sangster 1993)
5.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

8.37, 7.40; 7.33(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
7.16 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.68 (goldfish, 3% lipid by wt., static fish-water equilibration system, 23-d exposure, Bruggeman et al. 1981)
5.45 (goldfish, 10% lipid dry wt. in food, Bruggeman et al. 1981)
5.72 (guppy, 3.5% lipid by wt., Bruggeman et al. 1982,1984)
4.14; 3.90 (goldfish, exptl.; correlated, Mackay & Hughes 1984)
3.38–4.11 mean 4.00 (rainbow trout, 15°C, steady-state BCF, 7- to 96-d study, Oliver & Niimi 1985)
4.0 (rainbow trout, mean of 7–96 d exposure, Oliver & Niimi 1985)
4.53, 4.00 (rainbow trout: kinetic BCF; steady state BCF, Oliver & Niimi 1985)
4.26 (guppy, Gobas et al. 1987)
5.68 (goldfish, Noegrohati & Hammers 1992)
3.89; 3.42 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.0, 5.09 (rainbow trout, flow through 96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.89, 5.43 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.00; 4.13 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

4.83 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.01 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constants k = (0.024–0.038) min^{-1} with $t_{½}$ = 18–29 min, k = (0.033–0.048) min^{-1} with $t_{½}$ = 14–21 min and k = (0.13–0.14) min^{-1} with $t_{½}$ = 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constant k = (0.056–0.064) min^{-1} with $t_{½}$ = 11–12 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; rate constant k = (0.015–0.027) min^{-1} with $t_{½}$ = 26–47 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference: k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

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tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = (1.4 – 2.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = (2.0 – 4.2) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = (1.4 – 3.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 95% degradation at 24 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 920 d^{-1}; k_2 = 0.066 d^{-1} (23°C, goldfish, 3% lipid, Bruggeman et al. 1981; quoted, Waid 1986)

k_2 = 0.008 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

k_1 = 190 d^{-1}; k_2 = 0.11 d^{-1} (guppy, Bruggeman et al. 1984; quoted, Clark et al. 1990)

k_2 = 0.066, 0.0523 d^{-1} (goldfish, exptl., calculated, Mackay & Hughes 1984)

k_1 = 280 d^{-1}; k_2 = 0.0082 d^{-1} (rainbow trout, Oliver & Niimi 1985)

k_1 = 38.3, 49.2 h^{-1}; $1/k_2$ = 360, 220 h (goldfish, guppy, quoted, Hawker & Connell 1985)

k_1 = 1200 d^{-1} (guppy, Opperhuizen 1986)

k_1 = 122 d^{-1}; k_2 = 0.0089 d^{-1} (rainbow trout, calculated, Gobas & Mackay 1987)

log k_1 = 2.96, 3.07 d^{-1}; log $1/k_2$ = 0.96, 1.18 d (fish, quoted, Connell & Hawker 1988)

log $1/k_2$ = 2.1, 2.3 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)

log k_2 = – 0.96, –1.17 d^{-1} (fish, quoted, Thomann 1989)

k_1 = 2760 d^{-1}; k_2 = 0.368 d^{-1} (zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.004 d^{-1} with $t_{½}$ = 192 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 149 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 18–29 min, 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; $t_{½}$ = 11–12 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2; $t_{½}$ = 26–47 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: clearance $t_{½}$ = 10 d in goldfish (Bruggeman et al. 1981)

$t_{½}$ = 6.5 d in guppy (Bruggeman et al. 1984);

$t_{½}$ = 85 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and its muscle, $t_{½}$ = 56 d (Niimi & Oliver 1983).

depuration $t_{½}$ = 192 d for high-dose treatment, $t_{½}$ = 149 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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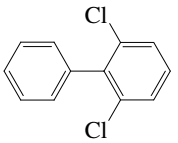
7.1.1.10 2,6-Dichlorobiphenyl (PCB-10)



Common Name: 2,6-Dichlorobiphenyl
Synonym: PCB-10, 2,6-dichloro-1,1′-biphenyl
Chemical Name: 2,6-dichlorobiphenyl
CAS Registry No: 33146-45-1
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
35.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
12.6 (differential scanning calorimetry, Miller et al. 1984)
Entropy of Fusion, ΔS_{fus} (J/mol K):
41.0 (Miller et al. 1984)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.789 (mp at 35.5°C)
0.801 Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
1.452 (shake flask-GC, Chiou et al. 1977)
1.390 (generator column-GC/ECD, Miller et al. 1984,1985)
0.294, 0.435, 0.245, 0.406 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
2.41 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.540 (generator column-GC/ECD, Opperhuizen et al. 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.288 (GC-RI correlation, Burkhard et al. 1985a)
0.365 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.336, 0.371 (supercooled P_L, GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)
0.347 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -3642/(T/K) + 11.74$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
47.83 (calculated-P/C, Burkhard et al. 1985b)
47.61 (calculated-MCI χ, Sabljic & Güsten 1989)
23.30 (wetted wall column-GC, Brunner et al. 1990)
42.86 (calculated-QSPR, Dunnivant et al. 1992)
27.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

5.30 (quoted, Kaiser 1983)
4.96 (calculated-TSA, Burkhard 1984)
5.31 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
4.93 (generator column-GC/ECD, Miller et al. 1984,1985)
4.97, 5.00, 4.97, 5.01 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.982 ± 0.013 (shake flask/slow stripping-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
4.99 (recommended, Sangster 1993)
4.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

7.18 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
log K_{OA} = – 4.84 + 3590/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
6.18 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

4.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.99 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: k = 0.043 min^{-1} with $t_{½}$ = 16 min, k = 0.082 min^{-1} with $t_{½}$ = 8 min and k = 0.30 min^{-1} with $t_{½}$ = 2 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constants k = 0.034 min^{-1} with $t_{½}$ = 20 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 µg/mL TiO_2; rate constants k = 0.052 min^{-1} with $t_{½}$ = 13 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.004 d^{-1} with $t_{½}$ = 183 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 93 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

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Surface water: $t_{½}$ = 16 min, 8 min and 2 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 20 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{½}$ = 13 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 56 d for high-dose treatment, $t_{½}$ = 53 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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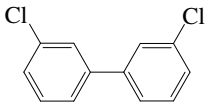
7.1.1.11 3,3′-Dichlorobiphenyl (PCB-11)



Common Name: 3,3′-Dichlorobiphenyl
Synonym: PCB-11, 3,3′-dichloro-1,1′-biphenyl
Chemical Name: 3,3′-dichlorobiphenyl
CAS Registry No: 2050-67-1
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
29 (Weast 1972–73, 1982–83; Lide 2003)
Boiling Point (°C):
320 (Lide 2003)
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.912 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
1.057 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0406, 0.102, 0.093, 0.0974 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.354 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0267 (P_S from GC-RT correlation, Westcott & Bidleman 1981; Westcott et al. 1981)
0.0865, 0.0952 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
0.0645 (supercooled liquid P_L, GC-RT correlation, Burkhard 1984)
0.0612 (GC-RI correlation, Burkhard et al. 1985a)
0.0646 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.091, 0.076 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.090 (selected P_L, supercooled liquid, Shiu & Mackay 1986)
log (P_L/Pa) = – 3936/(T/K) + 12.14; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0306–0.143; 0.0646–0.0953 (literature. P_S range; literature P_L range, Delle & Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C):
13.58 (calculated-P/C, Burkhard et al. 1985b)
23.61 (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
23.61; 38.69 (quoted exptl.; calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
23.61; 29.42 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.30 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)
5.34 (RP-TLC-k′ correlation, Bruggeman et al. 1982)

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5.30, 5.39, 5.22, 5.18 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.17 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.27 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

7.86, 7.90; 7.93 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

4.90 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.00 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 2.7×0^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)
k_{OH} = $(4.1 \pm 1.3) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 297 ± 2 K (relative rate method, Kwok et al. 1995)
tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2: 0.1385 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995)
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 5 d in rainbow trout, and $t_{½}$ < 5 d in its muscle (Niimi & Oliver 1983)

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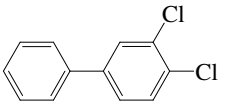
7.1.1.12 3,4-Dichlorobiphenyl (PCB-12)



Common Name: 3,4-Dichlorobiphenyl
Synonym: PCB-12, 3,4-dichloro-1,1′-biphenyl
Chemical Name: 3,4-dichlorobiphenyl
CAS Registry No: 2974-92-7
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
49–50 (Weingarten 1961)
Boiling Point (°C):
195–200 (Weast 1972–73)
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.566 (calculated, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
1.233 (calculated-TSA, supercooled liquid P_L, Burkhard et al. 1985b)
0.0523, 0.112, 0.0888, 0.128 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00791 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0138 (supercooled liquid P_L, calculated-mp, Dunnivant & Elzerman 1988)
0.280 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.091; 0.658 (quoted average of Brodsky & Ballschmiter 1988; calculated- χ, Patil 1991)
0.4004 (calculated-QSPR, Dunnivant et al. 1992)
0.930 (calculated-group contribution, Kühne et al. 1995)
0.268, 0.722 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
2.373 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0532 (supercooled liquid P_L, GT-RT correlation, Burkhard 1984)
0.0313 (GC-RI correlation, Burkhard et al. 1985a)
0.0532 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
0.078, 0.062 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.741 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -3885/(T/K) + 11.92$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.000736–0.0888; 0.0128–0.0783 (literature P_S range; literature P_L range, Delle Site 1997)
0.259 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Henry's Law Constant (Pa m^3/mol at 25°C):

20.77 (batch stripping/GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
14.18 (wetted-wall column-GC, Brunner et al. 1990)

Octanol/Water Partition Coefficient, log K_{OW}:

5.51 (Hansch & Leo 1979)
5.10, 5,51 (HPLC-RT correlation, calculated-π, Woodburn 1982; Woodburn et al. 1984)
5.29 (generator column-GC, Woodburn et al. 1984)
5.29 (generator column-GC/ECD, Doucette & Andren 1987)
5.26, 5.39, 5.22, 5.18 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.12 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.29 (recommended, Sangster 1993)
5.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

8.71, 7.80; 8.06(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

4.85 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
3.98 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constants k = (0.019–0.034) min^{-1} with $t_{½}$ = 21–36 min, k = (0.041–0.064) min^{-1} with $t_{½}$ = 11–17 min and k = (0.12–0.16) min^{-1} with $t_{½}$ = 4–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constants k = (0.013–0.029) min^{-1} with $t_{½}$ = 26–52 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 1.8×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 100% degraded by Nocardia strain NCIB 10603 within one week (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.010 d^{-1} with $t_{½}$ = 67 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the

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experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 21–36 min, 11–17 min and 4–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 26–52 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 88 d for high-dose treatment, $t_{½}$ = 67 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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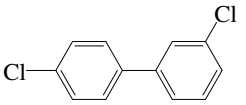
7.1.1.13 3,4′-Dichlorobiphenyl (PCB-13)



Common Name: 3,4′-Dichlorobiphenyl
Synonym: PCB-13, 3,4′-dichloro-1,1′-biphenyl
Chemical Name: 3,4′-dichlorobiphenyl
CAS Registry No: 2974-90-5
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 233.1
Melting Point (°C):
51 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
1.084 (supercooled liquid S_L, Burkhard et al. 1985a)
0.093 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.369 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0572 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0595 (GC-RI correlation, Burkhard et al. 1985b)
0.083, 0.067 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -3885/(T/K) + 11.92$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol):
12.36 (calculated-P/C, Burkhard et al. 1985b)
31.92 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
25.75 (calculated-QSPR, Dunnivant et al. 1992)
49.63 (calculated-QSPR, Achman et al. 1993)
7.44 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
21.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 51 \pm 25$ kJ/mol, $\Delta S_H = 0.13 \pm 0.09$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.10 (calculated-TSA, Burkhard 1984)
5.15 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.29 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.15 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:
7.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

4.90 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = 2.1×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)

tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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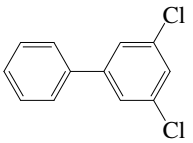
7.1.1.14 3,5-Dichlorobiphenyl (PCB-14)



Common Name: 3,5-Dichlorobiphenyl
Synonym: PCB-14, 3,5-dichloro-1,1′-biphenyl
Chemical Name: 3,5-dichlorobiphenyl
CAS Registry No: 34883-41-5
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
36 (Hinkel & Hay 1928)
31–32 (Weingarten 1961; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.872 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
1.05 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.00792, 0.0425, 0.0722, 0.109 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.128, 0.0662, 0.114 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0785 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.126, 0.117 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -3885/(T/K) + 12.13$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
16.72 (calculated-P/C, Burkhard et al. 1985b)
49.55 (calculated- QSAR-MCI χ, Sabljic & Güsten 1989)
42.63 (calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.37 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)
5.63, 5.56, 5.29, 5.16 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.28 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.17 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.41 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
8.82, 7.78 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.53 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF at 25°C or as indicated:

3.38–3.83 mean 3.79 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
3.82; 3.79 (rainbow trout: kinetic BCF, steady-state BCF, Oliver & Niimi 1985)

Sorption Partition Coefficient, log K_{OC}:

4.90 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 2.9×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)
$k_{OH} = (4.2 \pm 1.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 297 ± 2 K (relative rate method, Kwok et al. 1995)
tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 310 d^{-1}; k_2 = 0.046 d^{-1} (rainbow trout, Oliver & Niimi 1985)
log $1/k_2$ = 1.3, 2.5 h (fish, selected, calculated-K_{OW}, Hawker & Connell 1988)
$1/k_2$ = 21.7 d (rainbow trout, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 15 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985),
$t_{½}$ = 14 d in its muscle (Niimi & Oliver 1983).

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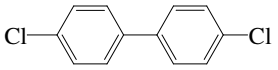
7.1.1.15 4,4′-Dichlorobiphenyl (PCB-15)



Common Name: 4,4′-Dichlorobiphenyl
Synonym: PCB-15, 4,4′-dichloro-1,1′-biphenyl
Chemical Name: 4,4′-dichlorobiphenyl
CAS Registry No: 2050-68-2
Molecular Formula: $C_{12}H_8Cl_2$
Molecular Weight: 223.098
Melting Point (°C):
149.3 (Lide 2003)
Boiling Point (°C):
317 (Lide 2003)
Density (g/cm^3 at 20°C): 1.0536
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point)
185.8 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.059 (Shiu & Mackay 1986)
0.0546 (Gobas et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
0.050 (Webb 1970)
0.060 (Hoover 1971)
0.080 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.056 (generator column-GC/ECD, Weil et al. 1974)
0.062 (20°C, shake flask-GC, Chiou et al. 1977; Freed et al. 1977)
0.046 (generator column-HPLC/UV, Billington 1982)
0.065 (generator column-HPLC/UV, Huang 1983)
0.058 (generator column-HPLC/UV, Billington et al. 1988)
0.151, 0.0774, 0.0952, 0.07055 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0363 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.057 ± 0.0021*(generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
ln x = –2.8677 – 4839.46/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
1.116, 0.959 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log S_L/(mol m^{-3}) = – 807/(T/K) + 0.41 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log S_L/(mol m^{-3}) = – 909/(T/K) + 0.68 (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00253* (Knudsen-effusion technique, extrapolated, Smith et al. 1964)
0.043 (P_L calculated from P_S using fugacity ratio F, Smith et al. 1964)
0.071, 0.084 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
0.0508 (supercooled liquid P_L, Burkhard 1984)
0.075, 0.059 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00313 (GC-RI correlation, Burkhard et al. 1985a)
0.0508 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0263 (extrapolated Antoine eq., Stephenson & Malanowski 1987)

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log (P_S/kPa) = – 5416/(T/K) + 12.585; temp range 50–87°C (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 10.10 – 4090/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0603, 0.0776 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3971/(T/K) + 12.18; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.00197* (gas saturation-GC/ECD, Wania et al. 1994)
log (P_S/Pa) = – 4977/(T/K) + 14.10; temp range –20 to 30°C (gas saturation-GC, solid, Wania et al. 1994)
0.0426 (supercooled liquid P_L, 20°C, from Falconer & Bidleman, Harner & Bidleman 1996)
0.00313–0.0219; 0518–0.0837 (literature P_S range; literature P_L range, Delle Site 1997)
0.223; 0.084 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI]; quoted lit., Saçan & Balcioğlu 1998)
log P/Pa = 14.10 – 4977/(T/K) temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0589, 0.0575 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 3931/(T/K) + 11.89 (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
log P_L/Pa = – 3829/(T/K) + 11.60 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

30.4 (calculated-P/C, Murphy et al. 1983)
11.04 (calculated-P/C, Burkhard et al. 1985b)
14.69 (calculated, Coates & Elzerman 1986)
17.0 (calculated-P/C, Shiu & Mackay 1986)
20.16 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
9.66 (wetted-wall column-GC/ECD, Fendinger & Glotfelty 1990)
18.95; 22.70 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln K_{AW} = – $\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 54 ± 3 kJ/mol, ΔS_H = 0.14 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
14.12, 13.49 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2921/(T/K) + 10.92 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

5.58 (shake flask-GC, Chiou et al. 1977)
5.17 (HPLC-RT correlation, Sugiura et al. 1978)
5.51 (Hansch & Leo 1979)
5.50 (shake flask-GC, Platford 1982)
5.36 ± 0.1; 5.28 (shake flask-GC; RP-TLC-k′ correlation, Bruggeman et al. 1982)
4.92 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
5.33 (generator column-GC/ECD; Woodburn et al. 1984)
4.82 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.30 (selected, Shiu & Mackay 1986)
5.33 (generator column-GC/ECD, Doucette & Andren 1987)
5.03, 5.39, 5.22, 5.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.17 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.23 (recommended, Sangster 1993)
5.58 (recommended, Hansch et al. 1995)
5.35, 5.36 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.67* (generator column-GC, measured range – 10 to 20°C, Harner & Mackay 1995)
log K_{OA} = – 5.10 + 3791.7/(T/K), temp range: – 10 to 20°C (generator column-GC, Harner & Mackay 1995)
7.88 (20°C, generator column-GC, Harner & Bidleman 1996)
log K_{OA} = –5.06 + 3792/(T/K); (temp range – 10 to + 20°C, Harner & Bidleman 1996)
8.87, 7.88; 7.89 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

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8.12 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.73; 7.77 (calibrated GC-RT correlation, GC-RT correlation, Wania et al. 2002)
7.65, 7.85 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4078/(T/K) – 5.83 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.97 (killifish, Goto et al. 1978)
2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
3.47 (calculated-S, Kenaga 1980)
3.58 (rainbow trout, highest value-non-equilibrated, Oliver & Niimi 1984)
4.27 (*picea omorika*, Reischl et al. 1989 from Reischl 1988)
4.06, 5.36 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

4.30 (calculated-solubility, Kenaga 1980)
4.91 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.65 (EPA-B2 river sediment, Coates & Elzerman 1986)
4.03 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated evaporation $t_{½}$ = 4.5 h for an initial concentration of 0.03 ppm in a 4.5 cm depth of water solution in a glass dish and $t_{½}$ = 1.7 h with stirring of the solution; while experimental observed $t_{½}$ = 4.0 h and 1.5 h under the same condition with stirring of the solution (Chiou et al. 1979).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = 1.4×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (SAR, Atkinson 1987)
tropospheric lifetime τ(calc) = 8–17 d for dichlorobiphenyls, based on k_{OH}(calc.) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for dichlorobiphenyls at room temp. (Atkinson 1987)
tropospheric lifetime τ(calc) = 3.4–7.2 d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, and the calculated k_{OH}(calc) = $(1.4 – 3.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50–80% biodegraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);
$t_{½}$ = 72 h for 50% degradation in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, and 55% degradation at 24 h in another PCB mixture by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986);
aerobic biodegradation $t_{½}$ = 1.42 d without the addition of polymer chitin, $t_{½}$ = 0.98 d with chitin and $t_{½}$ = 0.46 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.009 d^{-1} with $t_{½}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.007 d^{-1} with $t_{½}$ = 99 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

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Surface water: $t_{½}$ = 57.5 d in Lake Michigan, 57.5 d (Neely 1983);
aerobic biodegradation $t_{½}$ = 1.42 d without the addition of polymer chitin, $t_{½}$ = 0.98 d with chitin and $t_{½}$ = 0.46 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 27 d in *Picea omorika* (Reischl et al. 1989).
depuration $t_{½}$ = 81 d for high-dose treatment, $t_{½}$ = 99 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.15.1
Reported aqueous solubilities, vapor pressure and octanol-air partition coefficients of 4,4′-dichlorobiphenyl (PCB-15) at various temperatures

Aqueous solubility		Vapor pressure				log K_{OA}	
Shiu et al. 1997		Smith et al. 1964		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		Knudsen effusion		gas saturation-GC/ECD		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OA}
5	0.021	29.88	0.149	–10	1.206×10^{-5}	–10	9.36
15	0.0346	29.88	0.152	0	8.303×10^{-5}	0	8.83
25	0.0570	66.58	0.504	10	4.159×10^{-4}	10	8.35
35	0.106	66.58	0.432	20	1.197×10^{-3}	20	7.88
45	0.186	76.78	1.26	30	4.475×10^{-3}	25	7.67
		76.78	1.27				
		87.0	3.55	log P/Pa = A – B/(T/K)		ΔH_{OA}/(kJ mol^{-1}) = 72.6	
ΔH_{sol}/(kJ mol^{-1}) = 40.2		87.0	3.57	A	14.10		
at 5–45°C				B	4977	log K_{OA} = A + B/T	
		log P/mmHg = A – B/(T/K)		temp range –10 to30°C		A	–5.1
		A	13.460			B	3791.7
		B	5416	ΔH_{subl}/(kJ mol^{-1}) = 95.3			

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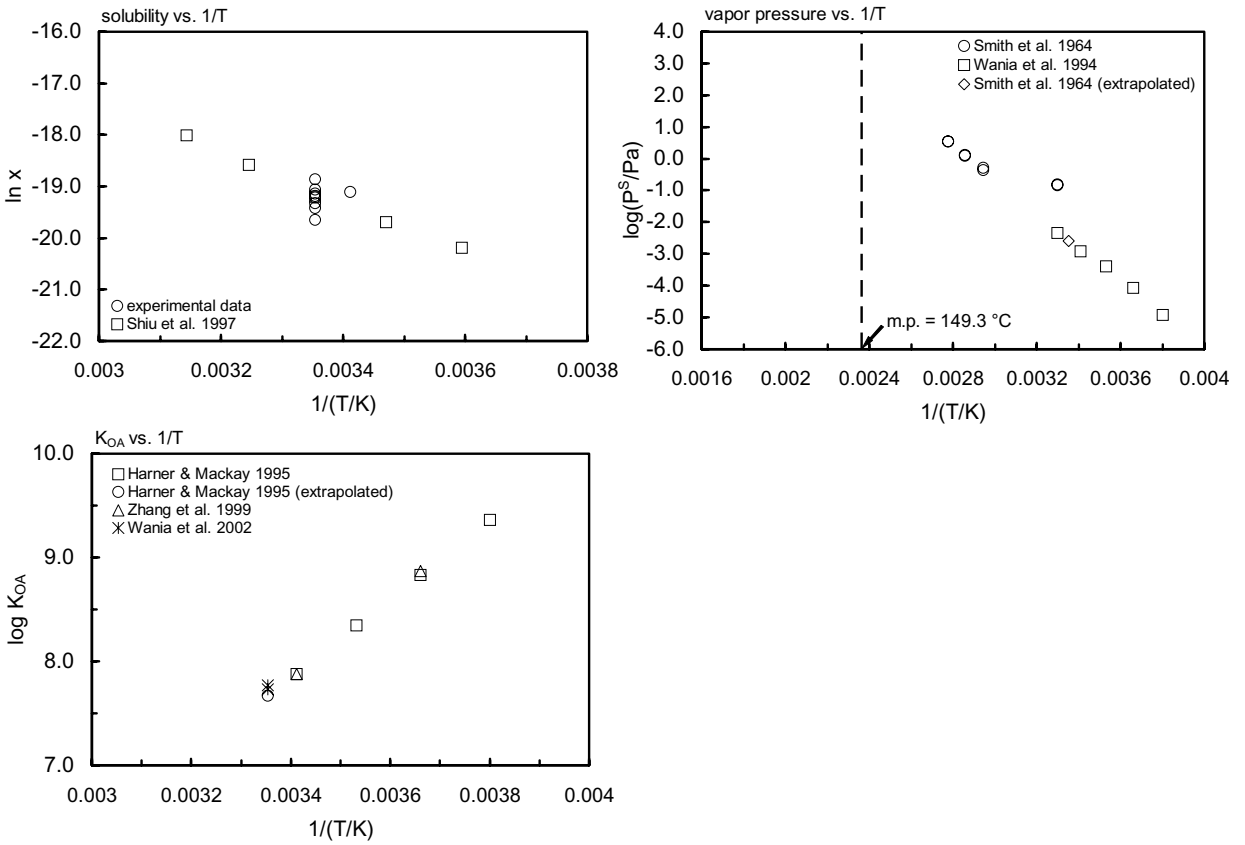

FIGURE 7.1.1.15.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 4,4′-dichlorobiphenyl (PCB-15).

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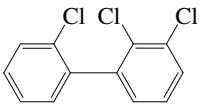
7.1.1.16 2,2′,3-Trichlorobiphenyl (PCB-16)



Common Name: 2,2′,3-Trichlorobiphenyl
Synonym: PCB-16, 2,2′,3-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,3-trichlorobiphenyl
CAS Registry No: 38444-78-9
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
28.1–28.8 (Weingarten 1961; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.934 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.505 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)
0.293 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.205 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.814 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)
0.674 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0522, 0.066, 0.033 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.069 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0538, 0.060 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0275 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.10 – 4100/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0427; 0.0427 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3935/(T/K) + 11.93 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0506; 0.0427 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI; quoted lit., Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
35.16 (calculated-P/C, Burkhard et al. 1985b)
80.0 (calculated-P/C, Shiu & Mackay 1986)
24.11 (20°C, calculated-P/C, Murphy et al. 1987)
81.77 (batch stripping, Atlas et al. 1982)
28.07 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
25.45 (calculated-QSPR, Dunnivant et al. 1992)
4.02, 11.74 (0, 15°C, from modified two-film exchange model, Hornbukle et al. 1994)
9.36 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
25.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

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ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.36 (calculated-TSA, Burkhard 1984)
4.15 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.31 (calculated-π const., Rapaport & Eisenreich 1984)
5.12 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.12 (recommended, Sangster 1993)
5.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations.:

7.22; 7.18 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log $K_{OA} = -6.50 + 4240/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.87, 7.98 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.32 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.16 (suspended particulate matter, Burkhard 1984)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.00 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.7 - 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(aq.) = 7.2×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(1.0 - 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degraded by Nocardia strain NCIB 10603 within 7 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008$ d^{-1} with $t_{½}$ = 90 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.010$ d^{-1} with $t_{½}$ = 72 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

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Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH· oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 90 d for high-dose treatment, $t_{½}$ = 72 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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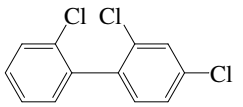
7.1.1.17 2,2′,4-Trichlorobiphenyl (PCB-17)



Common Name: 2,2′,4-Trichlorobiphenyl
Synonym: PCB-17, 2,2′,4-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,4-trichlorobiphenyl
CAS Registry No: 37680-66-3
Molecular Formula: $C_{12}H_8C_2$
Molecular Weight: 257.543
Melting Point (°C):
35 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.292 (supercooled liquid S_L, Burkhard et al. 1985a)
0.259 (supercooled liquid S_L, Murphy et al. 1987)
0.103 (RP-HLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.647 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.080 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0566, 0.0828, 0.0219 (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.0705, 0.0739 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0335 (supercooled liquid P_L, Murphy et al. 1987)
0.0692; 0.0526 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -3935/(T/K) + 12.05$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0692; 0.526 (P_L, quoted lit.; calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
52.18 (calculated-P/C, Burkhard et al. 1985b)
33.03 (calculated-P/C, Murphy et al. 1987)
40.63 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
37.82 (calculated-QSPR, Dunnivant et al. 1992)
26.04 (calculated-QSPR, Achman et al. 1993)
13.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.60, 5.76 (RP-HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenrich 1984)
5.39 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.50 (generator column-GC, Larsen et al. 1992)

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5.50 (recommended, Sangster 1993)
5.76 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
8.06; 7.74 (0; 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.24 (suspended particulate matter, Burkhard 1984)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.84 (calculated-QSAR-MCI $^1\chi$, Sabljic et al. 1995)
5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.7 – 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH-}(aq.) = 7.5×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(1.0 – 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.009 d^{-1} with $t_{½}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.007 d^{-1} with $t_{½}$ = 99 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 81 d for high-dose treatment, $t_{½}$ = 99 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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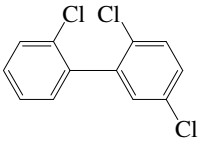
7.1.1.18 2,2′,5-Trichlorobiphenyl (PCB-18)



Common Name: 2,2′,5-Trichlorobiphenyl
Synonym: PCB-18, 2,2′,5-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,5-trichlorobiphenyl
CAS Registry No: 37680-65-2
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
43–44 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.648 (Mackay et al. 1980)
0.651 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.640 (shake flask-GC/ECD, Weil et al. 1974)
0.248 (shake flask-GC/ECD, Haque & Schmedding 1975)
0.016 (radioactive isotope-^{14}C labeled, Metcalf et al. 1975)
0.0614 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)
0.085 (Kenaga & Goring 1980; Kenaga 1980)
0.110 (shake flask GC/ECD, Bruggeman et al. 1981)
0.299 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.203, 0.135, 0.100, 0.112 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.510; 0.780 (generator column-GC/ECD, supercooled liquid S_L, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.267 (Neely 1981)
0.412 (P_L calculated from P_S using fugacity ratio F, Neely 1981)
0.012 (Neely 1983)
0.0904 (supercooled liquid P_L, Burkhard 1984)
0.0605 (GC-RI correlation, Burkhard et al. 1985a)
0.0904 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
0.0776, 0.0833 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.143; 0.220 (selected: solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
0.0352 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.10 – 4090/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0603, 0.0851 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3935/(T/K) + 12.09; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.033–0.0762; 0.035–0.116 (literature P_S range; literature P_L range, Delle Site 1997)

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Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101.53 (23°C, gas stripping-GC, Atlas et al. 1982)
20.26 (20°C, gas stripping-GC, Oliver 1985)
38.5 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
25.33 (wetted-wall column-GC/ECD, Brunner et al. 1990)
8.11, 12.07, 17.64, 25.358* ± 0.34, 34.14 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 9.5020 - 4197.74/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(34.9/kJ \cdot mol^{-1})/RT] + (0.079/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 $J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
25.3 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 35 \pm 3$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

3.89 (radiolabeled-^{14}C, Metcalf et al. 1975)
6.22 (shake flask, Hansch & Leo 1979)
5.88 (calculated after Rekker 1977, Könemann 1981)
5.64 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.59; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn 1982)
4.39, 5.55 (RP-HPLC-RT correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.60; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
4.97 (HPLC-RT correlation, DeVoe et al. 1987)
4.97, 5.68 (HPLC-k′ correlation, De Kock & Lord, 1987)
5.60 (generator column-GC/ECD, Doucette & Andren 1987,1988)
5.31, 5,37, 5,29, 5,37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.55 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.44 (generator column-GC, Larsen et al. 1992)
5.44 (recommended, Sangster 1993)
5.60 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

7.60; 7.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -6.00 + 4060/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
8.39 (10°C, estimated, Thomas et al. 1998)
8.70, 7.79 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.48 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.86, 3.76, 2.91, 3.81 (algae, snail, mosquito, fish, ^{14}C-labeled, Metcalf et al. 1975)
1.72 (green sunfish, 15 d in static water, Sanborn et al. 1975)
3.39 (calculated-S, Kenaga 1980)
5.52; 5.83 (goldfish: 10% lipid by wt. in food; 3% lipid, static equilibration system-GC/ECD, 23-d exposure studies, Bruggeman et al. 1981)
3.43–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.91, 4.23; 5.77 (rainbow trout, laboratory data: kinetic BCF(k_1/k_2), steady-state BCF (C_F/C_W); Lake Ontario field BCF, Oliver & Niimi 1985)
4.30 (fish, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
3.75 (*Picea omorika*, Reischl et al. 1989 from Reischl 1988)
4.23 (fish, Isnard & Lambert 1989)
5.82; 5.87 (goldfish; rainbow trout, Noegrohati & Hammers 1992)
4.11; 5.64 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

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2.60–4.19 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.08–6.01 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.23, 5.32 (rainbow trout, flow through-96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.30, 5.60 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.11, 5.64 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

4.50, 4.50, 5.0 (sediments: offshore Grand Haven 2.0% OC, nearshore Grand Haven 3.4% OC, Benton Harbor sediment 3.8% OC, batch equilibrium-sorption isotherm, Voice et al. 1983; Voice & Weber, Jr., 1985)
5.24 (suspended particulate matter, Burkhard 1984)
5.40; 5.50; 5.20(field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
5.1–6.3, 5.5; 7.0(suspended sediment, average; algae > 50 μm, Oliver 1987a)
4.57, 4.85 (natural solids, Aldrich humic acid, equilibrium dialysis, Chin & Weber 1989, Chin et al. 1990)
5.34 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.49 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
4.85, 4.15 (Aldrich humic acid substrate with methyl salicylate, organic polymers present in Huron River water, Chin et al. 1990)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.23 (soil, calculated-MCI, Sabljic et al. 1995)
4.53; 4.57 (soil, calculated-Characteristic Root Index [CRI]; quoted lit., Saçan & Balcioğlu 1996)
5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
4.85 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.7 – 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}-(aq.) = 6.9×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{½}$~4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(1.0 – 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: 50–80% being degraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 950 d^{-1}; k_2 = 0.048 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)
k_2 = 0.0037 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark 1990)
k_2 = 0.048, 0.0372 d^{-1} (goldfish, exptl., correlated, Mackay & Hughes 1984)
k_1 = 300 d^{-1}; k_2 = 0.0037 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 39.6 h^{-1}; $1/k_2$ = 500 h (goldfish, quoted, Hawker & Connell 1985)
log k_1 = 2.98 d^{-1}; log $1/k_2$ = 1.32 d (goldfish, quoted, Connell & Hawker 1988b)
log $1/k_2$ = 2.4, 2.4 d (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b).
log $1/k_2$ = 1.32 d (goldfish, quoted, Connell & Hawker 1988b; Thomann 1989)
k_1 = 3760 d^{-1}; k_2 = 0.292 d^{-1} (zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.020 d^{-1} with $t_{½}$ = 36 d and k_2 = 0.029 d^{-1} with $t_{½}$ = 24 d for food concn of 29 ng/g and 182 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

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k_2 = 0.009 d^{-1} with $t_{½}$ = 79 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.007 d^{-1} with $t_{½}$ = 96 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 43.1 d in Lake Michigan (Neely 1983); $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991).

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: 0.47 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 1.16 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC,1.21 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.17 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; 0.00838 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 0.00368 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 0.00357 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00062 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{½}$ = 190 d in rainbow trout, 190 d and its muscle 86 d (Niimi & Oliver 1983);
$t_{½}$ = 190 d in fish (rainbow trout, Niimi & Oliver 1983; Oliver & Niimi 1985);
$t_{½}$ = 26 d in worms at 8°C (Oliver 1987c);
$t_{½}$ = 25 d in omorika (Reischl et al. 1989)

Depuration $t_{½}$ = 32–42 d for a 32-d dietary exposure followed by a 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{½}$ = 79 d for high-dose treatment, $t_{½}$ = 96 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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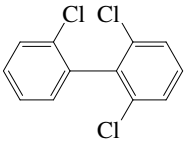
7.1.1.19 2,2′,6-Trichlorobiphenyl (PCB-19)



Common Name: 2,2′,6-Trichlorobiphenyl
Synonym: PCB-19, 2,2′6,-trichloro-1,1′-biphenyl
Chemical Name: 2,2′,6-trichlorobiphenyl
CAS Registry No: 38444-73-4
Molecular Formula: $C_{12}H_7Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
46 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.345 (supercooled liquid S_L, Burkhard et al. 1985a)
0.448 (supercooled liquid S_L, Murphy et al. 1987)
0.447, 0.408, 0.235, 0.246 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.814 (calculated-TSA, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.167 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.171 (GC-RI correlation, Burkhard et al. 1985b)
0.113, 0.131 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0529 (supercooled liquid P_L, Murphy et al. 1987)
log (P/mmHg) = 9.86 – 3970/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0933, 0.138 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3836/T + 11.93 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
124.6 (calculated-P/C, Burkhard et al. 1985b)
30.70 (calculated-P/C, Murphy et al. 1987)
45.09 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
23.30 (wetted-wall column-GC, Brunner et al. 1990)
44.74 (calculated-QSPR, Dunnivant et al. 1992)
13.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
3.75, 5.48 (RP-HPLC correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
4.88, 5.06, 5.03, 5.19 (RP-HPLC-k′ correction, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

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5.04 (recommended, Sangster 1993)
5.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
6.72 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.28 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.7 – 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(1.0 – 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.004 d^{-1} with $t_{½}$ = 155 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.008 d^{-1} with $t_{½}$ = 84 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–15 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 155 d for high-dose treatment, $t_{½}$ = 84 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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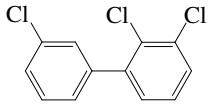
7.1.1.20 2,3,3′-Trichlorobiphenyl (PCB-20)



Common Name: 2,3,3′-Trichlorobiphenyl
Synonym: PCB-20, 2,3,3′-trichloro-1,1′-biphenyl
Chemical Name: 2,3,3′-trichlorobiphenyl
CAS Registry No: 38444-84-7
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
58 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
337 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.402 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.033 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)
0.0283 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0269 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
log (P/mmHg) = 10.40 – 4310/(T/K), (GC-RT correlation, Tateya et al. 1988)
0.0302 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.12$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry' Law Constant (Pa m^3/mol at 25°C):
81.77 (batch stripping-GC, Atlas et al. 1982)
17.23 (calculated-P/C, Burkhard et al. 1985b)
30.7 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
16.21 (wetted-wall column-GC/ECD, Brunner et al. 1990)
22.01 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.99, 5.57 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.57 (calculated-TSA, Hawker & Connell 1988a)
5.68 (generator column-GC, Larsen et al. 1992)
5.62 (recommended, Sangster 1993)
5.57 (recommended, Hansch et al. 1995)
5.4846 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} or as indicated:

9.51, 8.49 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
7.95 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

5.23 (suspended particulate matter, Burkhard 1984)
4.01–4.88; 5.20 (range, calculated from sequential desorption of 11 urban soils; lit. value, Krauss & Wilcke 2001)
5.13; 5.01, 4.88, 5.45 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.7 – 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(1.0 – 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 88 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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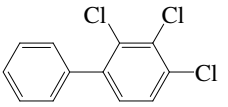
7.1.1.21 2,3,4-Trichlorobiphenyl (PCB-21)



Common Name: 2,3,4-Trichlorobiphenyl
Synonym: PCB-21, 2,3,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3,4-trichlorobiphenyl
CAS Registry No: 55702-46-0
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
101–102 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.176 (mp at 102°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.469 (calculated-TSA, Burkhard et al. 1985b)
0.224, 0.195, 0.142; 0.132 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00489 (GC-RI correlation, Burkhard et al. 1985a)
0.0269 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0295 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.11$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
14.79 (calculated-P/C, Burkhard et al. 1985b)
21.38 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
23.0 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.88 (calculated after Rekker 1977, Könemann 1981)
5.77 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.51, 5.61, 5.87, 5.73 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.860 ± 0.017(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990;)
5.68 (recommended, Sangster 1993)
5.86 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.16 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}

5.19 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constants k = 0.021 min^{-1} with $t_{½}$ = 33 min, k = 0.059min^{-1} with $t_{½}$ = 12 min and $t_{½}$ = 0.14 min^{-1} with $t_{½}$ = 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constants k = 0.0050 min^{-1} with $t_{½}$ = 139 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.7 – 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(1.0 – 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 33 min, 12 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; $t_{½}$ = 139 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

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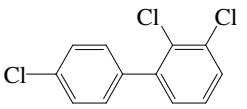
7.1.1.22 2,3,4′-Trichlorobiphenyl (PCB-22)



Common Name: 2,3,4′-Trichlorobiphenyl
Synonym: PCB-22, 2,3,4′-trichloro-1,1′-biphenyl
Chemical Name: 2,3,4′-trichlorobiphenyl
CAS Registry No: 38444-85-8
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
73 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)
69.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.335 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.397 (supercooled liquid S_L, Burkhard et al. 1985b)
0.142 (supercooled liquid S_L, Murphy et al. 1987)
0.408 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0696 (calculated-QSPR, Dunnivant et al. 1992)
0.187 (calculated-group contribution method, Kühne et al. 1995)
0.0677, 0.178 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.469 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0239 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0084 (GC-RI correlation, Burkhard et al. 1985b)
0.026, 0.023 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0111 (supercooled liquid P_L, Murphy et al. 1987)
0.0191, 0.0263(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.08$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0478 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C):
15.40 (calculated-P/C, Burkhard et al. 1985b)
20.16 (calculated-P/C, Murphy et al. 1987)
14.18 (wetted-wall column-GC/ECD, Brunner et al. 1990)
22.60 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
25.03; 19.35 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
13.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
31.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 31 \pm 1$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

4.84, 5.42 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.29 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.63 (generator column-GC, Larsen et al. 1992)
5.45 (recommended, Sangster 1993)
5.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.60; 8.58 (0; 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.70, 4.90 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.24 (suspended particulate matter, Burkhard 1984)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.90 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 7.4 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.012 d^{-1} with $t_{½}$ = 56 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.011 d^{-1} with $t_{½}$ = 64 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water: $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 56 d for high-dose treatment, $t_{½}$ = 64 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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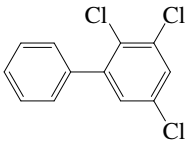
7.1.1.23 2,3,5-Trichlorobiphenyl (PCB-23)



Common Name: 2,3,5-Trichlorobiphenyl
Synonym: PCB-23, 2,3,5-trichloro-1,1′-biphenyl
Chemical Name: 2,3,5-trichlorobiphenyl
CAS Registry No: 55720-44-0
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
41 (Burkhard et al. 1985a)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.694 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.402 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.223 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0402 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0291 (GC-RI correlation, Burkhard et al. 1985b)
0.0447 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.36$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
25.74 (calculated-P/C, Burkhard et al. 1985a)
35.6 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
32.26 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.44 (calculated-TSA, Burkhard 1984)
5.53 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
5.57 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.6729 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

5.23 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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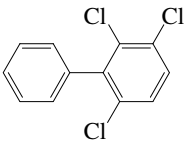
7.1.1.24 2,3,6-Trichlorobiphenyl (PCB-24)



Common Name: 2,3,6-Trichlorobiphenyl
Synonym: PCB-24, 2,3,6-trichloro-1,1′-biphenyl
Chemical Name: 2,3,6-trichlorobiphenyl
CAS Registry No: 55702-45-9
Molecular Formula: $C_{12}H_7Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
49 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.581 (mp at 49°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.507 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.132 (20°C, supercooled liquid, Murphy et al. 1987)
0.0677, 0.118, 0.0604, 0.098 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.167; 0.136, 0.358 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.132; 0.853 (quoted exptl., calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.087 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0899 (GC-RI correlation, Burkhard et al. 1985b)
0.0166 (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.6 – 4090/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0708 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 3935/(T/K) + 12.02 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
44.18 (calculated-P/C, Burkhard et al. 1985a)
32.12 (20°C, Murphy et al. 1987)
34.35 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
22.3 (wetted-wall column-GC, Brunner et al. 1990)
31.53 (calculated-QSPR, Dunnivant et al. 1992)
14.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 39 ± 21 kJ/mol, ΔS_H = 0.10 ± 0.07 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

4.52, 5.67 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

5.45, 5.42, 5.44, 5.46 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.44 (recommended, Sangster 1993)

5.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

7.75 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.16 (suspended particulate matter, Burkhard 1984)

6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: k = (0.019–0.029) min^{-1} with $t_{½}$ = 24–36 min, k = (0.041–0.059) min^{-1} with $t_{½}$ = 12–17 min and k = (0.12–0.22) min^{-1} with $t_{½}$ = 3–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constants, k = (0.0066–0.030) min^{-1} with $t_{½}$ = 23–105 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 µg/mL TiO_2; rate constant k = 0.022 min^{-1} with $t_{½}$ = 31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(aq.) = 7.6 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.009 d^{-1} with $t_{½}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime τ = 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime τ = 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

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Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
$t_{½}$ = 24–36 min, 12–17 min and 3–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 μg/mL TiO_2, respectively; $t_{½}$ = 23–105 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 μg/mL TiO_2; $t_{½}$ = 31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 μg/mL TiO_2 (Huang et al. 1996).
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 81 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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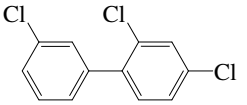
7.1.1.25 2,3′,4-Trichlorobiphenyl (PCB-25)



Common Name: 2,3′,4-Trichlorobiphenyl
Synonym: PCB-25, 2,3′,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,4-trichlorobiphenyl
CAS Registry No: 55712-37-3
Molecular Formula: $C_{12}H_3H_7$
Molecular Weight: 257.543
Melting Point (°C):
61 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.317 (supercooled liquid S_L, Burkhard et al. 1985a)
0.025 (supercooled liquid S_L, Murphy et al. 1987)
0.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.1025 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0313 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0327 (GC-RI correlation, Burkhard et al. 1985b)
0.0373, 0.0366 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.24×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0295, 0.0372(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
25.53 (calculated-P/C, Burkhard et al. 1985a)
43.27 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
32.04 (calculated-QSPR, Dunnivant et al. 1992)
17.20 (calculated-QSPR, Achman et al. 1993)
14.0 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.51 (calculated-TSA, Burkhard 1984)
5.67 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.54 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.63 (calculated, Miertus & Jakus 1990)
5.54 (recommended, Sangster 1993)
5.6793 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.31; 8.28; 8.23(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
7.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.7 – 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}-(aq.) = 7.2×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(1.0 – 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–5 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.008 d^{-1} with $t_{½}$ = 87 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.007 d^{-1} with $t_{½}$ = 102 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 87 d for high-dose treatment, $t_{½}$ = 102 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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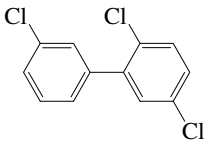
7.1.1.26 2,3′,5-Trichlorobiphenyl (PCB-26)



Common Name: 2,3′,5-Trichlorobiphenyl
Synonym: PCB-26, 2,3′,5-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,5-trichlorobiphenyl
CAS Registry No: 38444-81-4
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
40.0–40.5 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.705 (mp at 40.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.219, 0.166, 0.205, 0.155 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.253 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.138 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0353 (supercooled liquid P_L, Burkhard et al. 1984)
0.0262 (GC-RI correlation, Burkhard et al. 1985a)
0.0363 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0411, 0.0412 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0182 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0316, 0.389 (supercooled liquid P_L, GC-RI correlation, different stationary phases Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.28$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0112–0.0402; 0.0182–0.0449 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C):
32.93 (gas stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
20.27 (wetted-wall column-GC, Brunner et al. 1990)
12.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
30.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.76 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.52, 5.68, 5,72, 5,68 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.65 (recommended, Sangster 1993)
5.76 (recommended, Hansch et al. 1995):

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.30, 8.27; 8.24(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulate matter, Burkhard 1984)
6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 6.3 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 from lake sediments but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.007 d^{-1} with $t_{½}$ = 105 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 105 d for high-dose treatment, $t_{½}$ = 135 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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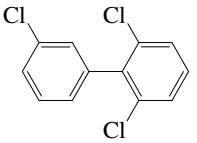
7.1.1.27 2,3′,6-Trichlorobiphenyl (PCB-27)



Common Name: 2,3′,6-Trichlorobiphenyl
Synonym: PCB-27, 2,3′,6-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,6-trichlorobiphenyl
CAS Registry No: 38444-81-4
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
45 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.404 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.039 (supercooled liquid S_L, Murphy et al. 1987)
0.256 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0653 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0676 (GC-RI correlation, Burkhard et al. 1985b)
0.0598, 0.0628 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.26×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0490, 0.0708 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -3935/(T/K) + 11.97$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
41.64 (calculated-P/C, Burkhard et al. 1985a)
49.95 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
41.0 (calculated-QSPR, Dunnivant et al. 1992)
22.17 (quoted as PCB-24 and 27, Achman et al. 1993)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.43 (calculated-TSA, Burkhard 1984)
5.44 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.52 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
5.50 (quoted as PCB-24 and 27, Murray & Andren 1992)
5.2417 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.23 (suspended particulate matter, Burkhard 1984)

6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 7.6 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.009 d^{-1} with $t_{½}$ = 81 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 81 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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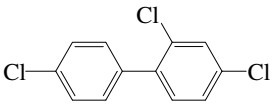
7.1.1.28 2,4,4′-Trichlorobiphenyl (PCB-28)



Common Name: 2,4,4′-Trichlorobiphenyl
Synonym: PCB-28, 2,4,4′-trichloro-1,1′-biphenyl
Chemical Name: 2,4,4′-trichlorobiphenyl
CAS Registry No:7012-37-5
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
57–58 (Hutzinger et al. 1971,1974)
Boiling Point (°C):
206–207 (Sengupta 1966)
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.6 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.482 (Mackay et al. 1980; Shiu & Mackay 1986)
0.482 (Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.085 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.260 (generator column-GC/ECD, Weil et al. 1974)
0.119 (Dexter & Pavlou 1978)
0.270 (20°C, supercooled liquid S_L, shake flask-GC/ECD, Chiou et al.1983; Chiou 1985)
0.142 (generator column-HPLC/UV, Huang 1983)
0.163 (generator column-GC/ECD, Miller et al. 1984)
0.312 (supercooled liquid P_L, calculated-TSA, Burkhard et al. 1985b)
0.116 (shake flask-GC/ECD, Chiou et al. 1986)
0.143 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixture, Murphy et al. 1987)
0.177, 0.107, 0.144,0.117 (RP-HPLC-k′ correlation, different stationary and mobile Brodsky & Ballschmiter 1988)
0.067 (22°C, generator column-GC, Opperhuizen et al. 1988)
0.117 (generator column-GC, Dunnivant & Elzerman 1988)
log [S_L/(mol/L)] = 0.232 – 975.5/(T/K); (supercooled liquid, Passivirta et al. 1999)
0.260, 0.228 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_L/(mol m^{-3})] = – 1147/(T/K) + 0.79 (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0277 (supercooled liquid P_L, Burkhard 1984)
0.014 (GC-RI correlation, Burkhard et al. 1985a)
0.0277 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0339, 0.0340(supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0149 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0277, 0.0335(supercooled liquid, Dunnivant & Elzerman 1988)
log (P/mmHg) = 10.40 – 4270/(T/K) (GC-RT correlation, Tateya et al. 1988)

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0.257, 0.0324(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4075/(T/K) + 12.20 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0210; 0.0436(solid, supercooled liquid, Passivirta et al. 1999)
log (P_S/Pa) = 15.15 – 5049/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 12.20 – 4075/(T/K) (supercooled liquid, Passivirta et al. 1999)
0.0234, 0.0269(supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log (P_L/Pa) = – 4157/(T/K) + 12.31 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log (P_L/Pa) = – 4007/(T/K) + 11.87 (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations

32.02 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
8.7, 21.2, 47.4, 50.3, 70.8, 120.6, 122.2 (10.4, 20, 30.1, 34.9, 42.1, 47.9, 48.4°C, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)
log [H/(Pa·m^3/mol)] = 11.97 – 3100/(T/K); (Passivirta et al. 1999)
13.13, 19.06, 27.18, 38.14 ± 0.37, 50.39 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[– (32.5/kJ·mol^{-1})/ RT] + (0.074/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
19.72 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 6.324 – 2467/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
36.5 (exptl. data, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 33 ± 2 kJ/mol, ΔS_H = 0.07 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
33.11, 30.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2010/(T/K) + 857 (LDV linear regression of literature data, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2860/(T/K) + 11.08 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

4.38 (shake flask-GC, Paris et al. 1978)
5.74 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.62 (shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.51, 5.77, 5.81, 5.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.68 (generator column-GC, Larsen et al. 1992)
5.59 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.71 (recommended, Sangster 1993)
5.62 (recommended, Hansch et al. 1995)
5.55, 5.66 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
log K_{OA} = – 6.12 + 4190/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.76 (10°C, estimated, Thomas et al. 1997)
9.43, 8.40 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.03 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.93, 7.85 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4102/(T/K) – 5.91 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.60–3.82 (various marine species, mean dry wt. BCF, Hope et al. 1998)
3.82–4.93 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.32, 5.62 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.74, 5.66 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)

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Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.50, 4.70 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.23 (calculated, Kenaga 1980)
4.38 (log K_{OM} soil organic matter, Wood burn soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
5.31 (suspended particulate matter, Burkhard 1984)
5.28 (sediment: suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
5.30; 4.59 (suspended solids-Lake Superior: calculated-K_{OW}, Baker et al. 1986)
4.40; 3.54 (Sanhedron soil-Suwannee River; humic acid, shake flask-GC, Chiou et al. 1986, 1987)
3.89; 3.57 (Sanhedron soil-Suwannee River; fulvic acid, shake flask-GC, Chiou et al. 1986, 1987)
4.84; 4.24 (Fluka-Tridom humic acid; Calcasieu River humic extract, Chiou et al. 1987)
3.53; 3.27 (Suwannee River water sample; Sopchoppy River water sample, Chiou et al. 1987)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.03–4.91; 5.30–5.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.25; 5.27, 4.91, 5.32 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolysis rate k_P(exptl) = 6×10^{-8} d^{-1} with $t_{½}$ = 133 d; k_P(calc) = 2.2×10^{-8} d^{-1} in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.7–1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(aq.) = 7.2×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(1.0–2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{½}$ = 7 h of biodegradation by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

49% degradation at 72 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.016 d^{-1} with $t_{½}$ = 44 d and k_2 = 0.015 d^{-1} with $t_{½}$ = 46 d for food concn of 16 ng/g and 108 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_1 = 0.00054 h^{-1}; k_2 = 0.089 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1(calc) = 11 (food lipid (mg)/(g worm lipid-d); k_2(calc) = 0.14 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

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Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995);
$t_{½}$ = 72 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis $t_{½}$ = 133 d in winter sunlight at 40°L in surface waters (Dulin et al. 1986);
half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
$t_{½}$ = 1450 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{½}$ = 26000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: 0.47 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 1.15 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 1.34 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.53 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; 0.00378 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 0.00183 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 0.0016 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00044 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).
$t_{½}$ = 26000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: depuration $t_{½}$ = 44–46 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$t_{½}$ = 7.8 h in blood plasma (ring doves, Drouillard & Norstrom 2000);
elimination $t_{½}$ = 5 d in earthworm given contaminated food (predicted, Wågman et al. 2001)
depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 88 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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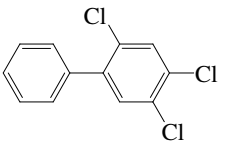
7.1.1.29 2,4,5-Trichlorobiphenyl (PCB-29)



Common Name: 2,4,5-Trichlorobiphenyl
Synonym: PCB-29, 2,4,5-trichloro-1,1′-biphenyl
Chemical Name: 2,4,5-trichlorobiphenyl
CAS Registry No: 15862-07-4
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
78.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
65.27 (Miller et al. 1984)
65.24, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.30 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.092 (generator column-GC/ECD, Weil et al. 1974)
0.119 (Dexter & Pavlou 1978)
0.140 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
0.142 (generator column-HPLC/UV, Huang 1983)
0.162 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.0.098, 0.107,0.138,0.120 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.106* ± 0.0045 (generator column-GC/ECD, Shiu et al. 1997)
0.0413, 0.0682, 0.106, 0.203, 0.33 (5, 15, 25, 35, 45°C, generator column-GC, Shiu et al. 1997)
ln x = – 3.06175 – 4633.86/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.479, 0.389 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log S_L/(mol m^{-3}) = – 824/(T/K) + 0.03 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log S_L/(mol m^{-3}) = – 977/(T/K) + 0.46 (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0443 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.0112 (GC-RI correlation, Burkhard et al. 1985a)
0.0320 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0453, 0.0464 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P_L/Pa) = – 4075/(T/K) + 12.20 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0263 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994; Harner & Bidleman 1996)
0.0447, 0.0457 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 3904/(T/K) + 11.75 (supercooled liquid, final adjusted eq., Li et al. 2003)

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Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

20.27 (wetted-wall column-GC, Brunner et al. 1990; quoted, Achman et al. 1993)
37.89* ± 0.53 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln K_{AW} = 9.863 – 4197.74/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[– (34.9/kJ·mol^{-1})/ RT] + (0.082/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
36.3 (exptl. data, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 35 ± 3 kJ/mol, ΔS_H = 0.08 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
32.36, 30.20 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 1674/(T/K) + 7.13 (LDV linear regression of literature data, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 2927/(T/K) + 11.30 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW} or as indicated and reported temperature dependence equations:

6.22 (Hansch & Leo 1979)
5.77 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.86 (HPLC-RT correlation, Woodburn 1982)
5.51 (generator column-GC/ECD, Miller et al. 1984)
5.81 (generator column-GC, Woodburn et al. 1984)
5.86 (HPLC-RT correlation, Woodburn et al. 1984)
6.25 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.66 (HPLC-RP/MS, Burkhard & Kuehl 1986)
5.81 (generator column-GC/ECD, Doucette & Andren 1987)
5.78, 5.82, 5.88, 5,76 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.86 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
5.901 ± 0.007 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.54 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.81 (recommended, Sangster 1993)
5.90 (recommended, Hansch et al. 1995)
5.74, 5.60 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.96* (generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)
log K_{OA} = – 4.80 + 3791.7/(T/K); temp range –10 to + 20°C (generator column-GC, Harner & Mackay 1995)
8.03 (20°C, generator column-GC, Harner & Bidleman 1996)
log K_{OA} = – 4.77 + 3792/(T/K); temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
9.15, 8.05 (0, 20°C, multi-column GC-k′ correlation; Zhang et al. 1999)
8.21 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.01; 8.03 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
7.80, 7.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4175/(T/K) – 6.22 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

4.97 (guppy, lipid wt. based, Gobas et al. 1989)
5.41 (guppy, corr. lipid wt. based, Gobas et al. 1989)
4.36, 5.53 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.26 (suspended particulate matter, Burkhard 1984)
4.51 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

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Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constants k = (0.019–0.022) min^{-1} with $t_{½}$ = 31–36 min, k = (0.033–0.048) min^{-1} with $t_{½}$ = 14–21 min and k = (0.13–0.14) min^{-1} with $t_{½}$ = 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; rate constants k = (0.0056–0.020) min^{-1} with $t_{½}$ = 35–123 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: half-life of biodegradation by *Alcaligenes* sp. strain Y-42 from lake sediments estimated to be less than 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

log k_2 = – 1.68 d^{-1} (fish, quoted, Hawker & Connell 1985; Thomann 1989)

k_2 = 0.004 d^{-1} with $t_{½}$ = 190 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.007 d^{-1} with $t_{½}$ = 100 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 31–36 min, 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2, respectively; $t_{½}$ = 35–123 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 190 d for high-dose treatment, $t_{½}$ = 100 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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TABLE 7.1.1.29.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficient log of 2,4,5-trichlorobiphenyl (PCB-29) at various temperatures

Solubility		Henry's law constant		log K_{OA}	
Shiu et al. 1997		Bamford et al. 2000		Harner & Mackay 1995	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	0.0413	4	12.12	–10	9.5
15	0.0682	11	18.04	0	8.97
25	0.106	18	28.37	10	8.51
35	0.203	25	37.89	20	8.03
45	0.330	31	51.03	25	7.96
		$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		ΔH_{OA}/(kJ mol^{-1}) = 72.6	
ΔH_{sol}/(kJ mol^{-1}) = 36.9		K_{AW}			
at 5–45°C		A	9.8629	$\log K_{OA} = A + B/T$	
		B	4197.74	A	–4.8
		enthalpy, entropy change:		B	3791.7
		ΔH/(kJ·mol^{-1}) = 34.9 ± 2.8			
		ΔS/(J·mol^{-1}·K^{-1}) = 82 ± 10			

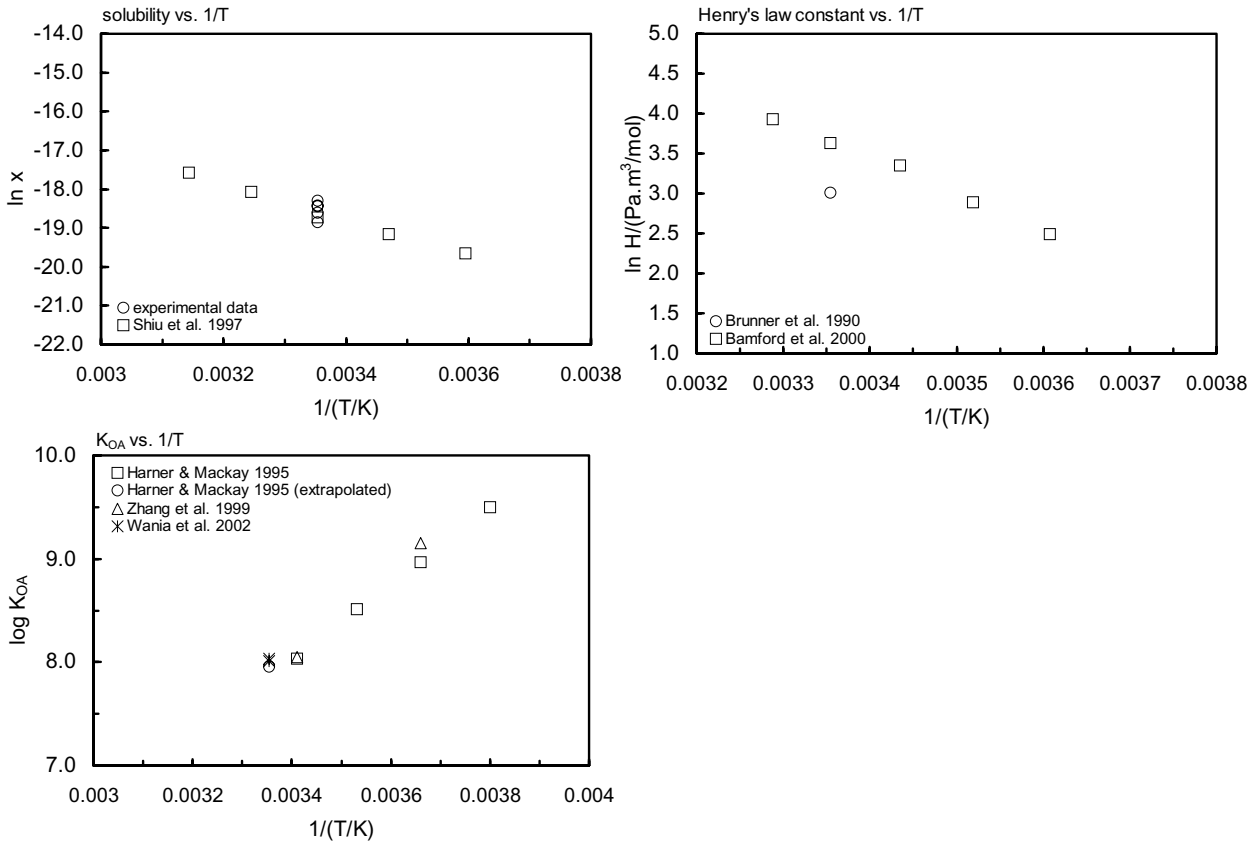

FIGURE 7.1.1.29.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,4,5-trichlorobiphenyl (PCB-29).

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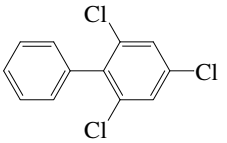
7.1.1.30 2,4,6-Trichlorobiphenyl (PCB-30)



Common Name: 2,4,6-Trichlorobiphenyl
Synonym: PCB-30
Chemical Name: 2,4,6-trichlorobiphenyl
CAS Registry No: 35693-92-6
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
62.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
16.5 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999))
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.37 (Miller et al. 1984)
49.36, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F :
0.427 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.226 (generator column/ECD, Miller et al. 1984,1985)
0.024, 0.0468, 0.0491, 0.0893 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.187* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988)
0.0803, 0.187, 0.435 (4, 25, 40°C, generator column-GC/ECD, Doucette & Andren 1988)
S/(mol/L) = 2.49×10^{-7} exp(0.047·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
log x = – 1742/(T/K) – 1.983, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)
0.252, 0.243 (generator column-GC, Dunnivant & Elzerman 1988)
0.236 (generator column-GC, Li et al. 1992)
0.235 (generator column-GC/ECD, Li et al. 1993)
0.217 (shake flask-GC/ECD, Li & Andren 1994)
ln x = – 4.5969 – 4004.7/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.031 (Augood 1953; quoted, Bidleman 1984)
0.0865, 0.0948(P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.030 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.0955, 0.144(supercooled liquid P_L calculated from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.0421 (GC-RI correlation, Burkhard et al. 1985a)
0.111, 0.135 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0946 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.110; 0.0851(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 3886/(T/K) + 12.02; (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0130–0.0637; 0.085–0.146 (literature P_S range; literature P_L range, Delle Site 1997)

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Henry's Law Constant (Pa m^3/mol at 25°C):

61.40 (calculated-P/C, Burkhard et al. 1985b)
49.51 (calculated-P/C, Shiu & Mackay 1986)
65.76 (batch stripping, Dunnivant et al. 1988 Dunnivant & Elzerman 1988)
47.51 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
58.04 (calculated-QSPR, Dunnivant et al. 1992)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.47 (generator column-GC/ECD, Miller et al. 1984, 1985)
5.57 (generator column-GC/ECD, Doucette & Andren 1987,1988)
5.77, 5.70, 5.51, 5.48 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.33, 5.57 (RP-HPLC-k′ correlation, different stationary phases, Sherblom & Eganhouse 1988)
5.711 ± 0.014 (shake flask/slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.75 (generator column-GC, Li et al. 1993)
5.62 (recommended, Sangster 1993)
5.71 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

7.28 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.24 (suspended particulates matter, Burkhard 1984)
4.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation: 30% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

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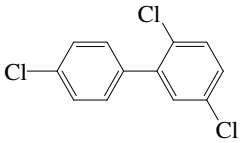
7.1.1.31 2,4′,5-Trichlorobiphenyl (PCB-31)



Common Name: 2,4′,5-Trichlorobiphenyl
Synonym: PCB-31, 2,4′,5-trichloro-1,1′-biphenyl
Chemical Name: 2,4′,5-trichlorobiphenyl
CAS Registry No: 16606-02-3
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
67 (Bellavita 1935; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.384 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.11 (Kilzer et al. 1979)
0.075 (shake flask-GC/ECD, Bruggeman et al. 1981)
0.265, 0.155, 0.179, 0.120 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.090 (generator column-GC/ECD, Opperhuizen et al. 1988)
0.143 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.220, 0.194 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -1123/(T/K) + 0.64$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0341, 0.0474 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
0.0132 (GC-RI correlation, Burkhard et al. 1985a)
0.0313 (supercooled liquid P_L, calculated-GC-RI correlation, Burkhard et al. 1985b)
0.0373, 0.0346 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0149 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/\text{mmHg}) = 10.40 - 4270/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.0263, 0.0347 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4058/(T/K) + 12.14$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.024, 0.0257 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log (P_L/\text{Pa}) = -4149/(T/K) + 12.29$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log (P_L/\text{Pa}) = -4010/(T/K) + 11.86$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
94.13 (gas-stripping-GC, Atlas et al. 1982)
20.26 (calculated, Murphy et al. 1983)
25.43 (calculated-P/C, Burkhard et al. 1985b)
26.75 (20°C, calculated-P/C, Murphy et al. 1987)

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28.47 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)
27.78 (calculated-QSPR, Dunnivant et al. 1992)
20.21 (calculated-QSPR, Achman et al. 1993)
12.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
30.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
37.15, 33.88 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -2887/(T/K) + 11.22$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.22 (Hansch & Leo 1979)
5.30 (HPLC-RT correlation, Woodburn 1982; Woodburn et al.1984)
5.77 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.79 (generator column-GC/ECD, Woodburn et al. 1984)
5.70 (selected, Shiu & Mackay 1986)
5.99, 6.22, 6.18, 6.33 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.79 (generator column-GC/ECD, Doucette & Andren 1987,1988)
5.59 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.68 (recommended, Sangster 1993)
5.79 (recommended, Hansch et al. 1995)
5.79, 5.78 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
$\log K_{OA} = -6.12 + 4190/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
9.43, 8.40; 8.23 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.93, 7.94 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4110/(T/K) - 5.84$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

3.45 (fish, Korte et al. 1978)
– 0.30, – 0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
6.15 (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
5.98 (goldfish, 10% lipid content in food, Bruggeman et al. 1981)
3.95, 3.95, 4.51 (algae, fish, activated sludge, Freitag et al. 1984,1985)
3.66 (salmon fry in humic water-steady state, Carlberg et al. 1986)
3.83 (salmon fry in lake water-steady state, Carlberg et al. 1986)
4.62 (fish, calculated-C_B/C_W or k_1/k_2 Connell & Hawker 1988; Hawker 1990)
4.66; 6.19 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4/09 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)
5.04 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
3.95, 4.65 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)
4.23, 5.23 (*Daphna*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.08, 6.04 (mussel: wet wt basis, dry wt basis, Geyer et al. 2000)
4.63, 5.93 (goldfish: wet wt basis, dry wt basis, Geyer et al. 2000)
4.67, 6.19 (zebrafish: wet wt basis, dry wt basis, Geyer et al. 2000

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_P$ or $\log K_d$

5.90, 4.80 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

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Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulates, Burkhard 1984)
5.5–6.3, 5.9; 6.80 (suspended sediment, average; algae > 50 µm, Oliver 1987a)
5.48 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.63 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.51 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
5.10 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH-}(aq.) = 7.2 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Biodegradation: 50–80% being degraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 890 d^{-1}; k_2 = 0.021 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986)
k_2 = 0.0035 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 37.1 h^{-1}; $1/k_2$ = 1142 h (goldfish, quoted, Hawker & Connell 1985)
log k_1 = 2.95 d^{-1}; log $1/k_2$ = 1.68 d (fish, quoted, Connell & Hawker 1988; Thomann 1989)
k_1 = 3950 d^{-1}; k_2 = 0.0867 d^{-1} (zebrafish, 30-d exposure, Fox et al. 1994)
k_1 = 5044 h^{-1}, k_2 = 0.411 h^{-1} (algae *Chlorella fusca*, Wang et al. 1996)
k_1 = 0.00447 h^{-1}; k_2 = 0.100 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1 = 14 L d^{-1} g^{-1} dry wt.; k_2 = 0.129 d^{-1} (Baltic Sea blue mussels, flow-through expt. Gustafsson et al. 1999)
k_2 = 0.008 d^{-1} with $t_{½}$ = 91 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.008 d^{-1} with $t_{½}$ = 88 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from, $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Groundwater:
Sediment:

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Soil:

Biota: $t_{½}$ = 196 d in rainbow trout, and $t_{½}$ = 81d in its muscle, (Niimi & Oliver 1983);

$t_{½}$ = 30 d in worms at 8°C (Oliver 1987c);

theoretical half-life to reach 90% steady-state tissue concn 5.4 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);

$t_{½}$ = 6.9 h in blood plasma (ring doves, Drouillard & Norstrom 2000).

depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 88 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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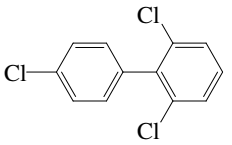
7.1.1.32 2,4′,6-Trichlorobiphenyl (PCB-32)



Common Name: 2,4′,6-Trichlorobiphenyl
Synonym: PCB-32, 2,4′,6-trichloro-1,1′-biphenyl
Chemical Name: 2,4′,6-trichlorobiphenyl
CAS Registry No: 38444-77-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
70 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.399 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.355, 0.182, 0.129, 0.0778 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0578 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.060 (GC-RI correlation, Burkhard et al. 1985b)
0.0543, 0.0562(supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P/mmHg) = 16.10 – 4100/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0427, 0.0589(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –3935/(T/K) + 11.93 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
37.29 (calculated-P/C, Burkhard 1984)
41.75 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
39.69 (calculated-QSPR, Dunnivant et al. 1990)
27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.60, 5.75 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.80 (selected, Shiu & Mackay 1986)
4.95, 5.29, 5.21, 5.52 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.47 (generator column-GC, Larsen et al. 1992)
5.49 (recommended, Sangster 1993)
5.75 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

7.72 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
log K_{OA} = –6.50 + 4240/(T/K); temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
8.89, 7.97; 7.92 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al 1999)
7.49 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.23 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 8.0 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.008 d^{-1} with $t_{½}$ = 85 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.006 d^{-1} with $t_{½}$ = 111 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 85 d for high-dose treatment, $t_{½}$ = 111 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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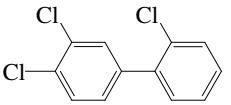
7.1.1.33 2,3′,4′-Trichlorobiphenyl (PCB-33)



Common Name: 2,3′,4′-Trichlorobiphenyl
Synonym: PCB-33, 2,3′,4′-trichlorobiphenyl, 2′,3,4-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,4′-trichlorobiphenyl
CAS Registry No: 38444-86-9
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
60–60.5 (Wallnöfer et al. 1973)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.1485
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.452 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.078 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.291 (calculated-TSA, Mackay et al. 1980)
0.0796 (quoted lit. average, Yalkowsky et al. 1983)
0.371 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b;)
0.246, 0.170, 0.103, 0.142 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0814 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.133 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.103 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.174 (calculated-MCI χ, Patil 1991)
0.152 (calculated-QSPR, Dunnivant et al. 1992)
0.209 (calculated-group contribution, Kühne et al. 1995)
0.0833, 0.219 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.576 (calculated–mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0107 (P_S from GC-RT correlation, Westcott & Bidleman 1981)
0.0133, 0.0160 (solid P_S, 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
log (P_S/mmHg) = 1.09 – 1510/(T/K), temp range 30–40°C (gas saturation-GC/ECD, Westcott et al. 1981)
0.030 (P_L calculated from P_S using fugacity ratio F, Westcott et al. 1981)
0.0115 (GC-RI correlation, Burkhard et al. 1985a)
0.0243 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0264, 0.0219 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0136, 0.030 (selected P_S, P_L, Shiu & Mackay 1986)
0.0119 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P_L/mmHg) = 10.40 – 4330/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0137; 0.0272 (quoted; calculated-UNIFAC, Banerjee et al. 1990)
0.0214, 0.0295(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)

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log (P_L/Pa) = – 4075/(T/K) + 12.09 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.00484–0.0270; 0.0119–0.030 (quoted lit. P_S range; lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

15.20 (calculated, Murphy et al. 1983)
16.92 (calculated-P/C, Burkhard et al. 1985b)
43.67 (calculated-P/C, Shiu & Mackay 1986)
22.70 (20°C, calculated-P/C, Murphy et al. 1987)
21.99 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
16.21 (wetted wall column-GC,/ECD, Brunner et al. 1990)
24.31 (calculated-QSPR, Dunnivant et al. 1992)
11.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
29.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 22$ kJ/mol, $\Delta S_H = 0.11 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.48, 5.66, 5.98, 5.71 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.872 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.71 (recommended, Sangster 1993)
5.87 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.52, 8.52 (0, 20°C, multi-column GC-k′ correlation; Zhang et al. 1999)
8.03 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.79 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)
3.79, 6.04 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.57, 5.87 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.26 (suspended particulate matter, Burkhard 1984)
4.64 (soil, calculated-S, Chou & Griffin 1986)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.20 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.7–1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 7.2×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(1.0–2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

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Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008\ d^{-1}$ with $t_{½} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008\ d^{-1}$ with $t_{½} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½} \sim 4$–11 d in freshwater systems, $t_{½} = 0.1$–10 d in cloud water, $t_{½} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 1.90\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.88\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.37\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00413\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00099\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00052\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{½} = 91$ d for high-dose treatment, $t_{½} = 88$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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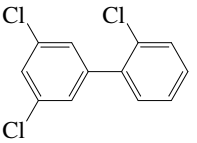
7.1.1.34 2,3′,5′-Trichlorobiphenyl (PCB-34)



Common Name: 2,3′,5′-Trichlorobiphenyl
Synonym: PCB-34, 2,3′,5′-trichlorobiphenyl, 2,3′,5′-trichloro-1,1′-biphenyl
Chemical Name: 2,3′,5′-trichlorobiphenyl
CAS Registry No: 37680-68-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
58.0 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.474 (mp at 58°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.319 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.129 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.205 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.036 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0177 (GC-RI correlation, Burkhard et al. 1985b)
0.0447 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4075/(T/K) + 12.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
29.08 (calculated-P/C, Burkhard 1984)
51.17 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
42.73 (calculated-QSPR, Dunnivant et al. 1992)
29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.51 (calculated-TSA, Burkhard 1984)
5.66 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.71 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988; recommended, Sangster 1993)
5.6522 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.72 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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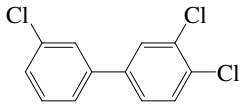
7.1.1.35 3,3′,4-Trichlorobiphenyl (PCB-35)



Common Name: 3,3′,4-Trichlorobiphenyl
Synonym: PCB-35
Chemical Name: 3,3′,4-trichlorobiphenyl
CAS Registry No: 37680-69-6
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
87.0 (Burkhard et al. 1985a)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.301 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0152 (quoted-3,4,4′-trichlorobiphenyl from Weil et al. 1974; Opperhuizen et al. 1988)
0.0814 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00246 (GC-RI correlation, Burkhard et al. 1985a)
0.00949 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.014, 0.0105 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0129 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4242/(T/K) + 12.37$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
8.13 (calculated-P/C, Burkhard et al. 1985b)
22.49 (calculated-MCI χ, Sabljic & Güsten 1989)
18.23 (calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.53 (calculated-TSA, Burkhard 1984)
5.82 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7151 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

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Sorption Partition Coefficient, log K_{OC}:

5.33 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

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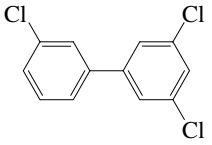
7.1.1.36 3,3′,5-Trichlorobiphenyl (PCB-36)



Common Name: 3,3′,5-Trichlorobiphenyl
Synonym: PCB-36, 3,3′,5-trichloro-1,1′-biphenyl
Chemical Name: 3,3′,5-trichlorobiphenyl
CAS Registry No: 38444-87-0
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
46 (estimated, Abramowitz & Yalkowsky)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.260 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.00469, 0.0155, 0.010 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0814 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0141 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0149 (GC-RI correlation, Burkhard et al. 1985b)
0.0191 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4242/(T/K) + 2.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
13.98 (calculated-P/C, Burkhard et al. 1985a)
51.47 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
17.40 (wetted-wall column-GC/ECD, Brunner et al. 1990)
34.10 (calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.57 (calculated-TSA, Burkhard 1984)
4.15 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
5.70 (selected, Shiu & Mackay 1986)
5.88 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.76, 5.86, 5.80 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.81 (recommended, Sangster 1993)
5.8293 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.37 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.7 – 1.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc)$ = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (1.0 – 2.1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc)$ = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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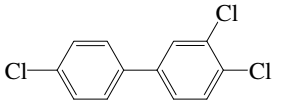
7.1.1.37 3,4,4′-Trichlorobiphenyl (PCB-37)



Common Name: 3,4,4′-Trichlorobiphenyl
Synonym: PCB-37
Chemical Name: 3,4,4′-trichlorobiphenyl
CAS Registry No: 38444-90-5
Molecular Formula: $C_{12}H_7Cl_3$
Molecular Weight: 257.543
Melting Point (°C):
86.8–87.8 (Weingarten 1961)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
198.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.244 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0152 (generator column-GC/ECD, Weil et al. 1974)
0.135 (calculated-TSA, Mackay et al. 1980)
0.296 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)
0.0853 (calculated-fragment solubility constants, Wakita et al. 1986)
0.072 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0110, 0.0142, 0.00853, 0.853 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0408 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.0287 (calculated-QSPR, Dunnivant et al. 1992)
0.0437, 0.115 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.170 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0566, 0.00897, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0084 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.0127, 0.0094 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00454 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00912, 0.0115 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4242/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0612 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
84.21 (batch stripping, Atlas et al. 1982)
7.34 (calculated-P/C, Burkhard et al. 1985b)
15.40 (20°C, calculated-P/C, Murphy et al. 1987)
14.59 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
15.41 (calculated-QSPR, Dunnivant et al. 1992)

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20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.90 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.00 (calculated-fragment const., Yalkowsky et al. 1983)
5.53 (calculated-TSA, Burkhard 1984)
4.94 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.58, 5.86, 5.84, 5.85 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.83 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.78 (recommended, Sangster 1993)
5.7373 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

8.97 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.58, 5.90 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.70, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.33 (suspended particulate matter, Burkhard 1984)
4.81 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.81 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
4.46 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

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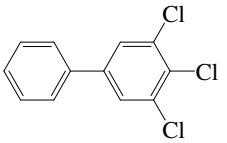
7.1.1.38 3,4,5-Trichlorobiphenyl (PCB-38)



Common Name: 3,4,5-Trichlorobiphenyl
Synonym: PCB-38, 3,4,5-trichloro-1,1′-biphenyl
Chemical Name: 3,4,5-trichlorobiphenyl
CAS Registry No: 53555-66-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
114 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.353 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0258 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0104 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0566, 0.0111, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
7.62 (calculated-P/C, Burkhard 1984)
20.97 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
2.027 (wetted-wall column-GC/ECD, Brunner et al. 1990)
23.54 (calculated-QSPR, Dunnivant et al. 1992)
19.30 (calculated-QSPR, Achman et al. 1993)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.48 (calculated-TSA, Burkhard 1984)
5.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7298 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.92 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.28 (suspended particulate matter, cal-K_{OW}, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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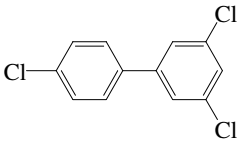
7.1.1.39 3,4′,5-Trichlorobiphenyl (PCB-39)



Common Name: 3,4′,5-Trichlorobiphenyl
Synonym: PCB-39, 3,4′,5-trichloro-1,1′-biphenyl
Chemical Name: 3,4′,5-trichlorobiphenyl
CAS Registry No: 38444-88-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 257.543
Melting Point (°C):
88 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.241 (mp at 88°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.353 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.0258 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0310 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0125 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0135, 0.00314, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.0203, 0.0174 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4242/(T/K) + 12.53$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
12.56 (calculated-P/C, Burkhard et al. 1985a)
43.57 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
30.32 (calculated-QSPR, Dunnivant et al. 1992)
20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.58 (calculated-TSA, Burkhard 1984)
5.89 (calculated-TSA, Hawker & Connell 1988a quoted, Hansch et al. 1995)
5.8173 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.79 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.38 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for trichlorobiphenyls, and the tropospheric lifetime τ(calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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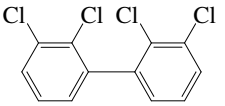
7.1.1.40 2,2′,3,3′-Tetrachlorobiphenyl (PCB-40)



Common Name: 2,2′,3,3′-Tetrachlorobiphenyl
Synonym: PCB-40
Chemical Name: 2,2′,3,3′-tetrachlorobiphenyl
CAS Registry No: 38444-93-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
119.5–121.5 (Wallnöfer et al. 1973; Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.113 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.034 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.070, 0.0583, 0.0232, 0.0385 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0156 (generator column-GC/ECD; Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0098 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.00134 (GC-RI correlation, Burkhard et al. 1985a)
0.0112 (supercooled liquid P_L, GC-RI correlation, Burkhard et al.)
0.00887, 0.00861 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00255; 0.0020 (selected solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
0.00452 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.70 – 4480/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00676, 0.012(supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4271/(T/K) + 12.32 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.000473–0.00957; 0.00450–0.0120 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
20.27 (calculated-P/C, Burkhard et al. 1985b;)
12.16 (20°C, batch stripping-GC, Oliver 1985)
21.94 (calculated-P/C, Shiu & Mackay 1986)
16.31 (20°C, calculated-P/C, Murphy et al. 1987)
20.47 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
45.14 (calculated-QSAR-χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
18.52 (calculated-QSPR, Dunnivant et al. 1992)
15.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)

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29.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
4.63 (HPLC-RT correlation, Sugiura et al. 1978)
5.56 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.80 (shake flask-GC, Chiou 1985)
5.48, 5.66, 5.84, 5.85 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.55 (generator column-GC/ECD, Hawker & Connell 1988a)
6.178 (slow stirring-GC; De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.67 (recommended, Sangster 1993)
6.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
8.05 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.08 (killifish, Goto et al. 1978)
3.36–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
4.69, 4.23; 5.38 (rainbow trout: laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
4.38, 4.23 (worms, fish, Oliver 1987c)
4.23 (fish, quoted, Isnard & Lambert 1988, 1989)

Bioaccumulation Factor, log BAF:
6.48 (rainbow trout, L/kg(Ip), quoted, Thomann 1989)

Biota Sediment Accumulation Factor, BSAF:
10 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:
5.57 (suspended particulate matter, Burkhard 1984)
5.50; 5.50 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
5.00 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
5.00 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 6.1×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

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Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0065\ d^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 320\ d^{-1}$; $k_2 = 0.0065\ d^{-1}$ (rainbow trout, Oliver & Niimi 1985)

log $1/k_2$ = 2.2, 2.9 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)

$k_2 = 0.006\ d^{-1}$ with $t_{½} = 107$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.006\ d^{-1}$ with $t_{½} = 112$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.20\ d^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.95\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.36\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; $k = 0.00155\ d^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00285\ d^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00258\ d^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00119\ d^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: half-life in rainbow trout, $t_{½}$ = 107 d and $t_{½}$ = 61 d its muscle (Niimi & Oliver 1983);

$t_{½}$ = 107d in rainbow trout (Oliver & Niimi 1985);

$t_{½}$ = 29 d in worms at 8°C (Oliver 1987c).

depuration $t_{½}$ = 107 d for high-dose treatment, $t_{½}$ = 112 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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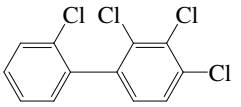
7.1.1.41 2,2′,3,4-Tetrachlorobiphenyl (PCB-41)



Common Name: 2,2′,3,4-Tetrachlorobiphenyl
Synonym: PCB-41, 2,2′,3,4-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4-tetrachlorobiphenyl
CAS Registry No: 52663-59-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
63 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.150 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.0648 (20°C, supercooled liquid S_L, Murphy et al. 1987)
0.0306, 0.0328, 0.0197, 0.0351 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0124 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0131 (GC-RI correlation, Burkhard et al. 1985b)
0.0110, 0.0098 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.59×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0776, 0.0120(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.22$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
23.91 (calculated-P/C, Burkhard et al. 1984)
20.37 (calculated-P/C, Murphy et al. 1987)
20.87 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990; quoted, Achman et al. 1993)
24.76 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.09, 6.11 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
5.73, 5.83, 5.82, 5.78 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.79 (recommended, Sangster 1993)
6.11 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.79, 8.82 (0, 20°C, RP-HPLC-RT, Zhang et al. 1999)
8.46 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.59 (suspended particulate matter, Burkhard 1984)
5.01 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.40 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 6.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.005$ d^{-1} with $t_{½}$ = 147 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 162 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 147 d for high-dose treatment, $t_{½}$ = 162 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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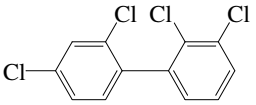
7.1.1.42 2,2′,3,4′-Tetrachlorobiphenyl (PCB-42)



Common Name: 2,2′,3,4′-Tetrachlorobiphenyl
Synonym: PCB-42, 2,2′,3,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′-tetrachlorobiphenyl
CAS Registry No: 36559-22-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
69.0 (Burkhard et al. 1985; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol 9K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.370 (mp at 69°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.150 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985a)
0.0608 (20°C, supercooled liquid S_L, Murphy et al. 1987)
0.032 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0334 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0131 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00507 (GC-RI correlation, Burkhard et al. 1985b)
0.0116, 0.0116 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.19×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.70 – 4480/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00912, 0.0135 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4229/(T/K) + 12.25 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
29.49 (calculated-P/C, Burkhard et al. 1985a)
32.02 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990)
25.92 (calculated-QSPR, Dunnivant et al. 1995)
10.13 (calculated-QSPR, Achman et al. 1993)
21.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
38.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 3$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated-TSA, Burkhard 1984)
5.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.72 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.72 (quoted values; recommended, Sangster 1993)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.19 (10°C, estimated, Thomas et al. 1998)
8.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.64 (suspended particulate matter, Burkhard 1984)
5.30 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
$k_{OH}(calc) = (0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.006$ d^{-1} with $t_{½}$ = 123 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½}$ = 140 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.20 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.89 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.23 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.35 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; k = 0.00066 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00309 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.0016 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00101 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)
Biota: depuration $t_{½}$ = 123 d for high-dose treatment, $t_{½}$ = 140 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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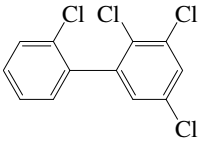
7.1.1.43 2,2′,3,5-Tetrachlorobiphenyl (PCB-43)



Common Name: 2,2′,3,5-Tetrachlorobiphenyl
Synonym: PCB-43
Chemical Name: 2,2′,3,5-tetrachlorobiphenyl
CAS Registry No: 70362-46-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.130 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0183 (P_L supercooled liquid, Burkhard et al. 1985a)
0.0194 (GC-RI correlation, Burkhard et al. 1985b)
0.0166, 0.0191 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0123, 0.0191 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.40$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
41.14 (calculated-P/C, Burkhard 1984)
35.26 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
33.94 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated-TSA, Burkhard 1984)
5.75 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8627 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.64 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 155 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 188 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 155 d for high-dose treatment, $t_{½}$ = 188 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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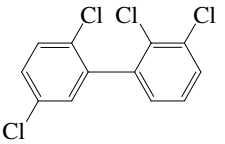
7.1.1.44 2,2′,3,5′-Tetrachlorobiphenyl (PCB-44)



Common Name: 2,2′,3,5′-Tetrachlorobiphenyl
Synonym: PCB-44
Chemical Name: 2,2′,3,5′-tetrachlorobiphenyl
CAS Registry No: 41464-39-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
46.5–47 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.608 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.170 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.080 (generator column-HPLC/UV, Billington 1982)
0.10 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.08 (generator column-HPLC/UV, Billington et al. 1988)
0.0463, 0.0394, 0.0254, 0.0343 (RP-HPLC-k′ correlation correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00943 (GC-RI correlation, Burkhard et al. 1985a)
0.0147 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0128, 0.013 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0152 (quoted, Eisenreich 1987)
0.0064 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00955, 0.0151 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4229/(T/K) + 12.29 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
79.28 (batch stripping, Atlas et al. 1982)
24.32 (calculated, Murphy et al. 1983)
32.83 (calculated-P/C, Burkhard et al. 1985b)
19.15 (20°C, calculated-P/C, Murphy et al. 1987)
25.43 (calculated-QSPR-MCI χ, Sabljic & Gusten 1989)
14.19 (wetted-wall column-GC, Brunner et al. 1990)
23.32 (calculated-QSPR, Dunnivant et al. 1992)
11.86, 16.02, 21.33, 28.05* ± 0.27, 35.13 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 5.8937 – 3103.2/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

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$K_{AW} = \exp[-(25.8/kJ{\cdot}mol^{-1})/RT] + (0.049/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where $R = 8.314\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)—see Comment by Goss et al. 2004

27.0 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

6.67 (calculated-fragment const., Yalkowsky et al. 1983)
5.84 (calculated-TSA, Burkhard 1984)
5.81 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.29 (calculated-S, Chou & Griffin 1986)
5.61, 5.78, 5.74, 5.79 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.75 (calculated-TSA, Hawker & Connell 1988b)
5.88 (calculated-MCI χ, Patil 1991)
5.73 (recommended, Sangster 1993)
5.81 (recommended, Hansch et al. 1995)
6.20, 4.79–6.67 (calculated-Characteristic Root Index [CRI]; minimum-maximum range, Saçan & Inel 1995)
5.6625 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.26 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

8.36 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
$\log K_{OA} = -6.20 + 4340/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
9.19 (10°C, estimated, Thomas et al. 1998)
9.67, 8.71; 8.41 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.58 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.04 (oyster, Vreeland 1974)
4.84; 6.37 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.04, 6.29 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.84, 5.37 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.60, 4.70 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

5.64 (suspended particulate matter, Burkhard 1984)
4.43 (soil, calculated-S, Chou & Griffin 1986)
5.60 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.67 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.05 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
5.40 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 25–60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

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k_{OH}(aq.) = 5.5×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation: 99% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 200 d^{-1}; k_2 = .0461 d^{-1} (Zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.014 d^{-1} with $t_{½}$ = 49 d and k_2 = 0.018 d^{-1} with $t_{½}$ = 38 d for food concn of 18 ng/g and 129 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_2 = 0.005 d^{-1} with $t_{½}$ = 146 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 175 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.23 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.98 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.32 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.38 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; k = 0.00090 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00253 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00161 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00122 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: depuration $t_{½}$ = 38–49 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½}$ = 146 d for high-dose treatment, $t_{½}$ = 175 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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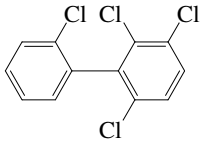
7.1.1.45 2,2′,3,6-Tetrachlorobiphenyl (PCB-45)



Common Name: 2,2′,3,6-Tetrachlorobiphenyl
Synonym: PCB-45, 2,2′,3,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,6-tetrachlorobiphenyl
CAS Registry No: 70362-45-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.115 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.146 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0398 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0416 (GC-RI correlation, Burkhard et al. 1985b)
0.0226, 0.0268 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0295 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4117/(T/K) + 12.16$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
101.1 (calculated-P/C, Burkhard 1984)
31.92 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
35.95 (calculated-QSPR, Dunnivant et al. 1992)
12.47 (calculated-QSPR, Achman et al. 1993)
25.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
43.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.88 (calculated-TSA, Burkhard 1984)
5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
4.84 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988
4.84 (recommended, Sangster 1993)
5.4616 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.68 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 6.7×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 7 food lipid (mg)/(g worm lipid-d); k_2 = 0.12 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 175 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 128 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 6 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{½}$ = 175 d for high-dose treatment, $t_{½}$ = 128 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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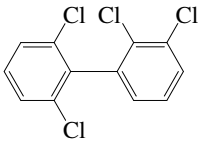
7.1.1.46 2,2′,3,6′-Tetrachlorobiphenyl (PCB-46)



Common Name: 2,2′,3,6′-Tetrachlorobiphenyl
Synonym: PCB-46, 2,2′,3,6′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,6′-tetrachlorobiphenyl
CAS Registry No: 41464-47-5
Molecular Formula: $C_{12}H_6H_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.114 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.106 (20°C, supercooled liquid, Murphy et al. 1987)
0.149 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0280 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0272 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0285 (GC-RI correlation, Burkhard et al. 1985b)
0.0186, 0.0206 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.04×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.0155 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.37$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
69.81 (calculated-P/C, Burkhard 1984)
26.04 (20°C, calculated-P/C, Murphy et al. 1987)
36.68 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
34.33 (calculated-QSPR, Dunnivant et al. 1992)
18.87 (calculated-QSAR, Achman et al. 1993)
18.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
34.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.89 (calculated-TSA, Burkhard 1984)
5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
4.84 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.86 (calculated, Miertus & Jakus 1990)

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4.84 (recommended, Sangster 1993)
5.2787 (calculated-molecular properties MNDO-AM1 method, Makino 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
9.49, 8.56 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1998)
7.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.69 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.006$ d^{-1} with $t_{½}$ = 112 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.006$ d^{-1} with $t_{½}$ = 907 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 112 d for high-dose treatment, $t_{½}$ = 107 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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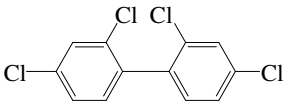
7.1.1.47 2,2′,4,4′-Tetrachlorobiphenyl (PCB-47)



Common Name: 2,2′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-47
Chemical Name: 2,2′,4,4′-tetrachlorobiphenyl
CAS Registry No: 2437-79-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
83 (Fichter & Adler 1926; Kühne et al. 1995; Ruelle & Kesselring 1997)
41–42 (Hall & Minhaj 1957; Wallnöfer et al. 1973)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.268 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.068 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.990 (supercooled liquid S_L, Johnstone et al. 1974)
0.0160, 0.0157, 0.0172, 0.0202 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0541 (22°C, generator column-GC, Opperhuizen et al. 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0115 (Neely 1983)
0.0111 (GC-RI correlation, Burkhard et al. 1985a)
0.0151 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0152, 0.0156 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0115, 0.0162 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.37$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
42.86 (calculated-P/C, Burkhard et al. 1985b)
17.38 (calculated-P/C, Shiu & Mackay 1986)
44.48 (calculated-QSAR- χ, Sabljic & Güsten 1989)
19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)
37.30 (calculated-QSPR, Dunnivant et al. 1992)
3.05, 8.91 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
12.67 (estimated-bond method, EPIWIN v3.04, Hardy 2002)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.68 (shake flask, Tulp & Hutzinger 1978)
5.20 (HPLC-k′ correlation, McDuffie 1981)

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6.29 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.17 (HPLC-k′ correlation, De Kock & Lord 1987)
5.93, 6.04, 5.86, 5.94 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.94 (recommended, Sangster 1993)
6.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.55, 8.56 (0, 20°C, multi-column GC-k′ correlation; Zhang et al. 1999)
8.01 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.98 (rainbow trout muscle, steady state, Branson et al. 1975; quoted, Waid 1986)
4.09 (rainbow trout, Neely et al. 1974)
3.95 (rainbow trout, Branson et al. 1975)
4.85; 4.782, 4.717 (quoted-whole fish; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
2.97, 2.71 (phytoplankton *Nanochloropsis oculata*, PCB concn at 50 ppb, after 4-d culture, Wang et al. 1998)
2.19, 2.11 (phytoplankton *Isochrysts galbana*, PCB concn at 500 ppb, after 4-d culture, Wang et al. 1998)
4.00, 5.52 (rainbow trout 8–10 g, muscle 3% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.46, 5.56 (rainbow trout 10–15 g, whole fish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.76 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.30, 4.70 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

4.61 (soil, calculated-solubility, Kenaga 1980)
5.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.68 (soil, calculated-S, Chou & Griffin 1986)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.04 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.70 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.65 (estimated-EPIWIN v3.04, Hardy 2002)

Sorption Partition Coefficient, log K_P:

5.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.18–5.64 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 0.2921 d from river, $t_{½}$ = 9.256 d from lake (estimated-EPIWIN v3.04, Hardy 2002).

Photolysis: photolysis rate $k_P = 0.553\ d^{-1}$ with $t_{½}$ = 13 d in summer sunlight; k_P(exptl) = $6 \times 10^{-8}\ d^{-1}$ with $t_{½}$ = 133 d, and k_P(calc) = $2.2 \times 10^{-8}\ d^{-1}$ in winter sunlight, at 40°L in surface waters (Dulin et al. 1986)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(aq.) = 6.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–0 d at room temp. (Kwok et al. 1995)

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Hydrolysis:
Biodegradation: no degradation observed after 98 d incubation by river dieaway test (Bailey et al. 1983).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 286\ d^{-1}$; $k_2 = 0.030\ d^{-1}$ (10–12°C, rainbow trout muscle, Branson et al. 1975; quoted, Waid 1986)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 177$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: $t_{½} = 49.2$ d in Lake Michigan (Neely 1983);
photolysis $t_{½} = 13$ d in summer sunlight and $t_{½} = 170$ d in winter sunlight at 40°L in surface waters (Dulin et al. 1986);
half-lives range from $t_{½} \sim 4$–11 d in freshwater systems, $t_{½} = 0.1$–10 d in cloud water, $t_{½} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
half-life of volatilization: $t_{½} = 0.2021$ d from river, and $t_{½} = 9.156$ d from lake, (estimated-EPIWIN v3.04, Hardy 2002).
Groundwater:
Sediment:
Soil:
Biota: $t_{½} = 28$ d in rainbow trout muscle (Branson et al. 1975; selected, Waid 1986).
depuration $t_{½} = 160$ d for high-dose treatment, $t_{½} = 177$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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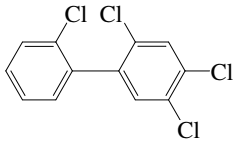
7.1.1.48 2,2′,4,5-Tetrachlorobiphenyl (PCB-48)



Common Name: 2,2′,4,5-Tetrachlorobiphenyl
Synonym: PCB-48, 2,2′,4,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5-tetrachlorobiphenyl
CAS Registry No: 70362-47-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
65.9 (Miller et al. 1984; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.4 (Miller et al. 1984; Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
69.04 (Miller et al. 1984)
Fugacity Ratio at 25°C, F:
0.393 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.121 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.030 (supercooled liquid S_L, Murphy et al. 1987)
0.0328, 0.0376, 0.0467, 0.0452 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0222, 0.0596 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0167 (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)
0.0177 (ΔG_v and GC-k′ correlation, Burkhard et al. 1985b)
0.0157, 0.016 (supercooled P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0265 (20°C, supercooled liquid, Murphy et al. 1987)
0.0115, 0.0170 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4229/(T/K) + 12.37 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.010 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI; Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
42.71 (calculated-P/C, Burkhard et al. 1985b)
26.64 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
30.67 (calculated-QSPR, Dunnivant et al. 1992)
19.30 (calculated-QSPR, Achman et al. 1993)
3.05, 8.91 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
22.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
39.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

5.86 (calculated-TSA, Burkhard 1984)
5.78 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.71, 5.79, 5.56 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.95 (calculated-solvatochromic parameters and intrinsic molar volume V_I, Kamlet et al. 1988)
5.69 (recommended, Sangster 1993)
5.9108 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

9.49, 8.50 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

4.41, 5.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.66 (suspended particulate matter, Burkhard 1984)
5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}-(aq.) = 6.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.004 d^{-1} with $t_{½}$ = 160 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 177 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 160 d for high-dose treatment, $t_{½}$ = 177 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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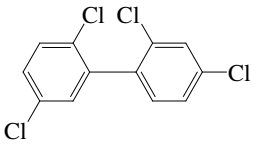
7.1.1.49 2,2′,4,5′-Tetrachlorobiphenyl (PCB-49)



Common Name: 2,2′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-49, 2,2′,4′,5-tetrachlorobiphenyl, 2,2′,4,5′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5′-tetrachlorobiphenyl
CAS Registry No: 41464-40-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
66.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.4 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
69.04 (Miller et al. 1984)
69.01, 64.3 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.392 (mp at 66.5°C)
0.411 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0164 (generator column-GC/ECD, Miller et al. 1984,1985)
0.0202, 0.0193, 0.0232, 0.0266 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00708 (GC-RI correlation, Burkhard et al. 1985a)
0.0170 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0167, 0.0162 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00742 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.60 – 4440/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0123, 0.0182 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4229/(T/K) + 12.41 (supercooled liquid P_L GC-RT correlation, Falconer & Bidleman 1994)
0.00955 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa m^3/mol at 25°C as indicated):
20.27 (calculated, Murphy et al. 1983)
47.72 (calculated-P/C, Burkhard et al. 1985b)
27.96 (20°C, calculated-P/C, Murphy et al. 1987)
37.90 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)
35.79 (calculated-QSPR, Dunnivant et al. 1992)
22.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
39.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.23 (calculated-π constant, Bruggeman et al. 1982)
5.73 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.22 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.86, 5.98, 5.77, 5.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.361 ± 0.046; 6.23 (slow stirring-GC, calculated-π const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.87 (recommended, Sangster 1993)
6.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

8.57 (20°C, generator column-GC, measured range –10 to 20°C, Harner & Bidleman 1996)
9.64, 9.08, 8.57, 8.21 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Bidleman 1996)
log K_{OA} = –4.96 + 3981/(T/K); temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
9.08 (10°C, estimated, Thomas et al. 1998)
9.50, 8.63; 8.48 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.34 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.84; 6.37 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.84, 6.38 (zebrafish, kinetic approach: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.71 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 6.2×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 3200 d^{-1}; k_2 = 0.0458 d^{-1} (zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{½}$ = 158 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 196 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

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Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.25 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.99 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.31 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.39 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00094 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00243 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00168 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00147 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{½}$ = 158 d for high-dose treatment, $t_{½}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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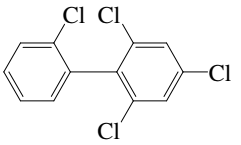
7.1.1.50 2,2′,4,6-Tetrachlorobiphenyl (PCB-50)



Common Name: 2,2′,4,6-Tetrachlorobiphenyl
Synonym: PCB-50, 2,2′,4,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,6-tetrachlorobiphenyl
CAS Registry No: 62796-65-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
45.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.092 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0320, 0.032, 0.030, 0.0412 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.1842 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.044 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C):
0.0451 (GC-RI correlation, Burkhard et al. 1985a)
0.0433 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
76.80 (gas stripping-GC, Atlas et al. 1982)
137.8 (calculated-P/C, Burkhard et al. 1985b)
58.57 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
61.76 (calculated-QSPR, Dunnivant et al. 1992)
28.68, 38.18, 49.84, 64.30 ± 1.4, 70.30 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 5.8937 - 2862.64/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(23.8/kJ{\cdot}mol^{-1})/RT] + (0.049/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where R = 8.314 $J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
60.5 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 4$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.96 (calculated-TSA, Burkhard 1984)
5.72, 5.84, 5.70, 5.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.63 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.87 (calculated-MCI χ, Patil 1991)
5.75 (recommended, Sangster 1993)
5.6545 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

7.89 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.26, 3.50, 3.81 (algae, fish, activated sludge, Freitag et al. 1984,1985)

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

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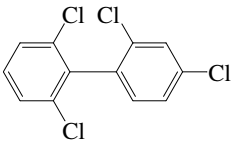
7.1.1.51 2,2′,4,6′-Tetrachlorobiphenyl (PCB-51)



Common Name: 2,2′,4,6′-Tetrachlorobiphenyl
Synonym: PCB-51
Chemical Name: 2,2′,4,6′-tetrachlorobiphenyl
CAS Registry No: 68194-04-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
66 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.396 (mp at 66°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0911 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.065 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.1842 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.044 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.033 (GC-RI correlation, Burkhard et al. 1985a)
0.0315 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 10.40 – 4330/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0263 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4117/(T/K) + 12.20 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
76.80 (gas stripping-GC, Atlas et al. 1982)
101.2 (calculated-P/C, Burkhard et al. 1985b)
49.04 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
51.73 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.96 (calculated-TSA, Burkhard 1984)
5.86, 5.98, 5.77, 5.86 (RP-HPLC-k′ correlation, different stationary phases, Brodsky & Ballschmiter 1988)
5.63 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.88 (calculated-MCI χ, Patil 1991)
5.51 (recommended, Sangster 1993)
5.4591 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.62 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 10 food lipid (mg)/(g worm lipid-d); $k_{2:}$ = 0.11 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.006 d^{-1} with $t_{½}$ = 126 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 150 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 6 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{½}$ = 126 d for high-dose treatment, $t_{½}$ = 150 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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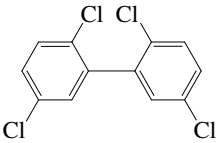
7.1.1.52 2,2′,5,5′-Tetrachlorobiphenyl (PCB-52)



Common Name: 2,2′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-52
Chemical Name: 2,2′,5,5′-tetrachlorobiphenyl
CAS Registry No: 35693-99-3
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
87–89 (Webb & McCall 1972; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point,)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
46.02 (Hinckley et al. 1990)
46.1 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.243 (calculated, assuming ΔS_{fus} = 56 J/mol K, Mackay et al. 1980)
0.316 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.046 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0265 (shake flask-GC/ECD, Haque & Schmedding 1975)
0.016 (shake flask-LSC, Metcalf et al. 1975)
0.0060 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
0.0223 (shake flask-GC/ECD from Aroclor 1242 mixture, Lee et al. 1979)
0.055 (generator column-GC/ECD, Bruggeman et al. 1981)
0.0365 (generator column-HPLC/UV, Huang 1983)
0.027 (generator column-GC/ECD, Miller et al. 1984; 1985)
0.0237, 0.0279, 0.0335, 0.0335 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.170 (generator column-HPLC/UV, Billington et al. 1988)
0.110; 0.461 (generator column-GC; supercooled liquid S_L, calculated-mp, Dunnivant & Elzerman 1988)
0.0153 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
0.0161 (shake flask-LSC, Eadie et al. 1990)
log (S_L/(mol/L)) = – 0.790 – 3352/(T/K) (supercooled liquid, Passivirta et al. 1999)
0.0923 (calculated-mp and K_{OW}, Ran et al. 2002)
0.199, 0.140 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log S_L/(mol m^{-3}) = –1103/(T/K) + 0.37 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00733 (solid P_S from GC-RT correlation, Westcott & Bidleman 1981)
0.00253, 0.0048(solid P_S, 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
log (P_S/mmHg) = 11.8 – 4920/(T/K), temp range 30–40°C (gas saturation-GC, Westcott et al. 1981)
0.104; 0.428(solid P_S; supercooled liq. P_L calculated from P_S using fugacity ratio F, Neely 1981)
0.0188, 0.0165(P_{GC} by GC-RT correlation, different GC stationary phases, Bidleman 1984)

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0.0104 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.0159, 0.0229(supercooled liquid P_L calculated from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.00492 (GC-RI correlation, Burkhard et al. 1985a)
0.00497; 0.0193(selected exptl. P_S; supercooled liquid P_L, GC-RI correlation, Burkhard et al.1985)
0.0184, 0.0173(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0049; 0.0020(selected solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
0.00904 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0127; 0.0546(calculated-S × HLC; solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
log (P/mmHg) = 10.60 – 4430/(T/K) (GC-RT correlation, supercooled liquid, Tateya et al. 1988)
0.0104, 0.008(supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.0188, 0.012 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (P_L/Pa) = 11.74 – 4127/(T/K) (GC-RT correlation, Hinckley et al. 1990)
0.0132, 0.020 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4220/(T/K) + 12.36 (supercooled liq. P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.00690; 0.00218 (solid P_S; supercooled liq. P_L, Passivirta et al. 1999)
log (P_S/Pa) = 14.77 – 5087/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 12.36 – 4220/(T/K) (liquid, Passivirta et al. 1999)
0.0033–0.013; 0.00901–0.0512 (literature P_S range; literature P_L range, Delle Site 1997)
0.00904 (supercooled liquid P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.0107, 0.0120 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log (P_L/Pa) = –4190/(T/K) + 12.08 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log (P_L/Pa) = –4059/(T/K) + 11.69 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

31.41–53.7 (calculated-P/C, Westcott et al. 1981)
14.1–53.7 (calculated-P/C, Westcott & Bidleman 1981)
94.15 (gas stripping-GC/ECD, Atlas et al. 1982)
22.29 (calculated-P/C, Murphy et al. 1983)
26.34 (calculated-P/C, Murphy 1984)
31.41–53.70 (calculated-P/C, Bidleman 1984)
53.20 (calculated-P/C, Burkhard et al. 1985b)
2.53 (batch stripping-GC, Hassett & Milicic 1985)
12.16 (20°C, gas stripping-GC, Oliver 1985)
47.59 (calculated-P/C, Shiu & Mackay 1986)
24.11 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
34.65 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
44.04 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
32.34 (calculated-QSPR, Dunnivant et al. 1992)
16.4* (20°C, gas stripping-HPLC/fluorescence, measured range 10–48°C, ten Hulscher et al. 1992)
17.0 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
28.78 ± 3.4 (gas stripping-GC/ECD, Girvin et al. 1997)
log [H/(Pa m^3/mol)] = 13.15 – 3552/(T/K) (Passivirta et al. 1999)
31.07* ± 0.42 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
K_{AW} = exp[–(30.5/kJ·mol^{-1})/ RT] + (0.066/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
28.27 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 2001)
log K_{AW} = 6.427 – 2530/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
31.3 (exptl. data, Bamford et al. 2002)
ln K_{AW} = $-\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 31 ± 3 kJ/mol, ΔS_H = 0.07 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
28.18, 25.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

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log [H/(Pa m^3/mol)] = –2189/(T/K) + 8.79 (LDV linear regression of literature data, Li et al. 2003)
log [H/(Pa m^3/mol)] = –2956/(T/K) + 11.32 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

3.91 (shake flask-radiolabeled-^{14}C-LSC, Metcalf et al. 1975)
5.81 (Hansch & Leo 1979)
6.26 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.09 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.81, 5.87, 5.43, 5,80 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.02 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
5.81 (generator column-GC, Larsen et al. 1992)
6.00 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
5.79 (recommended, Sangster 1993)
6.09 (recommended, Hansch et al. 1995)
6.10 (calculated, Passivirta et al. 1999)
6.00, 5.91 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

7.90 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
8.22; 7.73 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = –6.20 + 4340/(T/K); temp range: 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
9.10 (10°C, estimated, Thomas et al. 1998)
9.46, 8.49; 8.56 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.33 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.47; 8.44 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.22, 8.22 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4251/(T/K) – 6.04 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

3.87 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)
4.26, 4.60, 4.02, 4.07 (algae, snail, mosquito, fish, Metcalf et al. 1975)
2.66 (green sunfish, 15 d in static water, Sanborn et al. 1975)
6.21; 6.07 (goldfish, 3% lipid; 10% lipid dry wet in food, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
6.38 (guppy, 3.5% lipid, Bruggeman et al. 1982,1984; quoted, Gobas et al. 1987)
4.69, 4.98 (goldfish, exptl., correlated, Mackay & Hughes 1984)
3.49–4.26 highest value 4.26, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
5.30, 4.26; 6.28(rainbow trout, laboratory data: kinetic BCF (k_1/k_2), steady state BCF (C_F/C_W); Lake Ontario field BCF, Oliver & Niimi 1985)
4.26, 4.69 (guppy, goldfish, calculated-C_B/C_W, or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
4.26 (fish, quoted, Isnard & Lambert 1988,1989)
6.38; 5.76 (guppy, lipid wt. based, corrected lipid wt. based, Gobas et al. 1989)
4.25 (guppy, estimated, Banerjee & Baughman 1991)
6.21; 6.32 (lipid basis: goldfish; rainbow trout, Noegrahati & Hammers 1992)
4.54, 6.02; 4.782, 4.708 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
3.08–4.58 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.86–6.31 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.23 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
5.03, 4.67; 3.57, 4.76, 4.17, 5.39 (oligochaetes; chironomid larvae, Bott & Standley 2000)
3.36, 5.60 (*Daphnia*, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.87, 6.12 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)

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4.28, 6.23 (mussel *Mutilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.42, 6.34 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.63, 5.93 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.69, 5.99 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.92, 6.46 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.01; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Bioaccumulation Factor, log BAF at 25°C or as indicated:

7.38 (rainbow trout, lipid based-L/kg(Ip), quoted, Thomann 1989)
4.92; 6.43 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.60, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.73–5.15 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.67 (Woodburn soil silt loam, sorption isotherm measurement, Haque & Schmedding 1976)
5.91 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.60; 5.50; 5.70 (field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
4.54, 4.42 (Aldrich humic acid with 9.4 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
3.87, 4.36 (Huron River water with 7.8 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
4.87 (dissolved humic acid, gas purging-LSC, Hassett & Milicic 1985)
5.35 (suspended solids-Lake Superior; field measurement-GC/ECD, Baker et al. 1986)
5.70, 4.87 (Lake Superior suspended solids: calculated-KOW, Baker et al. 1986)
6.15 (Composite Condie silt soil 0.36% OC, batch sorption equilibrium, Anderson & Pankow 1986)
5.0–6.4, 5.9 (suspended sediment, range, average, Oliver 1987a)
6.12 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.65 (calculated, Bahnick & Doucette 1988)
3.48 (12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans 1988)
4.35 (calculated-polymaleic acid, Chin & Weber 1989)
5.88 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.88 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.83 (organic carbon from total suspended matter of raw water from Lake Michigan, Eadie et al. 1990)
5.00, 3.88 (Aldrich humic acid, natural DOC, reversed-phase separation, Eadie et al. 1990)
5.00; 4.38–4.81; 2.89–3.93 (Aldrich humic acid; humic acid from soil & water samples; fulvic acid & dissolved organic matter samples, Jota & Hassett 1991)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.41 (soil, batch sorption equilibration-GC, Paya-Perez et al. 1991)
6.04, 4.80 (Hamlet City lake sediment, WES reference soil, batch sorption equilibrium, Brannon et al. 1995)
4.73 (Ispra oil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.02, 6.04; 4.80 (sediments from Brown's Lake, Hamlet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)
4.97; 5.09 (soil, quoted lit.; calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.30–5.41 (soil-Catlin silt loam, f_{OC} = 0.0226, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.61–5.65 (Cloudland loam, f_{OC} = 0.0024, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997
5.30–5.31 (Kenoma silt loam, f_{OC} = 0.0153, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.38 (Kenoma silt loam, f_{OC} = 0.0092, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.43–5.53 (Kenoma silt loam, f_{OC} = 0.002, depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.26–5.44 (Norborne silt loam, f_{OC} = 0.0137, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)

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5.24–5.36 (Norborne silt loam, f_{OC} = 0.009, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.39–5.40 (Norborne silt loam, f_{OC} = 0.0057, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
5.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
5.50; 4.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
4.98 (sediment, Bott & Standley 2000)
5.02, 4.55 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
5.58 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)
3.79–6.07; 4.40–6.40(range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.32; 5.52, 5.38, 5.60(20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:

4.67 (Haque & Schmedding 1976; Chou & Griffin 1986)
4.67, 4.62 (quoted, calculated-MCI χ, Sabljic 1984)
3.88 (Great Lake DOC, reversed-phase separation, Eadie et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$(exptl) = 2.8 h of evaporation from an initial concentration of 0.005 ppm in a glass dish of 4.5 cm depth of water solution at 24°C and $t_{½}$ = 0.68 h with stirring of the solution (Chiou et al. 1979); depletion k = 34 d^{-1} from a 26-cm or 67-cm height purge vessels. from aqueous solution (Girvin et al. 1997).

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation: microbial degradation with pseudo first-order rate constant k = 0.1 yr^{-1} in the water column and k = 1.0 yr^{-1} in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.008 d^{-1} (11°C, rainbow trout, Guiney et al. 1977; quoted, Waid 1986)
k_2 = 0.003 d^{-1} (10–11°C, rainbow trout eggs and sac fry, Guiney et al. 1980; quoted, Waid 1986)
k_1 = 740 d^{-1}; k_2 = 0.015 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)
k_1 = 280 d^{-1}; k_2 = 0.0014 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 1200 d^{-1}; k_2 = 0.015 d^{-1} (guppy, Bruggeman et al. 1984)
k_2 = 0.015, 0.0134 d^{-1} (goldfish, exptl., correlated, Mackay & Hughes 1984)
k_1 = 2800 d^{-1}; k_2 = 0.0014 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 30.8 h^{-1}; $1/k_2$ = 1600 h (goldfish, quoted, Hawker & Connell 1985)
k_1 = 50.0 h^{-1}; $1/k_2$ = 1600 h (guppy, quoted, Hawker & Connell 1985)
k_1 = 1100 d^{-1} (guppy, Opperhuizen 1986)
log k_1 = 2.87 d^{-1}; log $1/k_2$ = 1.82 d (fish, quoted, Connell & Hawker 1988)
log $1/k_2$ = 2.9, 3.0 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b).
$1/k_2$ = 30.3 d (guppy, quoted, Clark et al. 1990)
$1/k_2$ = 61.7, 102 d (guppy, Gobas et al. 1989; quoted, Clark et al. 1990)
k_1 = 3230 d^{-1}; k_2 = 0.0387 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.011 d^{-1} with $t_{½}$ = 65 d and k_2 = 0.018 d^{-1} with $t_{½}$ = 39 d for food concn of 22 ng/g and 125 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_1 = 20 L d^{-1} g^{-1} dry wt.; k_2 = 0.118 d^{-1} (Baltic Sea blue mussels, flow-through experiment., Gustafsson et al. 1999)

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k_1 = 0.00061 h^{-1}; k_2 = 0.0115 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1(calc) = 9 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.09 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{½}$ = 158 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 196 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
k_2 = 0.015 d^{-1} with $t_{½}$ = 46.2 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1996);
$t_{½}$ = 1500 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{½}$ = 19.7 d in Lake Michigan (Neely 1983);
$t_{½}$ = 30000 h at 7°C for Baltic Proper environment (estimated, Sinkkonem & Passivirta 2000).

Groundwater:

Sediment: $t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.27 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.99 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.30 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.39 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00112 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00251 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00174 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00127 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).
$t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{½}$ = 1.76 yr in female rainbow trouts, $t_{½}$ = 1.43 yr in males (Guiney et al. 1980);
$t_{½}$ = 500 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985); and $t_{½}$ = 99 d in its muscle, (Niimi & Oliver 1983);
$t_{½}$ = 46 d in guppy (Bruggeman et al. 1984);
$t_{½}$ = 43 d in worms at 8°C, 43 d (Oliver 1987c)
depuration $t_{½}$ = 39–65 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
theoretical half-life to reach 90% steady-state tissue concn 5.9 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);
$t_{½}$ = 6.0 h in blood plasma (ring doves, Drouillard & Norstrom 2000)
elimination $t_{½}$ = 8 d in earthworm given contaminated food (predicted, Wågman et al. 2001).
depuration $t_{½}$ = 158 d for high-dose treatment, $t_{½}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
depuration $t_{½}$ = 46.2 d for juvenile carp in 100-d experiment (Stapleton et al. 2004)

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TABLE 7.1.1.52.1
Reported vapor pressures and Henry's law constants of 2,2′,5,5′-tetrachlorobiphenyl (PCB-52) at various temperatures and temperature dependence equations

Vapor pressure		Henry's law constant			
Westcott et al. 1981		ten Hulscher et al. 1992		Bamford et al. 2000	
gas saturation-GC/ECD		gas stripping-GC		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
25	0.00253	10.4	8.6	4	11.34
30	0.0048	20.0	16.4	11	16.13
		30.1	37.4	18	22.56
		34.9	38.8	25	31.07
$\log P = A - B/(T/K)$		42.1	68.7	31	40.43
	P/mmHg	47.9	109.2		
A	11.8	48.4	120.6		
B	4920			$\ln K_{AW} = -\Delta H/RT + \Delta S/R$	
temp range 30–40°C		$\ln K_{AW} = A - B/(T/K)$		A	7.9384
		A	23.387	B	3668.5
		B	6254.5		
				enthalpy, entropy change:	
		enthalpy of volatilization:		$\Delta H/(kJ \cdot mol^{-1}) = 30.5 \pm 2.8$	
		$\Delta H_{vol}/(kJ \cdot mol^{-1}) = 52.0 \pm 5$		$\Delta S/(J \cdot K^{-1}\ mol^{-1}) = 66 \pm 10$	
		entropy of volatilization, ΔS:			
		$T\Delta S_{vol}/(kJ \cdot mol^{-1}) = 57.0 \pm 6$			
		at 20°C			

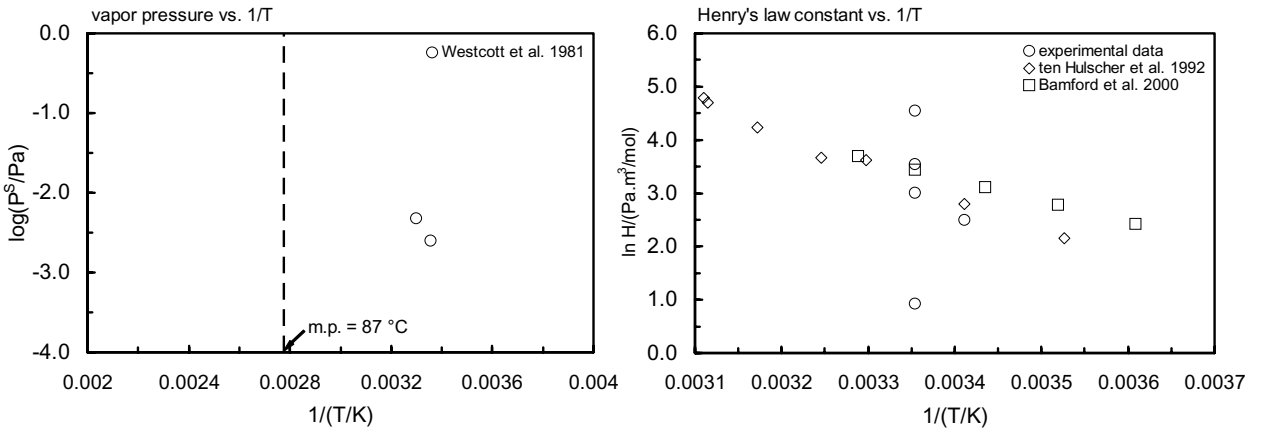

FIGURE 7.1.1.52.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for 2,2′,5,5′-tetrachlorobiphenyl (PCB-52).

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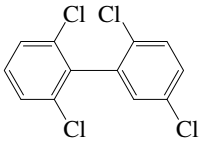
7.1.1.53 2,2′,5,6′-Tetrachlorobiphenyl (PCB-53)



Common Name: 2,2′,5,6′-Tetrachlorobiphenyl
Synonym: PCB-53, 2,2′,5,6′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,5,6′-tetrachlorobiphenyl
CAS Registry No: 41464-41-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
103–104.5 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.168 (mp at 104°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0923 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.109 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0945, 0.0786, 0.0717, 0.0335 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0476 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.288 (supercooled liquid S_L, calculated-mp, Dunnivant & Elzerman 1988)
0.292 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.044 (calculated-MCI χ, Patil 1991)
0.0520 (calculated-QSPR, Dunnivant et al. 1992)
0.0306 (calculated-group contribution, Kühne et al. 1995)
0.0114, 0.0306 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.114 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00493 (Neely 1983; quoted, Erickson 1986)
0.0273 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.0356 (supercooled liquid P_L, GC-RT correlation, Burkhard 1984)
0.0372 (GC-RI correlation, Burkhard et al. 1985a)
0.0356 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0268, 0.0331 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.011 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00671; 0.0405 (calculated-S × HLC, solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
log (P/mmHg) = 10.40 – 4310/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0214, 0.0347 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/)a) = – 4114/(T/K) + 12.24 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.0162 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994. Harner & Bidleman 1996)
0.00161–0.0204; 0.0107–0.0385 (literature P_S range; literature P_L range, Delle Site 1997)
0.00955 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], reported as 2,2′,5,6- Saçan & Balcioğlu 1998)

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Henry's Law Constant (Pa m^3/mol at 25°C as indicated):

30.40 (calculated-P/C, Murphy et al. 1983)
112.5 (calculated-P/C, Burkhard et al. 1985b)
28.67 (20°C, calculated-P/C, Murphy et al. 1987)
41.14 (batch stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
47.26 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
43.62 (calculated-QSPR, Dunnivant et al. 1992)
17.21 (calculated-QSPR, Achman et al. 1993)
44.8 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.96 (calculated-TSA, Burkhard 1984)
5.90 (calculated-regression analysis with chlorine substituents, Oliver 1987c)
5.39, 5.57, 5,43, 5.80 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.46 (generator column-GC, Hawker & Connell 1988a)
5.62 (calculated-TSA, Hawker & Connell 1988a)
5.87 (calculated-MCI χ, Patil 1991)
5.55 (recommended, Sangster 1993)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
5.98 (quoted, Hansch et al. 1995)
6.12, 5.55–5.90 (calculated-Characteristic Root Index CRI, min.-max. range, Saçan & Inel 1995)
5.4429 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.13 (calculated-CLOGP ver. 4, Ran et al. 2002)
5.67 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

9.28, 8.70, 8.24, 7.64 (0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
$\log K_{OA} = -5.26 + 3965/(T/K)$; temp range 0–30°C (generator column-GC, Harner & Bidleman 1996)
9.18, 8.18; 8.25 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}-(aq.) = 5.7×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

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Biodegradation: 91% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0019\ d^{-1}$ (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

$k_2 = 0.008\ d^{-1}$ with $t_{½} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008\ d^{-1}$ with $t_{½} = 88$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½} = 0.1$–10 d in cloud water, $t_{½} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil:

Biota: $t_{½} = 365$ d in rainbow trout, d and $t_{½} = 107$ d in its muscle 107 d (Niimi & Oliver 1983);

$t_{½} = 30$ d in worms at 8°C, 30 d (Oliver 1987c).

depuration $t_{½} = 91$ d for high-dose treatment, $t_{½} = 88$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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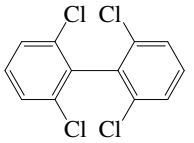
7.1.1.54 2,2′,6,6′-Tetrachlorobiphenyl (PCB-54)



Common Name: 2,2′,6,6′-Tetrachlorobiphenyl
Synonym: PCB-54, 2,2′,6,6′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,2′,6,6′-tetrachlorobiphenyl
CAS Registry No: 15968-05-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
198 (Van Roosmalen 1934; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0201 (mp at 198°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.412, 0.221, 0.143, 0.0882 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0027 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
0.0119 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0659 (supercooled liquid P_L, Burkhard 1984)
0.00132 (GC-RI correlation, Burkhard et al. 1985a)
0.0659 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0392, 0.0517 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0566 (supercooled liquid P_L, Dunnivant & Elzerman 1988)
0.00227; 0.118 (calculated-S × HLC, P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
log (P_L/Pa) = – 3751/(T/K) + 11.17 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
0.000396–0.0219; 0.00388–0.104 (literature P_S range; literature P_L range, Delle Site 1997)
0.0114 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
188.5 (calculated-P/C, Burkhard et al. 1985b)
15.0 (calculated, Coates & Elzerman 1986)
55.73 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
50.0 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
50.04 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.63 (calculated after Rekker 1977, Könemann 1981)
4.16, 713, 7.01 (HPLC-k′ correlation; calculated-π const.; calculated-fragment const., McDuffie 1981)

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5.94 (RP-TLC-retention, Bruggeman et al. 1982)
4.95, 5.27, 5.22, 5.52 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.48 (generator column-GC, Hawker & Connell 1988a)
5.936 ± 0.031 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.24 (recommended, Sangster 1993)
5.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
7.30 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
3.85; 5.38 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:
5.106, 4.91, 4.89, 4.72 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
5.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.63 (river sediment, Coates & Elzerman 1986)
4.79 (correlated literature values in soils, Sklarew & Girvin 1987)
5.01 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.11; 5.01 (soil, quoted lit.; calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
4.91, 4.84 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:
k_1 = 2740 d^{-1}; k_2 = 0.387 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{½}$ = 190 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.007 d^{-1} with $t_{½}$ = 100 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: photodegradation $t_{½}$ = 72.5 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5 kW high pressure Xenon lamp (De Felip et al. 1996).
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 190 d for high-dose treatment, $t_{½}$ = 100 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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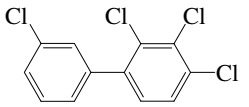
7.1.1.55 2,3,3′,4-Tetrachlorobiphenyl (PCB-55)



Common Name: 2,3,3′,4-Tetrachlorobiphenyl
Synonym: PCB-55, 2,3,3′,4-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4-tetrachlorobiphenyl
CAS Registry No: 74338-24-2
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
89 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.122 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.81×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00517 (GC-RI correlation, Burkhard et al. 1985b)
0.00579, 0.00349 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4382/(T/K) + 12.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
11.55 (calculated-P/C, Burkhard 1984)
23.51 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
18.48 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 2$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (calculated-TSA, Burkhard 1984)
6.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0161 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.66 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Live, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.008$ d^{-1} with $t_{½} = 91$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d^{-1} with $t_{½} = 157$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 91 d for high-dose treatment, $t_{½}$ = 157 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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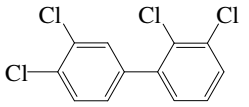
7.1.1.56 2,3,3′,4′-Tetrachlorobiphenyl (PCB-56)



Common Name: 2,3,3′,4′-Tetrachlorobiphenyl
Synonym: PCB-56, 2,3,3′,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′-tetrachlorobiphenyl
CAS Registry No: 41464-41-9
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
95 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.122 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0389 (20°C, supercooled liquid, Murphy et al. 1987)
0.0989 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0115 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.96×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00517 (GC-RI correlation, Burkhard et al. 1985b)
0.00434, 0.00327 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.17×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00331, 0.00468 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4382/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
9.45 (calculated-P/C, Burkhard 1984)
16.41 (20°C, calculated-P/C, Murphy et al. 1987)
13.27 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
15.34 (calculated-QSAR, Dunnivant et al. 1992)
8.24 (calculated-QSAR, Achman et al. 1993)
13.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
27.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 32 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (calculated-TSA, Burkhard 1984)
5.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.11 (calculated, Miertus & Jakus 1990)
5.85 (recommended, Sangster 1993)

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5.90 (calculated-TSA, Murray & Andren 1992)
5.9815 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.66 (suspended particulate matter, Burkhard 1984)
6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH-}(aq.) = 5.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota:

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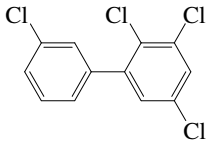
7.1.1.57 2,3,3′,5-Tetrachlorobiphenyl (PCB-57)



Common Name: 2,3,3′,5-Tetrachlorobiphenyl
Synonym: PCB-57
Chemical Name: 2,3,3′,5-tetrachlorobiphenyl
CAS Registry No: 70424-87-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 291.988
Melting Point (°C):
68 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0718 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00767 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
19.76 (calculated-P/C, Burkhard 1984)
37.59 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
27.40 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated, Burkhard 1984)
6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.1376 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.69 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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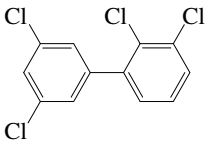
7.1.1.58 2,3,3′,5′-Tetrachlorobiphenyl (PCB-58)



Common Name: 2,3,3′,5′-Tetrachlorobiphenyl
Synonym: PCB-58
Chemical Name: 2,3,3′,5′-tetrachlorobiphenyl
CAS Registry No: 41464-43-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
68 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00558 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
9.62×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000167 (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 10.80 – 5600/(T/K) (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
16.11 (calculated-P/C, Burkhard 1984)
45.46 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
25.33 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.17 (calculated-TSA, Hawker & Connell 1988a)
6.17 (recommended, Hansch et al. 1995)
6.0904 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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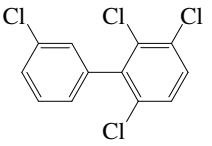
7.1.1.59 2,3,3′,6-Tetrachlorobiphenyl (PCB-59)



Common Name: 2,3,3′,6-Tetrachlorobiphenyl
Synonym: PCB-59
Chemical Name: 2,3,3′,6-tetrachlorobiphenyl
CAS Registry No: 74472-33-6
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
42 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.131 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00733 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0155 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0164 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
34.65 (calculated-P/C, Burkhard 1984)
36.58 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
30.81 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated, Burkhard 1984)
5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8476 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.64 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:

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Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.005 d^{-1} with $t_{½}$ = 132 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 132 d for high-dose treatment, $t_{½}$ = 135 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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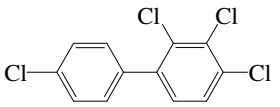
7.1.1.60 2,3,4,4′-Tetrachlorobiphenyl (PCB-60)



Common Name: 2,3,4,4′-Tetrachlorobiphenyl
Synonym: PCB-60, 2,3,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′-tetrachlorobiphenyl
CAS Registry No: 33025-41-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
128 (Weast 1972–73; Ruelle & Kesselring 1997)
142 (Saeki et al. 1971; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0695 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0168 (calculated-TSA, Mackay et al. 1980)
0.121 (calculated-TSA, supercooled liquid S_L, Burkhard et al. 1985b)
0.0389 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0902, 0.0485, 0.0254, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0359, 0.0273 (Nirmalakhandan & Speece 1989)
0.0146 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.045 (calculated-MCI χ, Patil 1991)
0.00274 (calculated-QSPR, Dunnivant et al. 1992)
0.0067, 0.0176 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000319 (GC-RI correlation, Burkhard et al. 1985a)
0.00427 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00527, 0.00414 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00217 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4660/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00331, 0.00458 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4282/(T/K) + 12.42 (supercooled liquid P_L, GC-RT correlation, Falconer Bidleman 1994)
0.0157 (supercooled liquid P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
84.20 (batch stripping, Atlas et al. 1982)
10.34 (calculated-P/C, Burkhard et al. 1985b)
16.41 (20°C, calculated-P/C, Murphy et al. 1987)

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15.40 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
15.48 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.87 (calculated-TSA, Burkhard 1984)
5.84 (HPLC-RT correlation calculated-π, Rapaport & Eisenreich 1984)
5.90 (selected, Shiu & Mackay 1986)
5.89, 6.15, 6.57, 6.37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.11 (calculated-TSA, Hawker & Connell 1988a)
5.88 (calculated-MCI χ, Patil 1991)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.01 (recommended, Sangster 1993)
5.84 (quoted, Hansch et al. 1995)
5.95, 5.33–6.24 (calculated-Characteristic Root Index CRI, minimum-maximum range, Saçan & Inel 1995)
6.0108 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.82 (10°C, estimated, Thomas et al. 1998)
9.21 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
6.20, 5.0 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
5.67 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.10 (organic carbon, obs., Murray & Andren 1992)
5.03 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 5.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 10 (food lipid mg)/(g worm lipid-d); k_2 = 0.10 d^{-1} (earthworm, Wågman et al. 2001)

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Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 7 d in earthworm given contaminated food (Wågman et al. 2001)

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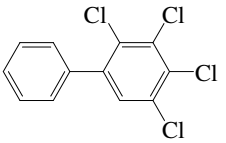
7.1.1.61 2,3,4,5-Tetrachlorobiphenyl (PCB-61)



Common Name: 2,3,4,5-Tetrachlorobiphenyl
Synonym: PCB-61, 2,3,4,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4,5-tetrachlorobiphenyl
CAS Registry No: 33284-53-6
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
92.2 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
25.2 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
69.45 (Miller et al. 1984)
69.25, 64.3 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.217 (Mackay et al. 1980)
0.218 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0192 (generator column-GC/ECD, Weil et al. 1974)
0.0209 (shake flask-GC/ECD, Haque & Schmedding 1975)
0.0099 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)
0.0209 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.0207, 0.030, 0.0180, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.014 (generator column-GC, Dunnivant & Elzerman 1988)
0.0137 (generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)
0.0136 (shake flask-GC/ECD, Li & Andren 1994)
0.0156* ± 0.0004 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
ln x = –3.967 – 4970.5/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0624 (calculated-mp and K_{OW}, Ran et al. 2002)
0.106, 0.101 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_L/(mol m^{-3})] = –839/(T/K) – 0.626 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log [S_L/(mol m^{-3})] = –1043/(T/K) + 0.037 (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0013 (GC-RT correlation, Burkhard et al. 1985a)
0.00558 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
log (P_L/Pa) = – 4382/(T/K) + 12.78 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
1.854 × 10^{-4}* (20°C, gas saturation-GC/ECD, measured range –20 to 20°C, Wania et al. 1994)
log (P_S/Pa) = 12.10 – 4632/(T/K); temp range –20 to + 20°C (gas saturation-GC, Wania et al. 1994)

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0.0144 (supercooled liq. P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.00724, 0.00692 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log (P_L/Pa) = -4330/(T/K) + 12.38$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log (P_L/Pa) = -4193/(T/K) + 11.91$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
11.45 (calculated-P/C, Burkhard et al. 1985b)
17.53 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
24.14 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
20.42, 19.95 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -3150/(T/K) + 11.87$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
5.78 (HPLC-RT correlation, Sugiura et al. 1979)
5.90 (shake flask-GC, Platford 1982)
6.39 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.74 (calculated-fragment const., Yalkowsky et al. 1983)
5.81 (calculated-TSA, Burkhard 1984)
5.72 (generator column-GC/ECD, Miller et al. 1984,1985)
5.90 (selected, Shiu & Mackay 1986)
6.38, 6.31, 6.57, 6.37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.18; 6.04 (generator column-GC/ECD; calculated-TSA, Hawker & Connell 1988a)
5.92, 6.74 (calculated-solvatochromic parameters and V_I, calculated- fragment additivity., Kamlet et al. 1988)
6.88, 6.74, 5.89, 6.04, 6.02 (calculated-π const., f const., MW, MCI χ, TSA, Doucette & Andren 1988)
6.39 (calculated-π const., De Bruijn et al. 1989)
6.406 ± 0.069 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
5.89 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.34 (generator column-GC, Li & Doucette 1993)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.44 (recommended, Sangster 1993)
6.41 (recommended, Hansch et al. 1995)
5.97, 5.72–6.74 (calculated-Characteristic Root Index CRI; minimum-maximum range, Saçan & Inel 1995)
6.1472 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.00 (calculated-QSPR, Yeh & Hong 2002)
6.51 (calculated-CLOGP ver. 4, Ran et al. 2002)
6.17, 6.11 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
8.901* (20°C, generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)
$\log K_{OA} = -2.90 + 3464/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Mackay 1995)
8.90 (20°C, generator column-GC, Harner & Bidleman 1996)
$\log K_{OA} = -2.89 + 3464.1/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
9.38–9.65 (10°C, estimated, Thomas et al. 1998)
10.19, 8.93; 8.90 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.80; 8.75 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.64, 8.55 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log K_{OA} = 4660/(T/K) - 7.08$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
4.29, 3.57, 3.94, 3.90 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

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Sorption Partition Coefficient, log K_{OC}:

5.61 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.93 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.038 d^{-1} (golden orfe, Sugiura et al. 1979)
k_2 = 0.0022 d^{-1} (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 312 d in rainbow trout, and $t_{½}$ = 93 d in its muscle 93 d (Niimi & Oliver 1983)

TABLE 7.1.1.61.1
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,3,4,5-tetrachlorobiphenyl (PCB-61) at various temperatures

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1997		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		gas saturation-GC/ECD		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
5	0.0056	–20	5.298 × 10^{-7}	–10	10.268
15	0.0102	–10	3.817 × 10^{-6}	0	9.80
25	0.0156	0	1.439 × 10^{-5}	10	9.40
35	0.0285	10	6.163 × 10^{-5}	20	8.901
45	0.0560	20	1.854 × 10^{-4}	25	8.74
		log (P/Pa) = A – B/(T/K)		ΔH_{OA}/(kJ mol^{-1}) = 66.3	
ΔH_{sol}/(kJ mol^{-1}) = 41.3		A	12.10		
for 5–45°C		B	4632	log K_{OA} = A + B/T	
		temp range –20 to20°C		A	–2.9
				B	3464.1
		ΔH_{subl}/(kJ mol^{-1}) = 88.7			

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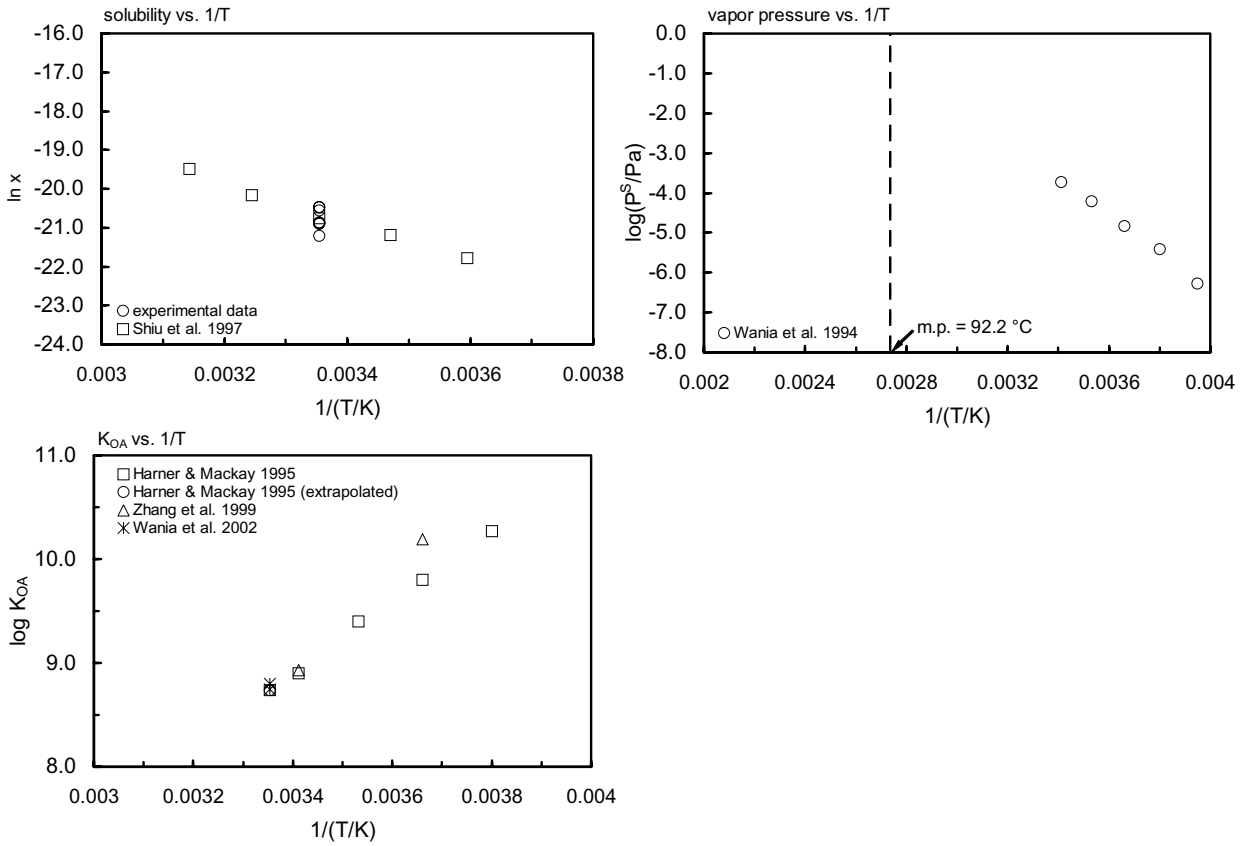

FIGURE 7.1.1.61.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,3,4,5-tetrachlorobiphenyl (PCB-61).

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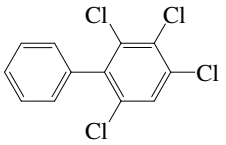
7.1.1.62 2,3,4,6-Tetrachlorobiphenyl (PCB-62)



Common Name: 2,3,4,6-Tetrachlorobiphenyl
Synonym: PCB-62
Chemical Name: 2,3,4,6-tetrachlorobiphenyl
CAS Registry No: 54230-23-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
77 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.151 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0463 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0158 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0167 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
30.70 (calculated-P/C, Burkhard 1984)
37.08 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC, Brunner et al. 1990)
37.47 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.79 (calculated, Burkhard 1984)
5.89 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0323 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.59 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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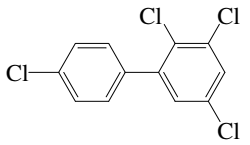
7.1.1.63 2,3,4′,5-Tetrachlorobiphenyl (PCB-63)



Common Name: 2,3,4′,5-Tetrachlorobiphenyl
Synonym: PCB-63, 2,3,4′,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,5-tetrachlorobiphenyl
CAS Registry No: 74472-34-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
83 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.105 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0263 (20°C, supercooled liquid, Murphy et al. 1987)
0.0496 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00727 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.36×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00681 (GC-RI correlation, Burkhard et al. 1985b)
2.64×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00724 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4382/(T/K) + 12.53$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
17.73 (calculated-P/C, Burkhard 1984)
29.28 (20°C, calculated-P/C, Murphy et al. 1987)
29.60 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
8.24 (calculated-QSAR, Achman et al. 1993)
25.59 (calculated-QSPR, Dunnivant et al. 1992)
24.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.10 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.10 (recommended, Sangster 1993)
6.1262 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.15, 9.06 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.003 d^{-1} with $t_{½}$ = 219 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 219 d for high-dose treatment, $t_{½}$ = 172 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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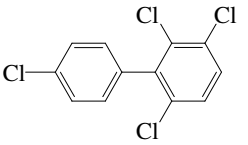
7.1.1.64 2,3,4′,6-Tetrachlorobiphenyl (PCB-64)



Common Name: 2,3,4′,6-Tetrachlorobiphenyl
Synonym: PCB-64, 2,3,4′,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,6-tetrachlorobiphenyl
CAS Registry No: 52663-58-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
57 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.130 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0937 (20°C, supercooled liquid, Murphy et al. 1987)
0.028 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0138 (P_L supercooled liquid, GC-RT correlation Burkhard et al. 1985a)
0.0146 (GC-RI correlation, Burkhard et al. 1985b)
5.51×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.70 – 4510/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00776, 0.0141 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4229/(T/K) + 12.30 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
31.01 (calculated-P/C, Burkhard 1984)
17.25 (20°C, calculated-P/C, Murphy et al. 1987)
28.37 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
14.2 (wetted-wall column-GC, Brunner et al. 1990)
27.59 (calculated-QSPR, Dunnivant et al. 1992)
24.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.84 (calculated-TSA, Burkhard 1984)
5.76 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0 (calculated-TSA, Murray & Andren 1992)
5.76 (recommended, Sangster 1993)
5.8251 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

8.41; 7.91 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = –6.43 + 4420/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.80 (quoted, Kömp & McLachlan 1997b)
9.62, 8.63; 8.74 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.54 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.64 (suspended particular matter, Burkhard 1984)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25 – 60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.005 d^{-1} with $t_{½}$ = 140 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 160 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 140 d for high-dose treatment, $t_{½}$ = 160 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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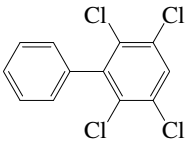
7.1.1.65 2,3,5,6-Tetrachlorobiphenyl (PCB-65)



Common Name: 2,3,5,6-Tetrachlorobiphenyl
Synonym: PCB-65, 2,3,5,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3,5,6-tetrachlorobiphenyl
CAS Registry No: 33284-54-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
77–77.5 (Bolgar 1973)
79.0 (Burkhard 1984; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.295 (mp at 79°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.162 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0099, 0.0216, 0.0119, 0.0279 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0431 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0151 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00467 (GC-RI correlation, Burkhard et al. 1985b)
0.0151 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0238 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C):
27.26 (calculated-P/C, Burkhard 1984)
31.01 (calculated-QSAR- MCI χ, Sabljic & Güsten 1989)
34.10 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.77 (calculated-TSA, Burkhard 1984)
6.07, 5.95, 5.98, 5.85 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.94; 5.86 (generator column-GC; calculated-TSA, Hawker & Connell 1988a)
5.96 (recommended, Sangster 1993)
7.8733 (calculated-UNIFAC group contribution method, Chen et al. 1993)

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5.86 (recommended, Hansch et al. 1995)
5.81; 5.46–5.96 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
6.0133 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
5.83 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:
8.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:
2.46 (*Poecillia reticulata*, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
5.57 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

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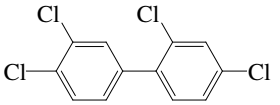
7.1.1.66 2,3′,4,4′-Tetrachlorobiphenyl (PCB-66)



Common Name: 2,3′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-66, 2,3′,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′-tetrachlorobiphenyl
CAS Registry No: 32598-10-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
124 (Saeki et al. 1971; Hutzinger et al. 1974)
127–127.5 (Webb & McCall 1972)
127–128 (Wallnöfer et al. 1973, Bolgar 1973)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.105 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0168 (calculated-TSA, Mackay et al. 1980)
0.098 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.00474 (calculated-fragment solubility constants, Wakita et al. 1986)
0.0368 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.068 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0273 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0116 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.045 (calculated-MCI χ, Patil 1991)
0.00446 (calculated-QSPR, Dunnivant et al. 1992)
0.0216 (calculated-group contribution method, Kühne et al. 1995)
0.0266 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00616 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.000494 (GC-RI correlation, Burkhard et al. 1985a)
0.00459 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00569, 0.00507 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00252 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4650/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00427, 0.0059 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4349/(T/K) + 12.38 (GC-RT correlation, Falconer & Bidleman 1994)
0.00347 (supercooled liquid P_L, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
84.20 (calculated-P/C, Murphy et al. 1983)
13.68 (calculated-P/C, Burkhard et al. 1985b)

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14.18 (quoted, Eisenreich 1987)
20.37 (20°C, calculated-P/C, Murphy et al. 1987)
25.84 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
12.16 (wetted-wall column-GC, Brunner et al. 1990)
20.55 (calculated-QSPR, Dunnivant et al. 1992)
36.97* ± 0.48 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln K_{AW} = 7.4573 – 3488.7/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(29.0/kJ{\cdot}mol^{-1})/RT] + (0.062/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where R = 8.314 $J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
35.4 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.90 (HPLC-RT correlation, Shaw & Connell 1982)
5.80, 6.31 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.98 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.31 (generator column-GC/ECD, Hawker & Connell 1988a)
6.09 (generator column-GC, Larsen et al.1992)
6.12 (recommended, Sangster 1993)
6.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9.22* (20°C, generator column-GC, measured range 0–30°C, Harner & Bidleman 1996)
log K_{OA} = –3.82 + 3827/(T/K); temp range 0–30°C (generator column-GC, Harner & Bidleman 1996)
9.73 (10°C, estimated, Thomas et al. 1998)
10.33, 9.29; 9.22 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.36 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
4.45 (worms, Oliver 1987c)
3.18–4.62 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.55–5.76 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.80, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
5.74 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.72 (soil, calculated-S, Chou & Griffin 1986)
5.23 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
4.90 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.10 (organic carbon, obs., Murray & Andren 1992)
4.90 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
5.20 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Hydrolysis:
Photolysis: photodegradation k = (0.11 ± 0.02) h^{-1} with $t_{½}$ = 7.1 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

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k_{OH}(aq.) = 5.1×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.001 d^{-1} (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

k_2 = 0.009 d^{-1} with $t_{½}$ = 82 d and k_2 = 0.013 d^{-1} with $t_{½}$ = 55 d for food concn of 21 ng/g and 158 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_2 = 0.004 d^{-1} with $t_{½}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.003 d^{-1} with $t_{½}$ = 225 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

photodegradation $t_{½}$ = (7.1 ± 1.5) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.067 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.75 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 1.18 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.32 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00081 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.0024 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00443 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.000295 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{½}$ = 670 d in rainbow trout, and $t_{½}$ = 108 d its muscle (Niimi & Oliver 1983)

$t_{½}$ = 33 d in worms at 8°C(Oliver 1987c)

depuration $t_{½}$ = 55–82 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½}$ = 164 d for high-dose treatment, $t_{½}$ = 225 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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TABLE 7.1.1.66.1
Reported Henry's law constants and octanol-air partition coefficients of 2,3′,4,4′-tetrachlorobiphenyl (PCB-66) at various temperatures and temperature dependence equations

Henry's law constant		log K_{OA}			
Bamford et al. 2000		Harner & Bidleman 1996		Zhang et al. 1999	
gas stripping-GC/MS		generator column-GC		multicolumn-GC-k′ correlation	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}	t/°C	log K_{OA}
4	14.17	0	10.21	0	10.33
11	19.80	10	9.65	20	9.29
18	27.25	20	9.22		
25	36.97	30	8.82		
31	47.51				
		ΔH_{OA}/(kJ mol^{-1}) = 73.28			
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$					
	K_{AW}	$\log K_{OA} = A + B/T$			
A	7.4573	A	–3.82		
B	3488.09	B	3827		

enthalpy, entropy change:

$\Delta H/(kJ \cdot mol^{-1}) = 29.0 \pm 2.6$

$\Delta S/(J \cdot mol^{-1} \cdot K^{-1}) = 62 \pm 8$

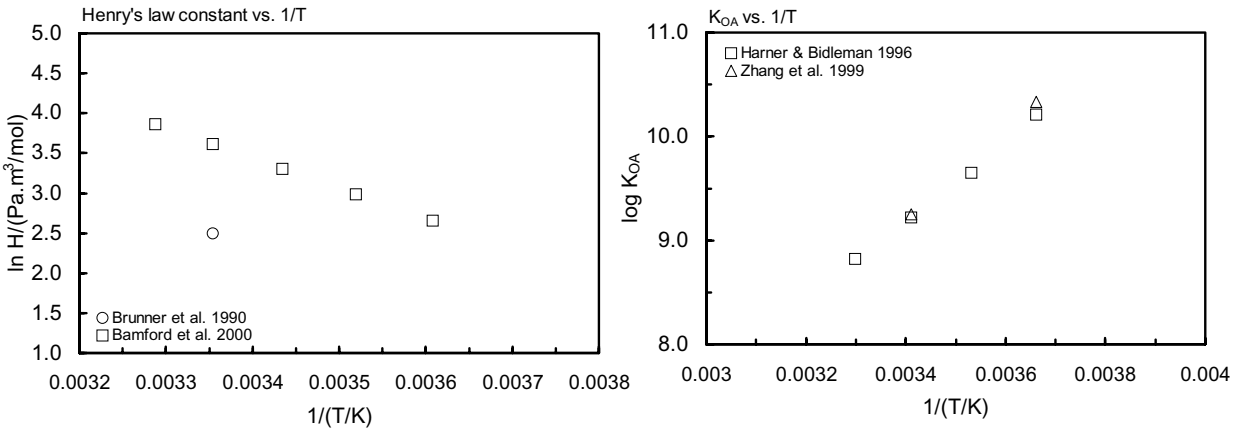

FIGURE 7.1.1.66.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,3′,4,4′-tetrachlorobiphenyl (PCB-66).

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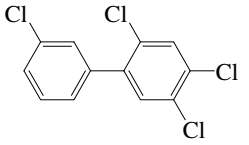
7.1.1.67 2,3′,4,5-Tetrachlorobiphenyl (PCB-67)



Common Name: 2,3′,4,5-Tetrachlorobiphenyl
Synonym: PCB-67, 2,3′,4,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,5-tetrachlorobiphenyl
CAS Registry No: 73575-53-8
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
83 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0987 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0351, 0.0298, 0.00804, 0.0266 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00654 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0070 (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 10.70 – 4530/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00708 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = –4382/(T/K) + 12.52, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
19.35 (calculated-P/C, Burkhard 1984)
29.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
23.70 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.93 (calculated-TSA, Burkhard 1984)
6.22, 6.32, 6.40, 6.33 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.32 (recommended, Sangster 1993)
6.2276 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.06 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.73 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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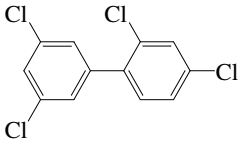
7.1.1.68 2,3′,4,5′-Tetrachlorobiphenyl (PCB-68)



Common Name: 2,3′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-68
Chemical Name: 2,3′,4,5′-tetrachlorobiphenyl
CAS Registry No: 73575-52-7
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
71 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.085 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.00679 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00726 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
23.30 (calculated-P/C, Burkhard 1984)
55.02 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
38.17 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.99 (calculated-TSA, Burkhard 1984)
6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.2624 (calculated molecular properties MNDO-AM method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.66 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.79 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:

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Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 11 (food lipid mg)/(g worm lipid-d); k_2 = 0.08 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 8 d in earthworm given contaminated food (Wågman et al. 2001)

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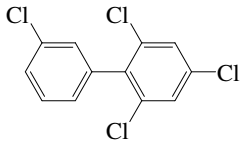
7.1.1.69 2,3′,4,6-Tetrachlorobiphenyl (PCB-69)



Common Name: 2,3′,4,6-Tetrachlorobiphenyl
Synonym: PCB-69
Chemical Name: 2,3′,4,6-tetrachlorobiphenyl
CAS Registry No: 60233-24-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
45 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.105 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0097, 0.0146, 0.0184, 0.0243 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0169 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0179, (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 10.60 – 4440/T (GC-RT correlation, Tateya et al. 1988)
0.01911 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = –4229/(T/K) + 12.43 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
47.12 (calculated-P/C, Burkhard 1984)
63.53 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)
51.22 (calculated-QSAR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.09,6.06, 6.09, 5.89 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0068 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.47 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.71 (suspended particulate matter, Burkhard et al. 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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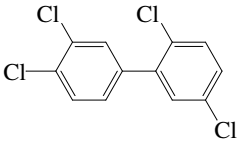
7.1.1.70 2,3′,4′,5-Tetrachlorobiphenyl (PCB-70)



Common Name: 2,3′,4′,5-Tetrachlorobiphenyl
Synonym: PCB-70, 2,3′,4′,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,3′,4′,5-tetrachlorobiphenyl
CAS Registry No: 32598-11-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
104 (Bellavita 1935; Hutzinger et al. 1974)
104–107 (Wallnöfer et al. 1973, Bolgar 1973)
Boiling Point (°C):

Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.168 (mp at 104°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.041 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.029 (calculated-TSA, Mackay et al. 1980)
0.022 (generator column-GC, Bruggeman et al. 1981)
0.099 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0091 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.0104 (calculated-fragment solubility constants, Wakita et al. 1986)
0.0362 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0254, 0.0368, 0.0432, 0.030 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0273 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.045 (calculated-MCI χ, Patil 1991)
0.0111 (calculated-QSPR, Dunnivant et al. 1992)
0.0114, 0.0306 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0463 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00544, 0.00642 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
0.00769 (calculated S × HLC, Burkhard et al. 1985a)
0.000919 (GC-RI correlation, Burkhard et al. 1985a)
0.00519 (supercooled liquid P_L, calculated-GC-RI, Burkhard et al. 1985b)
0.00526, 0.00551 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.0060 (selected P_L, supercooled liquid, Shiu & Mackay 1986)

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0.00236 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4640/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00447, 0.0063 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4431/(T/K) + 12.60 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

20.26 (calculated-P/C, Murphy et al. 1983)
15.30 (calculated-P/C, Burkhard et al. 1985b)
19.05 (20°C, calculated-P/C, Murphy et al. 1987)
19.15 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC, Brunner et al. 1990)
20.50 (calculated-QSPR, Dunnivant et al. 1992)
17.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

5.95 (shake flask-GC, Tulp & Hutzinger 1978)
5.95 (HPLC-k′ correlation, McDuffie 1981)
6.39 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.30 (HPLC-RT correlation, Shaw & Connell 1982)
5.72, 6.23 (HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.18 (HPLC-RT correlation, Opperhuizen et al. 1985)
6.01, 6.24, 6.36, 6.29 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.99 (generator column-GC, Larsen et al. 1992)
5.99 (HPLC-k′ correlation, Neogrohati & Hammers 1992)
5.7833 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.23 (recommended, Sangster 1993)
6.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.29, 9.22; 9.29 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.92 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

6.15 (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
6.20 (goldfish, 3% lipid, calculated-K_{OW}, Bruggeman et al. 1981)
4.62, 5.11 (goldfish, exptl., correlated, Mackay & Hughes 1984)
4.32, 5.50 (guppy, lipid phase, Opperhuizen et al. 1985)
4.92 (guppy, Gobas et al. 1987)
4.62, 4.32 (fish, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
5.08; 6.61 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.32, 5.62; 4.742, 4.257 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
5.08, 6.61 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

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Sorption Partition Coefficient, log K_{OC}:

5.02, 4.86, 4.85, 4.69 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
5.73 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.6–6.8, 6.3 (suspended sediment, average, Oliver 1987a)
7.20 (algae > 50 μm, Oliver 1987a)
4.81 (soil, calculated-S, Chou & Griffin 1986)
4.76 (correlated literature values in soils, Sklarew & Girvin 1987)
6.04 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.52 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.84 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.02; 5.07 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.86, 4.80 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 5.5×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~4–11 d in freshwater systems, 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 420 d^{-1}; k_2 = 0.01 d^{-1} (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986, Clark et al. 1990))
k_2 = 0.01, 0.0104 d^{-1} (goldfish, exptl., correlated, Mackay & Hughes 1984)
k_1 = 380 d^{-1}; k_2 = 0.018 d^{-1} (guppy, Opperhuizen et al. 1985)
k_1 = 17.5 h^{-1}; $1/k_2$ = 2400 h (goldfish, quoted, Hawker & Connell 1985)
log k_1 = 2.58, 2.62 d^{-1}; log $1/k_2$ = 1.74, 2.0 d (fish, quoted, Connell & Hawker 1988)
log k_2 = –2.0 d^{-1} (fish, quoted, Thomann 1989)
k_1 = 3340 d^{-1}; k_2 = 0.0280 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_1 = 0.00043 h^{-1}; k_2 = 0.170 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1 = 10 (food lipid mg)/(g worm lipid-d); k_2 = 0.09 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{½}$ = 167 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 217 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

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Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
photodegradation $t_{½}$ = 4.87 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

Groundwater:

Sediment:

Soil:

Biota: clearance $t_{½}$ = 60 d in goldfish (static equilibration system, 23-d exposure, Bruggeman et al. 1981)
$t_{½}$ = 38.6 d in guppy (Opperhuizen et al. 1985);
elimination $t_{½}$ = 8 d in earthworm given contaminated food (Wågman et al. 2001)
depuration $t_{½}$ = 167 d for high-dose treatment, $t_{½}$ = 217 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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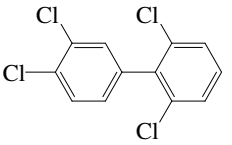
7.1.1.71 2,3′,4′,6-Tetrachlorobiphenyl (PCB-71)



Common Name: 2,3′,4′,6-Tetrachlorobiphenyl
Synonym: PCB-71
Chemical Name: 2,3′,4′,6-tetrachlorobiphenyl
CAS Registry No: 41464-46-4
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
57 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.123 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0278 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.59×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)
0.0102 (GC-RI correlation, Burkhard et al. 1985b)
0.00912, 0.00877 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00776, 0.0115 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4229/(T/K) + 12.14$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
22.80 (calculated-P/C, Burkhard 1984)
32.53 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
14.31 (calculated-QSPR, Achman et al. 1993)
31.82 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.86 (calculated-TSA, Burkhard 1984)
5.76 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.98 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.7206 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
9.78, 8.84; 8.98 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

5.66 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 5.7×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota:

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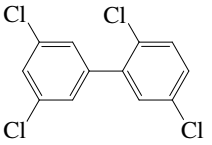
7.1.1.72 2,3′,5,5′-Tetrachlorobiphenyl (PCB-72)



Common Name: 2,3′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-72
Chemical Name: 2,3′,5,5′-tetrachlorobiphenyl
CAS Registry No: 41464-42-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
56 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0861 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0107 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.66×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00818, 0.00957 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.010, 0.00988 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4382/(T/K) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
25.34 (calculated-P/C, Burkhard 1984)
48.33 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
36.70 (calculated-QSAR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.98 (calculated, Burkhard 1984)
6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.2101 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.78 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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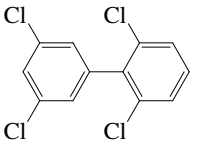
7.1.1.73 2,3′,5′,6-Tetrachlorobiphenyl (PCB-73)



Common Name: 2,3′,5′,6-Tetrachlorobiphenyl
Synonym: PCB-73
Chemical Name: 2,3′,5′,6-tetrachlorobiphenyl
CAS Registry No: 74338-23-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
66 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0142 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.0150, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
38.91 (calculated-P/C, Burkhard 1984)
61.81 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
52.69 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.91 (calculated-TSA, Burkhard 1984)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.8026 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
7.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:

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Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 - 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36 - 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–0 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–0 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

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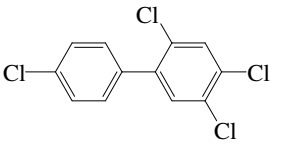
7.1.1.74 2,4,4′,5-Tetrachlorobiphenyl (PCB-74)



Common Name: 2,4,4′,5-Tetrachlorobiphenyl
Synonym: PCB-74, 2,4,4′,5-tetrachloro-1,1′-biphenyl
Chemical Name: 2,4,4′,5-tetrachlorobiphenyl
CAS Registry No: 32690-93-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
125 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.102 (calcd-assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0978 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0306 (20°C, supercooled liquid, Murphy et al. 1987)
0.0496 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00453 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0058 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00209, 0.000636, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00731, 0.00692 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.12×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.80 – 4600/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00479, 0.00631 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4382/(T/K) + 12.56 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0116 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
17.33 (calculated-P/C, Burkhard 1984)
21.18 (20°C,calculated-P/C, Murphy et al. 1987)
21.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)
21.76 (calculated-QSPR, Dunnivant et al. 1992)
23.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.16, 6.67 (HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.10 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.10 (recommended, Sangster 1993)
6.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.25, 9.14; 8.96 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.38–9.65 (10°C, estimated, Thomas et al. 1998)
9.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

51 (trout in Lake Ontario, Niimi 1996)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

5.74 (suspended particulate matter, Burkhard 1984)
6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.0 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.50 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH-}(aq.) = 5.4×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004$ d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d^{-1} with $t_{½}$ = 220 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

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Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 172 d for high-dose treatment, $t_{½}$ = 220 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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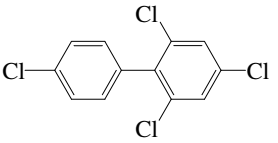
7.1.1.75 2,4,4′,6-Tetrachlorobiphenyl (PCB-75)



Common Name: 2,4,4′,6-Tetrachlorobiphenyl
Synonym: PCB-75, 2,4,4′,6-tetrachloro-1,1′-biphenyl
Chemical Name: 2,4,4′,6-tetrachlorobiphenyl
CAS Registry No: 32598-12-2
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
93.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.104 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.00967, 0.0127, 0.0122, 0.0180 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.091 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.045 (calculated-MCI χ, Patil 1991)
0.0804 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0204, 0.0158, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0150 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0179, 0.0202 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4229/(T/K) + 12.44$ (GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
42.25 (calculated-P/C, Burkhard et al. 1985b)
42.25 (batch stripping, Dunnivant & Elzerman 1988)
55.32 (calculated- QSPR-MCI χ, Sabljic & Güsten 1989)
47.07 (calculated-QSPR, Dunnivant et al. 1992)
35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.08, 6.10, 5.97, 5.97 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.03 (recommended, Sangster 1993)

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Octanol/Air Partition Coefficient, log K_{OA}:

8.19 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

5.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

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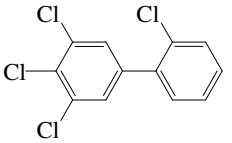
7.1.1.76 2,3′,4′,5′-Tetrachlorobiphenyl (PCB-76)



Common Name: 2,3′,4′,5′-Tetrachlorobiphenyl
Synonym: PCB-76, 2,3′,4′,5′-tetrachlorobiphenyl
Chemical Name: 2,3′,4′,5′-tetrachlorobiphenyl
CAS Registry No: 70362-48-0
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
89 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.114 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0551 (20°C, supercooled liquid, Murphy et al. 1987)
0.0569 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0150 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00512, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00602, 0.00426 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.44×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
0.00447, 0.00646 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4382/(T/K) + 12.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
12.16 (calculated-P/C, Burkhard 1984)
12.97 (20°C, calculated-P/C, Murphy et al. 1987)
22.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
10.13 (calculated-QSPR, Achman et al. 1993)
24.19 (calculated-QSPR, Dunnivant et al. 1992)
35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.88 (calculated-TSA, Burkhard 1984)
5.98 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.05 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.23 (Hawker & Connell 1988b)
5.90 (calculated-QSPR, Murray & Andren 1992)

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5.98 (recommended, Sangster 1993)
6.0763 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.68 (suspended particulate matter, Burkhard 1984)
6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}-(aq.) = 5.5×10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.005 d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 153 d for high-dose treatment, $t_{½}$ = 164 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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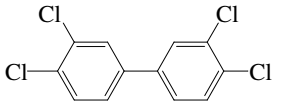
7.1.1.77 3,3′,4,4′-Tetrachlorobiphenyl (PCB-77)



Common Name: 3,3′,4,4′-Tetrachlorobiphenyl
Synonym: PCB-77, 3,3′,4,4′-tetrachloro-1,1′-biphenyl
Chemical Name: 3,3′,4,4′-tetrachlorobiphenyl
CAS Registry No: 32598-13-3
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
180 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2024
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.10 (Ruelle et al. 1993)
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.6 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.029 (calculated, assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)
0.0202 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.175 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
7.50×10^{-4} (generator column-GC/ECD, Weil et al. 1974)
5.69×10^{-4}* (generator column-GC/ECD, measured 4–32°C, Dickhut et al. 1986)
5.84×10^{-4}* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
ln x = –6098/(T/K) – 3.586, temp range 4–32°C, ΔH_{ss} = 50.7 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
log x = –2636/(T/K) – 1.558, ΔH_{ss} = 50.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
S/(mol/L) = 3.59×10^{-10} exp(0.072·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
8.23×10^{-4}, 1.01×10^{-3}, 1.16×10^{-3} (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0018 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
5.50×10^{-4}; 0.0161 (generator column-GC; supercooled liquid S_L, Dunnivant & Elzerman 1988)
6.10×10^{-4} (generator column-GC/ECD, room temp., Hong & Qiao 1995)
2.02×10^{-3}, 5.44×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
log S_L (mol/L) = – 0.246 + 1339/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln x = –3.58245 – 6074.34/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.00270* (generator column-GC/ECD, measured range 5–35°C. Huang & Hong 2002).—See Comment by van Noort 2004

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00219, 0.00196 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.0014 (supercooled liquid P_L, GT-RT correlation, Burkhard 1984)

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5.97×10^{-4}; 4.46×10^{-5}, 8.04×10^{-4} (calculated-MW, GC-RT correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0014 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00213, 0.00144 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.88×10^{-5}; 0.0020 (selected P_S, supercooled liquid P_L, Shiu & Mackay 1986)
0.00212 (supercooled liquid P_L, Dunnivant & Elzerman 1988)
1.82×10^{-5}; 5.26×10^{-4} (calculated-S × HLC, solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
0.00141, 0.00191(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4552/(T/K) + 12.61$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
1.202×10^{-3} (supercooled liquid P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
6.46×10^{-5}; 2.21×10^{-3} (solid, supercooled liquid, Passivirta et al. 1999)
$\log (P_S/Pa) = 15.56 - 5889/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 12.61 - 4552/(T/K)$ (liquid, Passivirta et al. 1999)
$(1.82 - 80.4) \times 10^{-5}$; $(4.71 - 22.0) \times 10^{-4}$ (quoted lit. P_S range; lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
4.37 (calculated-P/C, Burkhard et al. 1985b)
1.72 (calculated-P/C, Shiu & Mackay 1986)
9.52 (gas stripping-GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
40.88 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
10.39 (calculated-QSPR, Dunnivant et al. 1992)
$\log H$ (Pa m^3/mol) = 12.86 – 3214/(T/K) (Passivirta et al. 1999)
16.20* ± 0.41 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 11.0657 - 4787.1/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(39.8/kJ \cdot mol^{-1})/RT] + (0.092/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where $R = 8.314\ J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
16.7 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 40 \pm 6$ kJ/mol, $\Delta S_H = 0.09 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:
6.04 (HPLC-RT correlation, Sugiura et al. 1979)
6.52 (RP-TLC-retention, Bruggeman et al. 1982)
5.62 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.77 (HPLC-k′ correlation, De Kock & Lord 1987)
6.11, 6.40, 6.37 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.21 (generator column-GC, Hawker & Connell 1988a)
6.630 ± 0.018 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
6.13 (generator column-GC, Larsen et al. 1992)
5.98 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.11 (recommended, Sangster 1993)
6.63 (recommended, Hansch et al. 1995)
6.48 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
9.08 (calculated, Paterson et al. 1991)
9.96* (20°C, generator column-GC, measured range 0 to 30°C, Harner & Bidleman 1996)
$\log K_{OA} = -3.14 + 3828/(T/K)$; (temp range 0 to 30°C, Harner & Bidleman 1996)
10.92, 9.92; 10.03 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)

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9.70 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.29; 9.19 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.46 (killifish, Goto et al. 1978)
3.90, 3.24, 3.63, 4.15 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
2.77, 2.63 (human fat in lipid, wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
5.36; 6.89 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
4.59, 5.87; 4.745, 4.943 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW}, Lu et al. 1999)
2.56–4.26 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.19–5.23 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.36 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
5.36, 6.90 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.41, 6.37 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
2.62, 2.77 (human: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.75 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.41 (soil, calculated, Chou & Griffin 1986)
5.02 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.029, 0.0047 d^{-1} (golden orfe, guppy, Sugiura et al. 1979)
k_2 = 0.0157 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 5160 d^{-1}; k_2 = 0.0224 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_1 = 17 L d^{-1} g^{-1} dry wt.; k_2 = 0.073 d^{-1} (Baltic Sea blue mussel, flow-through expt., Gustafsson et al. 1999)
k_2 = 0.0251 d^{-1} with $t_{½}$ = 28 d (newly contaminated oysters, Gardinali et al. 2004)
k_2 = 0.0166 d^{-1} with $t_{½}$ = 42 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995);
$t_{½}$ = 1500 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{½}$ = 805 d in Lake Michigan (Neely 1983);
photodegradation $t_{½}$ = 528 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);
$t_{½}$ = 30000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

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Groundwater:
Sediment: $t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: $t_{½}$ = 44 d in rainbow trout, and its muscle, 29 d (Niimi & Oliver 1983);
theoretical half-life to reach 90% steady-state tissue concn 9.5 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)
Depuration $t_{½}$ = 28 d for newly contaminated oysters, and $t_{½}$ = 42 d for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 7.1.1.77.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 3,3′,4,4′-tetrachlorobiphenyl (PCB 77) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility				Henry's law constant		log K_{OA}	
Dickhut et al. 1986		Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
4	1.46×10^{-4}	5	1.25×10^{-3}	4	4.46	0	10.88
20	4.38×10^{-4}	15	1.77×10^{-3}	11	6.99	10	10.36
25	5.84×10^{-4}	25	2.70×10^{-3}	18	10.75	20	9.96
32	1.17×10^{-3}	35	4.35×10^{-3}	25	16.20	30	9.47
				31	22.69		
ln x = A – B/(T/K)		mp/°C	180–181			ΔH_{OA}/(kJ mol^{-1}) = 73.30	
A	–3.586			enthalpy, entropy change:			
B	6098.15	ΔH_{sol}/(kJ mol^{-1}) = 29.6		ΔH/(kJ·mol^{-1}) = 39.8 ± 6.0		log K_{OA} = A + B/T	
				ΔS/(J·mol^{-1}·K^{-1}) = 92 ± 20		A	–3.14
enthalpy of solution:						B	3828
ΔH_{sol}/(kJ mol^{-1}) = 50.7 ± 4.8				ln K_{AW} = –ΔH/RT + ΔS/R			
for 4–32°C				A	11.6567		
				B	4787.11		

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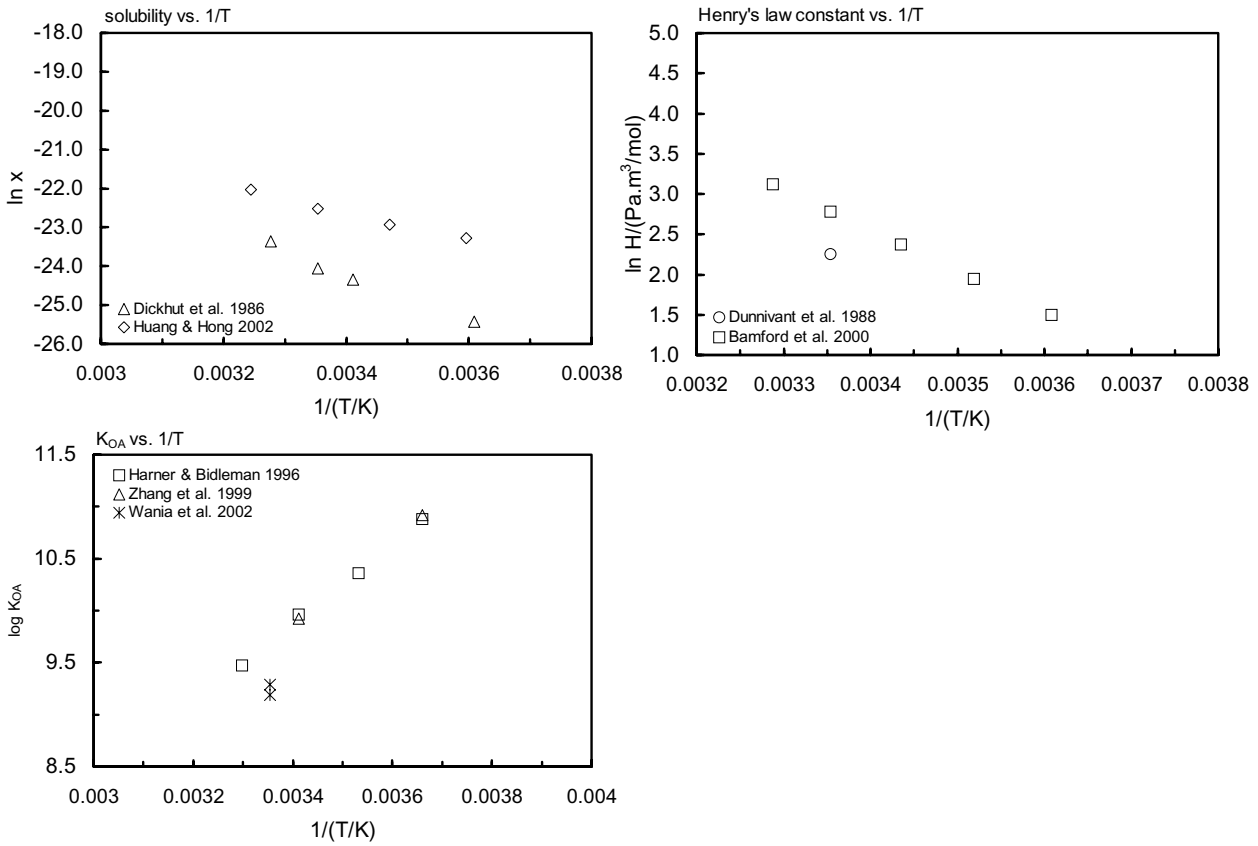

FIGURE 7.1.1.77.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 3,3′,4,4′-tetrachlorobiphenyl (PCB-77).

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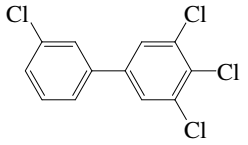
7.1.1.78 3,3′,4,5-Tetrachlorobiphenyl (PCB-78)



Common Name: 3,3′,4,5-Tetrachlorobiphenyl
Synonym: PCB-78
Chemical Name: 3,3′,4,5-tetrachlorobiphenyl
CAS Registry No: 70362-49-1
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
94 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0943 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00186 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00116, 0.000167, 0.000223 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00319, 0.00206 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P_L/Pa) = –4598/T + 12.92 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
5.76 (calculated-P/C, Burkhard 1984)
22.90 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
21.77 (calculated-QSPR, Dunnivant et al. 1992)
20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.95 (calculated, Burkhard 1984)
6.35 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.2278 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
5.75 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1: 8 (food lipid mg)/(g worm lipid-d); k_2: 0.09 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 7 d in earthworm given contaminated food (Wågman et al. 2001)

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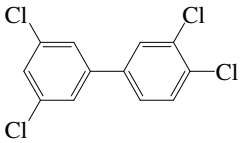
7.1.1.79 3,3′,4,5′-Tetrachlorobiphenyl (PCB-79)



Common Name: 3,3′,4,5′-Tetrachlorobiphenyl
Synonym: PCB-79
Chemical Name: 3,3′,4,5′-tetrachlorobiphenyl
CAS Registry No: 41464-48-6
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
83 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0815 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0036 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.07×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.00224, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00341, 0.00206 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4598/(T/K) + 12.95$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
7.39 (calculated-P/C, Burkhard 1984)
11.75 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
3.94 (calculated-QSPR, Achman et al. 1993)
12.73 (calculated-QSAR, Dunnivant et al. 1992)
20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.00 (calculated-TSA, Burkhard 1984)
6.42 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.3035 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.67 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

5.80 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.4–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.36–1.7) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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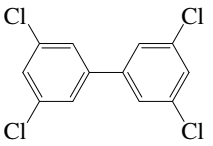
7.1.1.80 3,3′,5,5′-Tetrachlorobiphenyl (PCB-80)



Common Name: 3,3′,5,5′-Tetrachlorobiphenyl
Synonym: PCB-80, 3,3′,5,5′-tetrachloro-1,1′-biphenyl
Chemical Name: 3,3′,5,5′-tetrachlorobiphenyl
CAS Registry No: 33284-52-5
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
164 (Van Roosmalen 1934; Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.2 (calculated-Le Bas method at normal boiling point)
211.6 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0421 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0712 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.000306, 0.000496, 0.000786, 0.000902 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00124 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0295 (supercooled liquid S_L, calculated-mp, Dunnivant & Elzerman 1988)
0.00292 (calculated-TSA, Abramowitz & Yalkowsky 1990)
2.92×10^{-3}, 7.68×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
4.96×10^{-3} (calculated–mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000859, 0.000139, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00305 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00547, 0.00511 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4598/(T/K) + 13.16$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
12.46 (calculated-P/C, Burkhard et al. 1985b)
63.02 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
38.0 (calculated-QSPR, Dunnivant et al. 1992)
20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.85 (HPLC-RT correlation, Sugiura et al. 1978; quoted, Hansch et al. 1995)
6.58 (RP-TLC-retention, Bruggeman et al. 1982)

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6.77, 6.77, 6.45, 6.41 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.60 (recommended, Sangster 1993)
6.48, 6.85 (quoted lit. values, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.26 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
5.85 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

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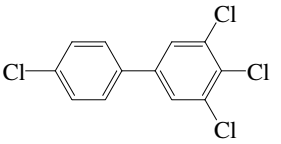
7.1.1.81 3,4,4′,5-Tetrachlorobiphenyl (PCB-81)



Common Name: 3,4,4′,5-Tetrachlorobiphenyl
Synonym: PCB-81
Chemical Name: 3,4,4′,5-Tetrachlorobiphenyl
CAS Registry No: 70362-50-4
Molecular Formula: $C_{12}H_6Cl_4$
Molecular Weight: 291.988
Melting Point (°C):
137 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0929 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985)
0.00292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0010 (room temp., generator column-GC/ECD, Hong & Qiao 1995)—see comment by van Noort 2004
0.00313 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)
0.00140, 0.00213, 0.00313, 0.00505 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00165 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.0204, 0.0018, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00290, 0.00182. (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4598/(T/K) + 12.88$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.20 (calculated-P/C, Burkhard et al. 1985a)
15.0 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
10.06 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
12.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
25.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 33 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.96 (calculated-TSA, Burkhard 1984)
6.36 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.1949 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.53; 6.16 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
6.64, 6.24 (calculated-MCI χ, calculated-molecular properties MNDO-MI method, Yeh & Hong 2002)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.88 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.10, 6.40 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.76 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.4–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 25–60 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.36–1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for tetrachlorobiphenyls, and the tropospheric lifetime τ(calc) = 8.5–40 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.0185 d^{-1} with $t_{½}$ = 37 d (newly contaminated oysters, Gardinali et al. 2004)

k_2 = 0.0186 d^{-1} with $t_{½}$ = 37 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: clearance $t_{½}$ = 21 d in guppy for tetrachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for tetrachlorobiphenyls: $t_{½}$ = 2–290 d in trout, $t_{½}$ = 29–127 d in trout muscle; $t_{½}$ = 51–81 d in goldfish, $t_{½}$ = 7–200 d in carp and $t_{½}$ = 4–53 d in guppy (Niimi 1987)

Depuration $t_{½}$ = 37 d for newly contaminated oysters, and $t_{½}$ = 37 d for chronically contaminated oysters (Gardinali et al. 2004)

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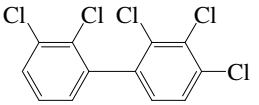
7.1.1.82 2,2′,3,3′,4-Pentachlorobiphenyl (PCB-82)



Common Name: 2,2′,3,3′,4-Pentachlorobiphenyl
Synonym: PCB-82
Chemical Name: 2,2′,3,3′,4-pentachlorobiphenyl
CAS Registry No: 52663-62-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
85 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0467 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0291 (20°C, supercooled liquid, Murphy et al. 1987)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0028 (calculated-QSPR, Dunnivant et al. 1992)
0.00622 (calculated-group contribution method, Kühne et al. 1995)
0.0221 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0020 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00218, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.06×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.0 – 4780/(T/K) (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
12.46 (calculated-P/C, Burkhard 1984)
11.86 (20°C, calculated-P/C, Murphy et al. 1987)
12.36 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
14.82 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
16.3 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 8$ kJ/mol, $\Delta S_H = 0.11 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.20 (calculated-TSA, Burkhard 1984)
6.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.30 (estimated, Girvin & Scott 1997)
6.0458 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.73 (calculated-CLOGP ver. 4, Ran et al. 2002)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.00 (suspended particulate matter, Burkhard 1984)

4.770 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

5.80 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 174 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 196d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 174 d for high-dose treatment, $t_{½}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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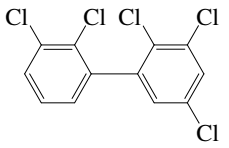
7.1.1.83 2,2′,3,3′,5-Pentachlorobiphenyl (PCB-83)



Common Name: 2,2′,3,3′,5-Pentachlorobiphenyl
Synonym: PCB-83
Chemical Name: 2,2′,3,3′,5-pentachlorobiphenyl
CAS Registry No: 60145-20-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
65 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle et al. 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.405 (mp at 65°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0045 (generator column-GC/ECD, Weil et al. 1974)
0.023 (shake flask-GC/ECD, Wallnöfer et al. 1973)
0.046 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0282 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0260 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.0103, 0.0278 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00735, 0.00324, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00299 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00274, 0.00303 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00154 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.0 – 4760/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00204 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4522/(T/K) + 12.60 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
21.28 (calculated-P/C, Burkhard et al. 1985b)
16.62 (20°C, calculated-P/C, Murphy et al. 1987)
26.65 (calculated- QSPR-MCI χ, Sabljic & Güsten 1989)
21.46 (calculated-QSPR, Dunnivant et al. 1992)
23.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
45.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 6$ kJ/mol, $\Delta S_H = 0.07 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.24 (calculated-TSA, Burkhard 1984)
6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.51 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
6.0458 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.44, 9.39 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.01 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.04 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.748 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.004 d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 217 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1996).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 172 d for high-dose treatment, $t_{½}$ = 217 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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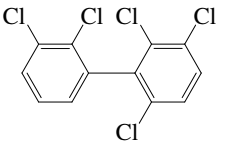
7.1.1.84 2,2′,3,3′,6-Pentachlorobiphenyl (PCB-84)



Common Name: 2,2′,3,3′,6-Pentachlorobiphenyl
Synonym: PCB-84, 2,2′,3,3′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,6-pentachlorobiphenyl
CAS Registry No: 52663-60-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
91 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.047 (20°C, supercooled liquid, Murphy et al. 1987)
0.0542 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.48×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00693, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00372, 0.00441 supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.64×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.0 – 4740/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00302, 0.0055 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4399/(T/K) + 12.32 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
51.68 (calculated-P/C, Burkhard 1984)
17.63 (20°C,calculated-P/C, Murphy et al. 1987)
24.82 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.97 (calculated-QSPR, Achman et al. 1993)
25.45 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.04 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
5.60 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.24 (generator column-GC, Larsen et al. 1992)
5.96 (recommended, Sangster 1993)
6.04 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = –5.84 + 4360/(T/K); (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.80 (quoted, Kömp & McLachlan 1997b)
10.28, 9.28 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
8.94 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

80 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

6.09 (suspended particulate matter, Bukhard 1984)
4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(aq.) = 4.7 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{½}$ = 141 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water: half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 135 d for high-dose treatment, $t_{½}$ = 141 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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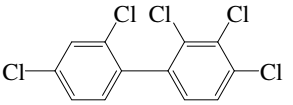
7.1.1.85 2,2′,3,4,4′-Pentachlorobiphenyl (PCB-85)



Common Name: 2,2′,3,4,4′-Pentachlorobiphenyl
Synonym: PCB-85, 2,2′,3,4,4′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′-pentachlorobiphenyl
CAS Registry No: 65510-45-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
87 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0428 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0219 (20°C, supercooled liquid, Murphy et al. 1987)
0.00782 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00233 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00253, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00472, 0.00218 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.12×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/Pa) = -4522/(T/K) + 12.54$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.00248 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
17.83 (calculated-P/C, Burkhard 1984)
16.72 (20°C, calculated-P/C, Murphy et al. 1987)
24.82 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
6.69 (wetted-wall column-GC/ECD, Brunner et al. 1990)
19.49 (calculated-QSPR, Dunnivant et al. 1992)
26.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
47.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 7$ kJ/mol, $\Delta S_H = 0.05 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.61 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
6.18 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.18 (recommended, Sangster 1993)
6.61 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.29 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.07 (suspended particulate matter, Burkhard 1984)
4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.70 (soil-organic carbon, Girvin & Scott 1997)
5.51 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.70 (soil, calculated-$K_{OW,}$ Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

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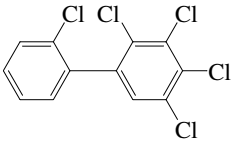
7.1.1.86 2,2′,3,4,5-Pentachlorobiphenyl (PCB-86)



Common Name: 2,2′,3,4,5-Pentachlorobiphenyl
Synonym: PCB-86, 2,2′,3,4,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5-pentachlorobiphenyl
CAS Registry No: 55312-69-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
100 (Mackay et al. 1980; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.181 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0098 (generator column-GC/ECD, Weil et al. 1974)
0.0349 (generator column-HPLC/UV, Huang 1983)
0.034 (generator column-HPLC, Billington et al. 1988)
0.00334, 0.00554, 0.00297, 0.00651 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00933 (quoted, Neely 1981)
0.051 (P_L calculated from P_S using fugacity ratio F, Neely 1981)
0.00643 (supercooled liquid P_L, Neely 1981)
0.000077 (calculated, Neely 1983; quoted, Erickson 1986)
0.00133, 0.00245, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0128 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00288 (supercooled liquid P_L, GC-RI correlations, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.61$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
84.1 (calculated-P/C, Burkhard et al. 1985b)
17.23 (calculated-MCI χ, Sabljic & Güsten 1989)
24.14 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.38 (Neely 1983; quoted, Erickson 1986)
7.49 (calculated-fragment const., Yalkowsky et al. 1983)
6.22 (calculated-TSA, Burkhard 1984)

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6.38 (calculated-π const., Woodburn et al. 1984)
6.20 (selected, Shiu & Mackay 1986)
6.44, 6.38, 6.43, 6.29 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.23 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.26 (calculated-MCI χ, Patil 1991)
6.39 (recommended, Sangster 1993)
6.325 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.97 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/air Partition Coefficient, log K_{OA}:
9.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
4.43 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)

Sorption Partition Coefficient, log K_{OC}:
6.02 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.770 (marine humic substances, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2 – 0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.3 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Biodegradation: microbial degradation with pseudo first-order rate constant k = 0.005 yr^{-1} in the water column and k = 0.05 yr^{-1} in the sediment (Furukawa et al. 1978; quoted, Neely 1981).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water: $t_{½}$ = 108 d in Lake Michigan (Neely 1983).
Groundwater:
Sediment:
Soil:
Biota:

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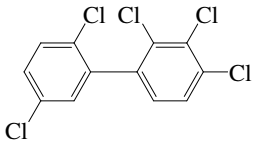
7.1.1.87 2,2′,3,4,5′-Pentachlorobiphenyl (PCB-87)



Common Name: 2,2′,3,4,5′-Pentachlorobiphenyl
Synonym: PCB-87, 2,2′,3,4,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5′-pentachlorobiphenyl
CAS Registry No: 38380-02-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
111.5–113 (Hutzinger et al. 1974; Erickson 1986)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.132 (Mackay et al. 1980)
0.138 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.022 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0045 (generator column-GC/ECD, Weil et al. 1974)
0.0294 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0082, 0.00783, 0.00543, 0.0070 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00226 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.000392 (GC-RI correlation, Burkhard et al. 1985a)
0.00141, 0.00262 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00261, 0.00248 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00116 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.10 – 4800/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0017, 0.00275(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4562/(T/K) + 12.66 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
33.44 (calculated, Murphy et al. 1983)
19.86 (calculated-P/C, Burkhard et al. 1985b)
24.81 (calculated-P/C, Shiu & Mackay 1986)
12.87 (20°C, calculated-P/C, Murphy et al. 1987)
18.24 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
7.50 (wetted-wall column-GC, Brunner et al. 1990)
18.61 (calculated-QSPR, Dunnivant et al. 1992)
5.966 (calculated-QSPR, Achman et al. 1993)

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37.71 ± 0.69 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
12.97, 18.83, 26.86, 37.71, 49.80 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 8.9006 – 3909.07/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[– (32.5/kJ·mol^{-1})/ RT] + (0.074/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
36.5 (exptl. data, Bamford et al. 2002)
ln K_{AW} = $-\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 33 ± 4 kJ/mol, ΔS_H = 0.07 ± 0.01 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.85 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.30 (HPLC-RT correlation, Shaw & Connell 1982)
5.45, 6.37 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
6,63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.14, 6.23, 6.24, 6.27 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.36 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.23 (recommended, Sangster 1993)
6.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
9.96 (10°C, estimated, Thomas et al. 1998)
9.25 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:
4.43 (oyster, Vreeland 1974)
5.38; 6.91 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:
4.54 (Koch 1983)
6.07 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.88 (calculated, Bahnick & Doucette 1988)
4.761, 4.748 (marine humic substances of 5 mg/L DOC, selected, calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
4.76, 4.87, 4.85, 3.75 (marine humic substance in concentrations. of 5,10, 20, 40 mg/L DOC, reported as log K_h, Lara & Ernst 1989)
6.18 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.08 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.73 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted and selected, Baker et al. 2000)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.62 (soil, calculated-MCI, Sabljic et al. 1995)
5.02 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
6.00 (soil, calculated-K_{OW}, Girvin & Scott 1997)
5.80; 4.50 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Sorption Partition Coefficient, log K_{OM}:
4.50, 4.85 (selected, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:

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Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2 – 0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.3 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.0045 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 0.049 h^{-1}; k_2 = 0.013 h^{-1} (mayfly-sediment model II, Gobas et al. 1989)
k_1 = 3360 d^{-1}; k_2 = 0.0140 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.005 d^{-1} with $t_{½}$ = 154 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 195 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.027 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.57 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and k = 0.27 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: k = 0.00152 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00223 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and k = 0.0039 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).
Biota: $t_{½}$ = 155 d in rainbow trout and $t_{½}$ = 62 d its muscle (Niimi & Oliver 1983).
depuration $t_{½}$ = 154 d for high-dose treatment, $t_{½}$ = 195 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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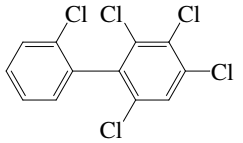
7.1.1.88 2,2′,3,4,6-Pentachlorobiphenyl (PCB-88)



Common Name: 2,2′,3,4,6-Pentachlorobiphenyl
Synonym: PCB-88
Chemical Name: 2,2′,3,4,6-pentachlorobiphenyl
CAS Registry No: 55215-17-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
100 (Mackay et al. 1980; Burkhard et al. 1985a; Opperhuizen et al. 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.182 (Mackay et al. 1980)

Water Solubility (g/m^3 or mg/L at 25°C):
0.012 (generator column-GC/ECD, Weil et al. 1974)
0.0129 (calculated-TSA, Mackay et al. 1980)
0.0385 (supercooled liquid S_L, calculated- TSA, Burkhard et al. 1985b)
0.00242 (calculated-fragment solubility constants, Wakita et al. 1986)
0.009 (calculated-MCI χ, Nirmalakhandan & Speece 1989)
0.0206 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI χ, Patil 1991)
0.00801 (calculated-group contribution, Kühne et al. 1995)
0.0124, 0.00472 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0265 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00309 (GC-RI correlation, Burkhard et al. 1985a)
0.0161 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00646 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4399/(T/K) + 12.53$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
136.8 (calculated-P/C, Burkhard et al. 1985b)
34.65 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
38.97 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)–see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.51 (calculated-fragment const., Yalkowsky et al. 1983)

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6.31 (calculated-TSA, Burkhard 1984)
6.07 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.26 (calculated-MCI χ, Patil 1991)
6.1452 (calculated-molecular properties, MNDO-AM1 method, Makino 1998)
6.84 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA}:
9.39 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
6.11 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.611 (marine humic substances, calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L of DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

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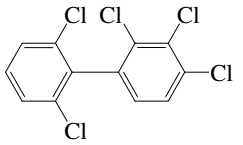
7.1.1.89 2,2′,3,4,6′-Pentachlorobiphenyl (PCB-89)



Common Name: 2,2′,3,4,6′-Pentachlorobiphenyl
Synonym: PCB-89, 2,2′,3,4,6′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,6′-pentachlorobiphenyl
CAS Registry No: 73575-57-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0382 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0542 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
4.82×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00522 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
41.64 (calculated-P/C, Burkhard 1984)
29.49 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
30.18 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
30.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 21 \pm 6$ kJ/mol, $\Delta S_H = 0.04 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (calculated-TSA, Burkhard 1984)
6.07 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.60 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.40 (calculated-TSA, Murray & Andren 1992)
5.60 (recommended, Sangster 1993)
5.8981 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.11 (suspended particulate matter, Burkhard 1984)

4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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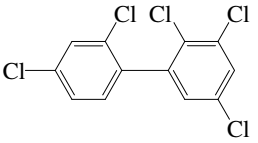
7.1.1.90 2,2′,3,4′,5-Pentachlorobiphenyl (PCB-90)



Common Name: 2,2′,3,4′,5-Pentachlorobiphenyl
Synonym: PCB-90, 2,2′,3,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5-pentachlorobiphenyl
CAS Registry No: 68194-07-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
67 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0375 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01344 (20°C, supercooled liquid S_L, Murphy et al. 1987)
0.00494 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00714 (calculated-group contribution method, Kühne et al. 1995)
0.00107, 0.00198 (generator column-GC/ECD, estimated, Hong & Qiao 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00375 (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 11.0 – 4740/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00347 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4522/(T/K) + 12.69, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
30.19 (calculated-P/C, Burkhard 1984)
39.11 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
29.83 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.32 (calculated-TSA, Burkhard 1984)
6.32 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988a)
6.36 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.32 (recommended, Sangster 1993)
6.339 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.92 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.12 (suspended particulate matter, Burkhard 1984)

4.66, 4.68, 4.75, 3.75 (marine humic substance in concentrations of 5,10, 20, 40 mg/L DOC, reported as log K_h, Lara & Ernst 1989)

4.659, 4.726 (marine humic substance, observed, calculated-MCI, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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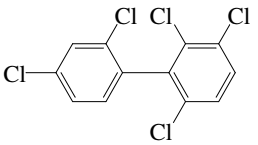
7.1.1.91 2,2′,3,4′,6-Pentachlorobiphenyl (PCB-91)



Common Name: 2,2′,3,4′,6-Pentachlorobiphenyl
Synonym: PCB-91, 2,2′,3,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,6-pentachlorobiphenyl
CAS Registry No: 58194-05-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0395 (20°C, supercooled liquid, Murphy et al. 1987)
0.0221 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00803 (GC-RI correlation, Burkhard et al. 1985b)
0.00487, 0.00667 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.32×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4650/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0038, 0.00589(supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4399/(T/K) + 12.44 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
73.16 (calculated-P/C, Burkhard 1984)
27.46 (20°C, calculated-P/C, Murphy et al. 1987)
35.78 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
12.16 (wetted-wall column-GC/ECD, Brunner et al. 1990)
35.05 (calculated-QSPR, Dunnivant et al. 1992)
9.03 (calculated-QSPR, Achman et al. 1993)
42.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
54.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 10 \pm 5$ kJ/mol, $\Delta S_H = 0.00 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
6.31 (calculated-TSA, Burkhard 1984)

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5.87 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.87 (recommended, Sangster 1993)
5.9623 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.07 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.11 (suspended particulate matter, Burkhard 1984)
4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 10 (food lipid mg)/(g worm lipid-d); k_2 = 0.08 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.08 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{½}$ = 166 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 217 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 8 d in earthworm given contaminated food (Wågman et al. 2001)
depuration $t_{½}$ = 166 d for high-dose treatment, $t_{½}$ = 217 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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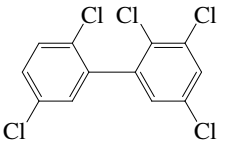
7.1.1.92 2,2′,3,5,5′-Pentachlorobiphenyl (PCB-92)



Common Name: 2,2′,3,5,5′-Pentachlorobiphenyl
Synonym: PCB-92, 2,2′,3,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,5′-pentachlorobiphenyl
CAS Registry No: 52663-61-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
53 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0379 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00494 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.92×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00422, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00394, 0.00458 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P/mmHg) = 11.0 – 4740/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00302, 0.00447 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4522/(T/K) + 12.76 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
33.64 (calculated-P/C, Burkhard 1984)
32.63 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
26.35 (calculated-QSPR, Dunnivant et al. 1992)
5.97 (calculated-QSPR, Achman et al. 1993)
28.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
48.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 6$ kJ/mol, $\Delta S_H = 0.05 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.05, 6.97 (RP-HPLC-k′ correlation:uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.32 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.11 (generator column-GC, Larsen et al. 1992)
6.32 (recommended, Sangster 1993)
6.97 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA}:

8.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.11 (suspended particulate matter, Burkhard 1984)

4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d^{-1} with $t_{½}$ = 135 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 141 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 135 d for high-dose treatment, $t_{½}$ = 141 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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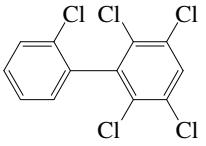
7.1.1.93 2,2′,3,5,6-Pentachlorobiphenyl (PCB-93)



Common Name: 2,2′,3,5,6-Pentachlorobiphenyl
Synonym: PCB-93, 2,2′,3,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,6-pentachlorobiphenyl
CAS Registry No: 73575-56-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
91 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0411 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0149, 0.0164, 0.00986, 0.0119 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0151 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.0160, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00708 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4399/(T/K) + 12.57$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
120.6 (calculated-P/C, Burkhard 1984)
28.78 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
34.49 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
5.99, 6.06, 6.07, 6.12 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.06 (recommended, Sangster 1993)
6.1176 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.09 (suspended particulate matter, Burkhard 1984)

4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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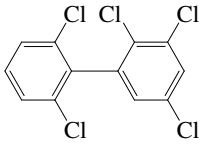
7.1.1.94 2,2′,3,5,6′-Pentachlorobiphenyl (PCB-94)



Common Name: 2,2′,3,5,6′-Pentachlorobiphenyl
Synonym: PCB-94
Chemical Name: 2,2′,3,5,6′-pentachlorobiphenyl
CAS Registry No: 73575-55-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
79 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
7.24×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00774, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
70.62 (calculated-P/C, Burkhard 1984)
43.98 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.69 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.36 (calculated-TSA, Burkhard 1984)
6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.0371 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.16 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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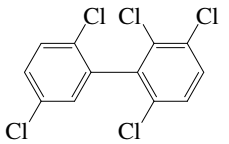
7.1.1.95 2,2′,3,5′,6-Pentachlorobiphenyl (PCB-95)



Common Name: 2,2′,3,5′,6-Pentachlorobiphenyl
Synonym: PCB-95, 2,2′,3,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5′,6-pentachlorobiphenyl
CAS Registry No: 38379-99-6
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
98.5–100 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.184 (mp at 100°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0336 (supercooled liquid S_L, calculated-TSA, Burkhard 1985b)
0.0541 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0291, 0.0216, 0.0192, 0.0156; 0.021 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0259 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI χ, Patil 1991)
0.00190 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00735, 0.00905, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00849 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00537, 0.00744 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00335 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 10.90 – 4650/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00427, 0.00741 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4399/(T/K) + 12.48 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
0.00295 (20°C, supercooled liquid P_L, from Falconer & Bidleman 1994; Harner & Bidleman 1996)
0.00211 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
82.78 (calculated-P/C, Burkhard 1985b)
20.06 (20°C, calculated-P/C, Murphy et al. 1987)
29.38 (calculated-molecular connectivity indices χ, Sabljic & Güsten 1989)
30.39 (calculated-QSPR, Dunnivant et al. 1992)
30.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 21 \pm 5$ kJ/mol, $\Delta S_H = 0.04 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

5.18 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
5.67, 5.98, 5.86, 6.05 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.08 (generator column-GC, Larsen et al. 1992)
5.92 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

9.06 (20°C, generator column-GC, measured range – 10 to 30°C, Harner & Bidleman 1996)
10.51, 9.06, 9.51, 9.06, 8.55 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
log K_{OA} = – 4.30 + 3904/(T/K); temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = – 5.84 + 4360/(T/K); (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
8.80 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
10.07, 9.06; 9.07 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.04 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.3–6.8, 6.1; 7.40 (suspended sediment, average; algae > 50 μm, Oliver 1987a)
6.30 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.60, 4.66, 4.61, 3.70 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
4.603, 4.589 (marine humic substances, observed; calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L DOC, Sabljic et al. 1989)
5.68, 5.70, 5.64 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.55 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.00030 h^{-1}; k_2 = 0.184 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_2 = 0.004 d^{-1} with $t_{½}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 225 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

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Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{½}$ = 8.29 min when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 164 d for high-dose treatment, $t_{½}$ = 225 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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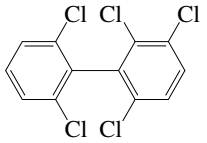
7.1.1.96 2,2′,3,6,6′-Pentachlorobiphenyl (PCB-96)



Common Name: 2,2′,3,6,6′-Pentachlorobiphenyl
Synonym: PCB-96
Chemical Name: 2,2′,3,6,6′-pentachlorobiphenyl
CAS Registry No: 73575-54-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
53 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0368 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0157 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00166, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
139.8 (calculated-P/C, Burkhard 1984)
38.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
41.56 (calculated-QSPR, Dunnivant et al. 1992)
62.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 15 \pm 3$ kJ/mol, $\Delta S_H = 0.02 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.33 (calculated-TSA, Burkhard 1984)
5.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
5.5365 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:
8.77 (20°C, generator column-GC/ECD, measured range –10 to 30°C, Harner & Bidleman 1996)
10.28, 9.72, 9.22, 8.77, 8.30 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
log $K_{OA} = -4.60 + 3913/(T/K)$, temp range –10 to 30°C (Harner & Bidleman 1996)
9.87, 8.79; 8.76 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
8.82 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.13 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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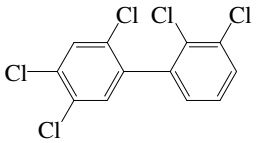
7.1.1.97 2,2′,3,4′,5′-Pentachlorobiphenyl (PCB-97)



Common Name: 2,2′,3,4′,5′-Pentachloro
Synonym: PCB-97
Chemical Name: 2,2′,3′,4,5-pentachlorobiphenyl
CAS Registry No: 41464-51-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
82 (Burkhard et al. 1984b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.77 (quoted, Shiu & Mackay 1986)
Fugacity Ratio at 25°C, F:
0.279 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0431 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0284 (20°C, supercooled liquid, Murphy et al. 1987)
0.00622, 0.00651, 0.00383, 0.00682 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0099 (literature average, Paya-Perez et al. 1991)
0.00847 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.01×10^{-3}, 8.05×10^{-4}, 8.04×10^{-4} (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00251, 0.00265 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.31×10^{-3} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.10 – 4790/(T/K) (GC-RT correlation, Tateya et al. 1988)
1.85×10^{-3}, 2.88×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4522/(T/K) + 12.56 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.0026 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
20.67 (calculated-P/C, Burkhard 1984)
15.1 (20°C, calculated-P/C, Murphy et al. 1987)
18.14 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)
18.23 (calculated-QSPR, Dunnivant et al. 1992)

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23.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
45.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 6$ kJ/mol, $\Delta S_H = 0.07 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.75, 6.67 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.25, 6.33, 6.35, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.31 (recommended, Sangster 1993)
6.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
10.49, 9.44 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.21 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:
5.43; 6.96 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:
6.07 (suspended particulate matter, Burkhard 1984)
4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)
5.83, 5.89, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.69 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.10 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 3400$ d^{-1}; $k_2 = 0.0126$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.004$ d^{-1} with $t_{½} = 163$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 188$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

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Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 163 d for high-dose treatment, $t_{½}$ = 188 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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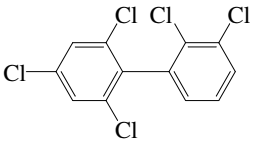
7.1.1.98 2,2′,3,4′,6′-Pentachlorobiphenyl (PCB-98)



Common Name: 2,2′,3,4′,6′-Pentachlorobiphenyl
Synonym: PCB-98
Chemical Name: 2,2′,3,4′,6′-pentachlorobiphenyl
CAS Registry No: 60233-25-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
268.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0333 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0153, 0.0116, 0.0124 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.05×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00753, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00615, 0.00751 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00692 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4399/(T/K) + 12.54$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
68.90 (calculated-P/C, Burkhard 1984)
50.26 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.69 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.36 (calculated-TSA, Burkhard 1984)
5.98, 6.16, 5.99 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.071 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, Burkhard 1984)

4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.005 d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 153 d for high-dose treatment, $t_{½}$ = 164 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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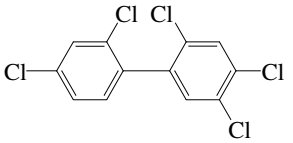
7.1.1.99 2,2′,4,4′,5-Pentachlorobiphenyl (PCB-99)



Common Name: 2,2′,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-99, 2,2′,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,5-pentachlorobiphenyl
CAS Registry No: 38380-01-7
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
81.0 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0353 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0222 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00366 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0103 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI χ, Patil 1991)
0.00597 (estimated-EPIWIN v3.04, Hardy 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0029 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
0.00735, 0.00342, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00316 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
0.00328, 0.00375 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00147 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.0 – 4740/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.0024, 0.00347 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4533/(T/K) + 12.68 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
0.00229 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.000293 (estimated-EPIWIN v3.04, Hardy 2002)

Henry's Law Constant (Pa m^3/mol at 25°C):
29.28 (calculated-P/C, Burkhard et al. 1985b)
21.68 (20°C, calculated-P/C, Murphy et al. 1987)
30.50 (calculated-QSAR MCI χ, Sabljic & Güsten 1989)
7.90 (wetted-wall column-GC/ECD, Brunner et al. 1990)
57.0 (calculated-QSPR, Dunnivant et al. 1992)
9.39 (estimated-bond method EPIWIN v3.04, Hardy 2002)
35.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
51.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 16 ± 6 kJ/mol, ΔS_H = 0.02 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.29, 7.21 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.41 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
6.39 (calculated-TSA, Hawker & Connell 1988a)
6.26 (calculated-MCI χ, Patil 1991)
6.41 (recommended; Sangster 1993)
7.21 (recommended, Hansch et al. 1995)
6.60, 6.26–7.21 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
6.4014 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.9795 (estimated-EPIWIN v3.04, Hardy 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.38 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.09 (fish, microcosm, Garten & Trabalka 1983)
5.14 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

6.14 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.73 (marine humic substance, calculated-MCI χ, reported as log K_h at 5 mg /L DOC, Sabljic et al. 1989)
7.00 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.68 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.54 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.10 (soil, calculated-K_{OW}, Girvin & Scott 1997)
4.87 (estimated-EPIWIN v3.04, Hardy 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 0.6419 d from river, $t_{½}$ = 13.31 d from lake (estimated-EPIWIN v3.04, Hardy 2002).
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 8 (food lipid mg)/(g worm lipid-d); k_2 = 0.07 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.003 d^{-1} with $t_{½}$ = 2252 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

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Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: volatilization $t_{½}$ = 0.6419 d from river, $t_{½}$ = 13.31 d from lake (estimated-EPIWIN v.3.04, Hardy 2002).

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 9 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{½}$ = 252 d for high-dose treatment, $t_{½}$ = 172 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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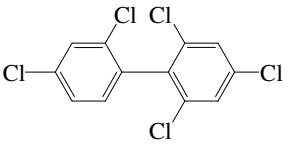
7.1.1.100 2,2′,4,4′,6-Pentachlorobiphenyl (PCB-100)



Common Name: 2,2′,4,4′,6-Pentachlorobiphenyl
Synonym: PCB-100, 2,2′,4,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,6-pentachlorobiphenyl
CAS Registry No: 39485-83-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
95 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0275 (supercooled liq. S_L, calculated-TSA, Burkhard et al. 1985b)
0.031 (unpublished data of Weil 1978; quoted, Kilzer et al. 1979; Geyer et al. 1980)
0.00666, 0.00580, 0.00941 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.011 (calculated-MCI χ, Patil 1991)
0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.00735, 0.00872, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al 1985a)
0.00818 (supercooled liquid, GC-RT correlation, Burkhard et al. 1985b; quoted, Eisenreich 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
97.27 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
62.62 (calculated-MCI χ, Sabljic & Güsten 1989)
56.98 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.23, 6.37, 6.08 (RP-HPLC-RI correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.23 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:
8.66 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:
1.11, 1.06 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
0.32 (rodent, Garten & Trabalka 1983)
4.06, 3.91 (algae, calculated, Geyer et al. 1984)
4.06, 3.37, 4.44 (algae, fish, activated sludge, Freitag et al. 1984,1985; quoted, Halfon & Reggiani 1986)

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Sorption Partition Coefficient, log K_{OC}:

6.24 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

4.567 (marine humic substance, calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.010 d^{-1} (10°C, sandworm, Goerke & Ernst 1977; quoted, Waid 1986)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

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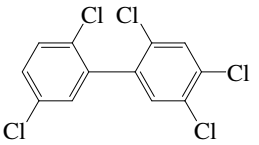
7.1.1.101 2,2′,4,5,5′-Pentachlorobiphenyl (PCB-101)



Common Name: 2,2′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-101, 2,2′,4,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 37680-72-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
78.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.56 (Miller et al. 1984)
53.7, 65.6 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C, F:
0.318 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)
0.0321 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.031 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)
0.0103 (shake flask-GC/ECD, Haque & Schmedding 1975; Chiou et al. 1977)
0.0042 (generator column-GC/ECD, Weil et al. 1974)
0.019 (shake flask-LSC, Metcalf et al. 1975)
0.010 (24°C, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)
0.00424 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
0.0005; 0.004 (generator column-HPLC/UV; RP-HPLC-RT correlation, Swann et al. 1983)
0.0194 (generator column-GC/ECD, Miller et al. 1984, 1985)
0.0356 (supercooled liquid P_L, calculated-TSA, Burkhard et al. 1985b)
0.0154* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
ln x = –3837/(T/K) – 8.0159, temp range 4–32°C, ΔH_{ss} = 31.9 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
log x = – 1664/(T/K) – 3.478, ΔH_{ss} = 31.8 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
S/(mol/L) = 1.54×10^{-10} exp(0.046·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
0.011 (shake flask-GC/ECD, Chiou et al. 1986, 1991)
0.0263 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00402, 0.00517, 0.0070, 0.0070 (RP-HPLC-k′ correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00674; 0.0222(generator column-GC/ECD, supercooled liquid S_L, Dunnivant & Elzerman 1988)
log [S_L/(mol/L)] = 0.875 – 982.6/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln x = – 8.026 – 3836.44/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

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0.0334 (calculated-mp and K_{OW}, Ran et al. 2002)
0.0312, 0.0333 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -1113/(T/K) - 0.27$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0016 (P_S from GC-RT correlation, Westcott & Bidleman 1981)
0.00096, 0.00173 (solid P_S: 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
$\log (P/\text{mmHg}) = 11.1 - 4840/(T/K)$; temp range 30–40°C (gas saturation-GC, Westcott et al. 1981)
0.0031 (P_L calculated from P_S using fugacity ratio F, Westcott & Bidleman 1981)
0.0053, 0.00316 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.00315 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.00336, 0.00402 (supercooled liquid P_L, calculated from P_{GC}, GC-RT correlation, different stationary phases, Bidleman 1984)
0.00358 (supercooled liquid P_L, GC-RT correlation, Burkhard 1984, Burkhard et al. 1985b)
0.00225, 0.00118, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00361, 0.00403 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00109; 0.0035 (selected solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
0.00142 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00359 (supercooled liquid P_L, Dunnivant & Elzerman 1988)
0.000527; 0.00173 (calculated-S × HLC, solid P_S; supercooled liquid P_L, Dunnivant & Elzerman 1988)
$\log (P/\text{mmHg}) = 11.0 - 4750/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
0.00152 (calculated-UNIFAC group contribution, Banerjee et al. 1990)
0.00315, 0.00296 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.00504, 0.0034 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log (P_L/\text{Pa}) = 12.13 - 4369/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
0.00257, 0.00398 (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -4514/(T/K) + 12.67$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
1.86×10^{-3} (supercooled liquid P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
1.33×10^{-4}, 4.16×10^{-4} (solid, supercooled liquid, Passivirta et al. 1999)
$\log (P_S/\text{Pa}) = 15.47 - 5495/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa}) = 12.67 - 4514/(T/K)$ (liquid, Passivirta et al. 1999)
$(4.04–22.5) \times 10^{-4}$; $(1.46–40.4) \times 10^{-3}$ (literature solid P_S range; literature liquid P_L range, Delle Site 1997)
0.0020 (supercooled P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
0.0024, 0.00245 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/\text{Pa} = -4632/(T/K) + 12.92$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
$\log P_L/\text{Pa} = -4346/(T/K) + 11.94$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
11.46–35.46 (calculated-P/C, Westcott et al. 1981)
32.73 (calculated-P/C, Burkhard et al. 1985b)
7.09 (20°C, gas stripping-GC, Oliver 1985)
35.48 (calculated-P/C, Shiu & Mackay 1986)
18.14 (20°C, calculated-P/C, Murphy et al. 1987)
25.43 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
47.19 (calculated-QSAR-χ, Sabljic & Güsten 1989)
9.12 (wetted-wall column-GC/ECD, Brunner et al. 1990)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
1.424, 4.166 (0, 15°C, from modified two-film model, Hornbuckle et al. 1994)
$\log H$ (Pa m^3/mol) $= 13.55 - 3531/(T/K)$ (Passivirta et al. 1999)
42.07* ± 0.70 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 7.9384 - 3572.29/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(29.7/\text{kJ·mol}^{-1})/RT + (0.066/\text{kJ·mol}^{-1}\text{·K}^{-1})/R]$; where $R = 8.314$ J·K^{-1}·mol^{-1} and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)

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43.2 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
31.62, 24.0 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = – 3233/(T/K) + 12.21 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
4.12 (radiolabeled-^{14}C, Metcalf et al. 1975)
6.11 (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)
7.64 (Hansch & Leo 1979)
6.44 (HPLC-RT correlation, Veith et al. 1979)
6.85 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.42 (HPLC-RT correlation, Swann et al. 1983)
5.92 (generator column-GC/ECD, Miller et al. 1984)
6.15, 7.07 (RP-HPLC-k′ correlation, Rapaport & Eisenreich 1984)
7.64 (HPLC-RT correlation, Woodburn et al. 1984)
6.50 (generator column-HPLC, Woodburn et al. 1984)
6.88, 7.0 (HPLC-k′ correlation, calculated, De Kock & Lord 1987)
6.50 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
6.36, 6.39, 6.18, 6.27 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.88 (HPLC-RT correlation, Doucette & Andren 1988)
6.23, 6.18 (RP-HPLC-k′ correlation, different stationary phases, Sherblom & Eganhouse 1988)
6.41 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.16 (recommended, Sangster 1993)
6.50 (recommended, Hansch et al. 1995)
6.15, 6.33 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.
8.30 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
9.31* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = – 3.82 + 3841/(T/K); temp range –10 to 30°C (generator Column-GC, Harner & Bidleman 1996)
8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = – 5.84 + 4360/(T/K) (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
9.79 (10°C, estimated, Thomas et al. 1998)
10.49, 9.44; 9.29 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.37 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.14; 9.05 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
8.90, 8.73 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4291/(T/K) – 5.50 (LDV linear regression of literature data, Li et al. 2003)
log K_{OA} = 3785/(T/K) – 5.35 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:
3.18 (green sunfish, 15 d in static water, Sanborn et al. 1975)
3.74, 4.78, 4.08, 4.24 (algae, snail, fish, mosquito, Metcalf et al. 1975)
4.66 (fish, flowing water, Kenaga & Goring; Kenaga 1980)
3.92, 3.60 (calculated-S, calculated-K_{OC}, Kenaga 1980)
4.09 (fish, microcosm, Garten & Trabalka 1983)
3.30–4.15 highest value, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
> 5.40, 4.15; 6.92 (rainbow trout, laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
2.73, 2.60 (human fat of lipid, wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
4.15 (fish, quoted, Isnard & Lambert 1988)

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6.55 (rainbow trout, lipid basis, Noegrohati & Hammers 1992)
5.47; 7.00 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.32–5.15 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.84–6.26 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.06, 6.06 (*Daphnia*, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.47, 7.0 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.10, 7.02 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.03; 3.98 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d
5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:
4.63 (Kenaga & Goring 1980)
4.74, 4.80 (estimated-S, K_{OW}, Lyman 1982)
5.13, 4.67 (estimated-BCF, Lyman 1982)
4.70; 5.45 (soil, slurry method; HPLC-RT correlation, Swann et al. 1983)
6.14 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.60; 5.50; 6.60 (field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
5.65 (suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
6.68, 5.58 (suspended solids-Lake Superior: calculated-K_{OW}, Baker et al. 1986)
4.87, 4.07 (Sanhedron soil, Suwannee River, humic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
4.12, 4.10 (Sanhedron soil, Suwannee River, fulvic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
5.1–6.7, 6.2 (suspended sediment, average, Oliver 1987a)
5.41, 5.41, 4.81, 4.09, 4.01 (Aldrich humic acid Na salt, Fluka-Tridon humic acid, Calcasieu River humic extract, Suwannee River water sample, Sopchoppy River water sample, Chiou et al. 1987)
6.25 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.77, 4.86, 4.80, 3.86 (humic substances, in concentrations. of 5, 10, 20, 40 mg C/L, reported as log K_h, Lara & Ernst 1989)
4.772, 4.726 (marine humic substances of 5 mg/L DOC, reported as association coefficient log K_h, quoted exptl; calculated-MCI χ, Sabljic et al. 1989)
5.86 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.58 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.81, 5.83, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.67 (soil, shake flask-GC, Paya-Perez et al. 1991)
5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
4.63 (soil, Sabljic et al. 1995)
5.80; 5.58 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.90; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
5.73 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)
4.78–7.03; 4.60–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.59; 6.19, 5.53, 6.04 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:
4.63, 4.84 (quoted, calculated-molecular connectivity indices χ, Sabljic 1984)

Sorption Partition Coefficient, log K_P:
4.87–5.35 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

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Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photodegradation rate constants k = (0.20 ± 0.01) h^{-1}, (0.20 ± 0.04) h^{-1}, with $t_{½}$ = 3.4 h, 3.7 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(aq.) = 4.6 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: degradation rate, k = 1.5 × 10^{-8} nmol $cell^{-1}$ h^{-1} by species of Alcaligenes and Acinetobacter (Furukawa et al. 1978, selected, NAS 1979);

85% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986);

aerobic biodegradation $t_{½}$ = 1.32 d with the addition of polymer chitin, $t_{½}$ = 0.80 d with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 > 0.0007 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

k_1 = 180 d^{-1}; k_2 = 0.0007 d^{-1} (rainbow trout, Oliver & Niimi 1985)

k_1 = 0.049 h^{-1}; k_2 = 0.014 h^{-1} (mayfly-sediment model II, Gobas et al. 1989)

log $1/k_2$ > 3.1, 3.6 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b).

k_1 = 3850 d^{-1}; k_2 = 0.0130 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.054 d^{-1} with an elimination $t_{½}$ = 12.9 d (earthworm, Belfroid et al. 1995)

k_2 = 0.005 d^{-1} with $t_{½}$ = 131 d and k_2 = 0.012 d^{-1} with $t_{½}$ = 56 d for food concn of 20 ng/g and 148 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_1 = 0.00082 h^{-1}; k_2 = 0.160 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1(calc) = 6 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.06 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.003 d^{-1} with $t_{½}$ = 246 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995);

suggested $t_{½}$ = 3000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: aerobic biodegradation $t_{½}$ = 1.32 d with the addition of polymer chitin, $t_{½}$ = 0.80 d with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990);

half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

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photodegradation $t_{½}$ = (3.4 ± 015) h, (3.7 ± 0.8) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995);

$t_{½}$ = 60000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: k = 0.039 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.65 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.54 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.24 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are k = 0.00064 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, k = 0.00188 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, k = 0.00073 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and k = 0.00247 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

$t_{½}$ = 87600 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{½}$ 1000 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{½}$ = 85 d in its muscle, (Niimi & Oliver 1983);

elimination $t_{½}$ = 12.9 from earthworm (Belfroid et al. 1995)

depuration $t_{½}$ = 56–131 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$t_{½}$ = 4.3 h in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination $t_{½}$ = 12 d in earthworm given contaminated food (predicted, Wågman et al. 2001).

depuration $t_{½}$ = 172 d for high-dose treatment, $t_{½}$ = 24446 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.101.1
Reported aqueous solubilities, vapor pressures, Henry's law constants and octanol-air partition coefficients of 2,2′,4,5,5′-pentachlorobiphenyl (PCB-101) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure		Henry's law constant		log K_{OA}	
Dickhut et al. 1986		Westcott et al. 1981		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas saturation-GC		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
4	0.0061	25	0.00096	4	15.75	–10	10.70
20	0.0121	30	0.00173	11	22.20	0	10.31
25	0.0154			18	30.78	10	9.78
32	0.0223			25	42.07	20	9.31
		log P/mmHg = A – B/(T/K)		31	54.40	30	8.78
ln *x* = A – B/(T/K)		A	11.1				
A	–8.0159	B	4840	ln K_{AW} = –ΔH/RT + ΔS/R		ΔH_{OA}/(kJ mol^{-1}) = 73.54	
B	3836.90	temp range 30–40°C		A	7.9384		
				B	3572.3	log K_{OA} = A + B/T	
ΔH_{sol}/(kJ mol^{-1}) = 31.9 ±1.9						A	–3.82
for 4–32°C				enthalpy, entropy change:		B	3841
				ΔH/(kJ·mol^{-1}) = 29.7 ± 3.2			
				ΔS/(J·mol^{-1}·K^{-1}) = 66 ± 10			

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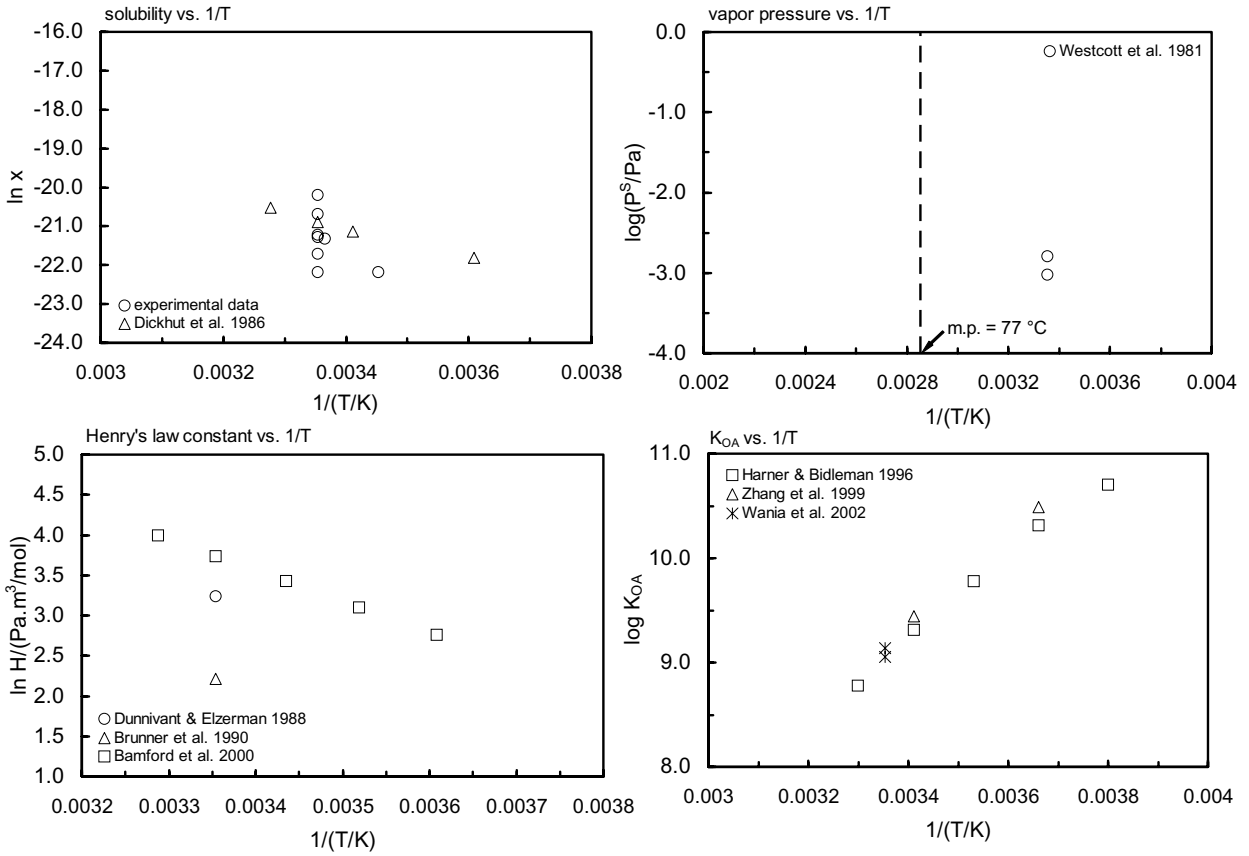

FIGURE 7.1.1.101.1 Logarithm of mole fraction solubility, vapor pressure, Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,4,5,5′-pentachlorobiphenyl (PCB-101).

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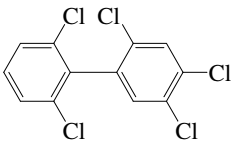
7.1.1.102 2,2′,4,5,6′-Pentachlorobiphenyl (PCB-102)



Common Name: 2,2′,4,5,6′-Pentachlorobiphenyl
Synonym: PCB-102, 2,2′,4,5,6′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5,6′-pentachlorobiphenyl
CAS Registry No: 68194-06-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
93 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0314 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0065 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.61×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00706, 0.00184 (calculated-MW, GC-RI correlation, calculated-χ, Burkhard et al. 1985b)
0.00527, 0.00667 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P/mmHg) = 10.80 – 4630/(T/K) (GC-RT correlation, Tateya et al. 1988)
log (P_L/Pa) = – 4399/(T/K) + 12.48 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
68.60 (calculated-P/C, Burkhard 1984)
35.26 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
9.12 (wetted-wall column-GC/ECD, Brunner et al. 1990)
37.6 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (calculated-TSA, Burkhard 1984)
6.16 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.0959 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.13 (calculated-QSPR/quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.19 (suspended particulate matter, Burkhard 1984)

4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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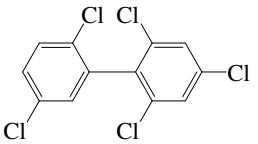
7.1.1.103 2,2′,4,5′,6-Pentachlorobiphenyl (PCB-103)



Common Name: 2,2′,4,5′,6-Pentachlorobiphenyl
Synonym: PCB-103, 2,2′,4,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,5′,6-pentachlorobiphenyl
CAS Registry No: 60145-21-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0275 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00986, 0.00859, 0.0164, 0.0113 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.23×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00983, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00887, 0.0112 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00617 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4399/(T/K) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
109.43 (calculated-P/C, Burkhard 1984)
56.24 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
51.02 (calculated-QSPR, Dunnivant et al. 1992)
51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.44 (calculated-TSA, Burkhard 1984)
6.11, 6.25, 5.92, 6.14 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.22 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.11 (recommended, Sangster 1993)
8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.1499 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.24 (suspended particulate matter, Burkhard 1984)

4.567 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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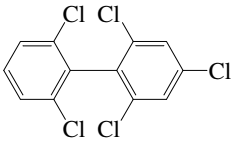
7.1.1.104 2,2′,4,6,6′-Pentachlorobiphenyl (PCB-104)



Common Name: 2,2′,4,6,6′-Pentachlorobiphenyl
Synonym: PCB-104, 2,2′,4,6,6′-pentachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,6,6′-pentachlorobiphenyl
CAS Registry No: 56558-16-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
85.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.258 (mp at 85°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.030 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0156 (generator column-GC, Dunnivant & Elzerman 1988)
0.0411 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.00986 (calculated-group contribution method, Kühne et al. 1995)
0.00651, 0.0175 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.0666 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C):
0.017 (supercooled liquid P_L, Burkhard 1984)
0.00735, 0.018, 0.00419 (supercooled liquid P_L, calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.0170 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00434 (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
0.00434 (calculated-S × HLC, solid P_S, Dunnivant & Elzerman 1988)
0.00225 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
185.4 (calculated-P/C, Burkhard et al. 1985b)
90.9 (gas stripping, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
55.4 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
75.11 (calculated-QSPR, Dunnivant et al. 1992)
39.40, 47.17, 56.0, 66.0* ± 1.4, 75.50 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 2.1650 - 1774.05/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(14.5/kJ{\cdot}mol^{-1})/RT] + (0.018/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where R = 8.314 $J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
62.0 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 15 \pm 3$ kJ/mol, $\Delta S_H = 0.02 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.40 (calculated-TSA, Burkhard 1984)
5.37 (generator column-GC, Hawker & Connell 1988a; quoted, Sangster 1993)
5.81 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.61 (calculated-Characteristic Root Index CRI, Saçan & Inel 1995)
5.7636 (calculated-molecular properties MNDO-AM1, Makino 1998)
5.96 (calculated-QSPR, Yeh & Hong 2002)
6.59 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

8.46 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.20 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.431 (marine humic substances, reported as association coefficient log K_h at 5 mg L^{-1} DOC, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 > 0.0007 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 6 (food lipid mg)/(g worm lipid-d); k_2 = 0.10 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ > 1000 d in rainbow trout, and $t_{½}$ = 101 d in its muscle (Niimi & Oliver 1983);
elimination $t_{½}$ = 7 d in earthworm given contaminated food (Wågman et al. 2001)

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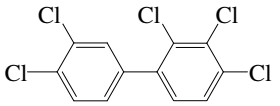
7.1.1.105 2,3,3′,4,4′-Pentachlorobiphenyl (PCB-105)



Common Name: 2,3,3′,4,4′-Pentachlorobiphenyl
Synonym: PCB-105, 2,3,3′,4,4′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′-pentachlorobiphenyl
CAS Registry No: 32598-14-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
103 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, assuming ΔS_{fus} = 56 J/mol K, F: 0.164 (at mp 103°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0405 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00236, 0.0119, 0.00636, 0.00517 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00190 (calculated-QSPR, Dunnivant et al. 1992)
0.000982, 0.00190(generator column-GC/ECD, estimated, Hong & Qiao 1995)
0.00166* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
0.0362, 0.08243(supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log $[S_L/(\text{mol m}^{-3})]$ = – 1285/(T/K) + 0.18 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.7×10^{-4}, 9.35×10^{-4} (supercooled liquid P_L by GC-RT correlation, different stationary phases, Bidleman 1984)
7.07×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00124, 0.000132, 0.000233 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
8.85×10^{-4}, 6.77×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.62×10^{-4}, 7.76×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4758/(T/K) + 12.90 (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
6.76×10^{-4} (supercooled liquid P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
2.54×10^{-3} (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)
8.71×10^{-4}, 1.23×10^{-3} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = – 4554/(T/K) + 12.29 (supercooled liquid P_L, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
5.68 (calculated-P/C, Burkhard 1985a)
6.08 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
10.06 (calculated-QSPR, Dunnivant et al. 1992)
2.43 (calculated-QSPR, Achman et al. 1993)

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33.6* ± 1.3 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln K_{AW} = 26.221 – 9093.1/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
K_{AW} = exp[–(75.6/kJ·mol^{-1})/ RT] + (0.218/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
33.9 (exptl. data, Bamford et al. 2002)
ln K_{AW} = – ΔH_H/RT + ΔS_H/R; R is the ideal gas constant, ΔH_H = 76 ± 8 kJ/mol, ΔS_H = 0.22 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
33.88, 13.80 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log H/(Pa m^3/mol) = –3269/(T/K) + 12.1 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:
6.41, 6.68, 7.14, 6.93 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.82 (generator column-GC; Hawker & Connell 1988a)
6.79 (recommended, Sangster 1993)
6.65 (recommended, Hansch et al. 1995)
4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)
6.61 (generator column-GC/ECD, Yeh & Hong 2002)
6.61, 6.82 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
10.27* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = – 5.68 + 4678/(T/K); (temp range –10 to 30°C, Harner & Bidleman 1996)
11.41, 10.20; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4630/(T/K) – 6.0 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF or log K_B:
2.82–4.26 (various marine species, mean dry weight, Hope et al. 1998)

Sorption Partition Coefficient, log K_{OC}:
6.09 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.906 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)
5.81 (soil, shake flask-GC, Paya-Perez et al. 1991)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 molecule^{-1} s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

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$k_2 = 0.014\ d^{-1}$ with $t_{½} = 48$ d and $k_2 = 0.014\ d^{-1}$ with $t_{½} = 50$ d for food concn of 17 ng/g and 133 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 181$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003\ d^{-1}$ with $t_{½} = 204$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment: $t_{½} = 7$ yr (Geyer et al. 2000)

Soil:

Biota: reported biological $t_{½} = 155$ to > 1000 d for trout, $t_{½} = 62$–101 d for trout muscle; $t_{½} = 73$ to > 200 d for carp for pentachlorobiphenyls (Niimi 1987)

Depuration $t_{½} = 49$–50 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½} = 181$ d for high-dose treatment, $t_{½} = 204$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.105.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,3,3′,4,4′-pentachlorobiphenyl (PCB 105) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	$S/g \cdot m^{-3}$	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	5.58×10^{-4}	4	3.09	–10	12.12
15	8.89×10^{-4}	11	7.10	0	11.43
25	1.66×10^{-3}	18	15.73	10	10.84
35	2.98×10^{-3}	25	33.6	20	10.27
		31	62.5	30	9.77
$\ln x = A - B/(T/K)$					
mole fraction x		$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 89.57$	
A		A	26.2208		
B	$\Delta H_{sol}/R$	B	9093.1	$\log K_{OA} = A + B/T$	
				A	–5.68
mp/°C	116.5–117.5	enthalpy, entropy change:		B	4678
$\Delta H_{sol}/(kJ\ mol^{-1}) = 40.1$		$\Delta H/(kJ \cdot mol^{-1}) = 75.6 \pm 8.4$			
		$\Delta S/(J \cdot mol^{-1} \cdot K^{-1}) = 218 \pm 28$			

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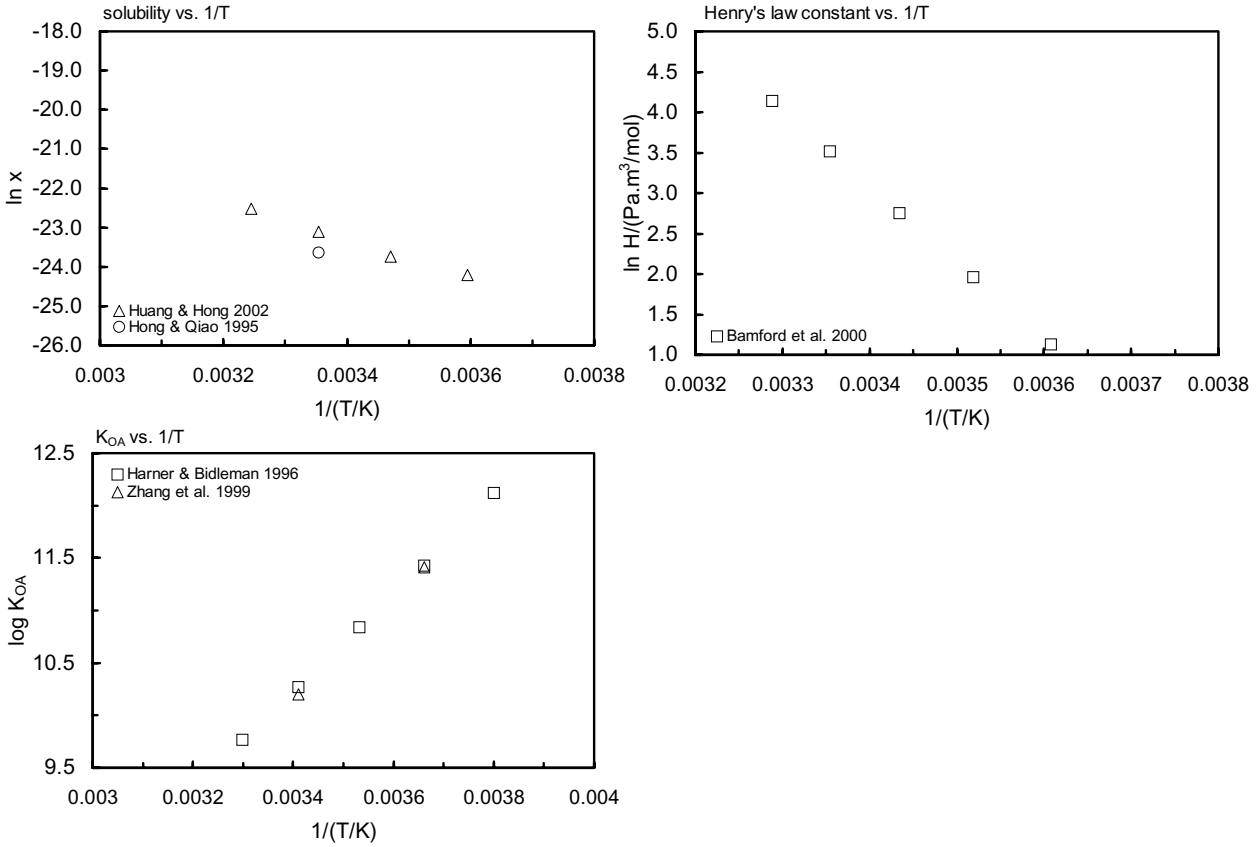

FIGURE 7.1.1.105.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,3,3′,4,4′-pentachlorobiphenyl (PCB-105).

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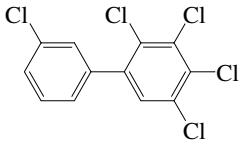
7.1.1.106 2,3,3′,4,5-Pentachlorobiphenyl (PCB-106)



Common Name: 2,3,3′,4,5-Pentachlorobiphenyl
Synonym: PCB-106, 2,3,3′,4,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5-pentachlorobiphenyl
CAS Registry No: 70424-69-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
105 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0411 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0082, 0.0088, 0.00517, 0.0058 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0050 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.0180, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00138, 0.00127 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4688/(T/K) + 12.86$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
39.82 (calculated-P/C, Burkhard 1984)
19.66 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
16.7 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
6.79, 6.79, 7.22, 6.89 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.64 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.92 (recommended, Sangster 1993)
6.6213 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.09 (suspended particulate matter, Burkhard 1984)

4.906 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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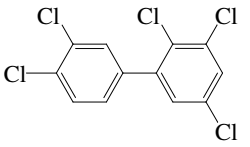
7.1.1.107 2,3,3′,4′,5-Pentachlorobiphenyl (PCB-107)



Common Name: 2,3,3′,4′,5-Pentachlorobiphenyl
Synonym: PCB-107, 2,3,3′,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5-pentachlorobiphenyl
CAS Registry No: 70424-68-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
105 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0359 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0148 (20°C, supercooled liquid, Murphy et al. 1987)
0.0026 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00105 (P_L supercooled liquid, Burkhard et al. 1985a)
0.00735, 0.00116, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
2.61×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
0.00105, 0.00132 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4688/(T/K) + 12.82$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
9.63 (calculated-P/C, Burkhard 1984)
8.61 (20°C, calculated-P/C, Murphy et al. 1987)
20.27 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
16.13 (calculated-QSPR, Dunnivant et al. 1992)
3.94 (calculated-QSPR, Achman et al. 1993)
16.1 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
40.1 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 43 \pm 7$ kJ/mol, $\Delta S_H = 0.11 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.34 (calculated-TSA, Burkhard 1984)
6.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.5952 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.58 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.14 (suspended particulate matter, Burkhard 1984)

4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.004 d^{-1} with $t_{½}$ = 194 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.002 d^{-1} with $t_{½}$ = 283 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 194 d for high-dose treatment, $t_{½}$ = 283 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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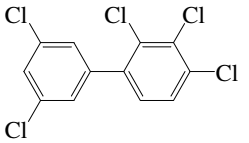
7.1.1.108 2,3,3′,4,5′-Pentachlorobiphenyl (PCB-108)



Common Name: 2,3,3′,4,5′-Pentachlorobiphenyl
Synonym: PCB-108, 2,3,3′,4,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5′-pentachlorobiphenyl
CAS Registry No: 70362-41-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
73 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0356 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0153 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00517 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00103 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00115, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00142, 0.00118 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00105 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4688/(T/K) + 12.87 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
9.57 (calculated-P/C, Burkhard 1984)
35.26 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
17.81 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 7$ kJ/mol, $\Delta S_H = 0.15 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.34 (calculated-TSA, Burkhard 1984)
6.57 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.6672 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.86 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.14 (suspended particulate matter, Burkhard 1984)

4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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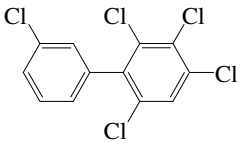
7.1.1.109 2,3,3′,4,6-Pentachlorobiphenyl (PCB-109)



Common Name: 2,3,3′,4,6-Pentachlorobiphenyl
Synonym: PCB-109, 2,3,3′,4,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,6-pentachlorobiphenyl
CAS Registry No: 74472-35-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
73 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0434 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.0063 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00675, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
47.52 (calculated-P/C, Burkhard 1984)
28.56 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
39.42 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.27 (calculated-TSA, Burkhard 1984)
6.48 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.5063 (quoted exptl., calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.59 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.07 (suspended particulate matter, Burkhard 1984)
4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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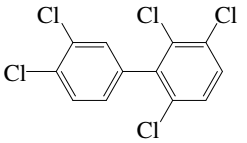
7.1.1.110 2,3,3′,4′,6-Pentachlorobiphenyl (PCB-110)



Common Name: 2,3,3′,4′,6-Pentachlorobiphenyl
Synonym: PCB-110, 2,3,3′,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,6-pentachlorobiphenyl
CAS Registry No: 38380-03-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
79 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0434 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.0288 (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00731 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0082 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.011 (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00735, 0.00248, 0.000804(calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00228 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00182, 0.00199(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.48×10^{-4} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.0 – 4780/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00141, 0.00224 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4522/(T/K) + 12.43 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
0.00258 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
37.48 (calculated-P/C, Murphy et al. 1983)
17.12 (calculated-P/C, Burkhard et al. 1985b)
10.74 (20°C, calculated-P/C, Murphy et al. 1987)
19.15 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
19.89 (calculated-QSPR, Dunnivant et al. 1992)
5.966 (calculated-QSPR, Achman et al. 1993)
18.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
42.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 38 \pm 7$ kJ/mol, $\Delta S_H = 0.09 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.20 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
6.48 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.22 (generator column-GC, Larsen et al. 1992)
6.20 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence equations:

9.06; 8.58 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = – 6.16 + 4540/(T/K); (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
10.14 (10°C, estimated, Thomas et al. 1998)
9.06 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
10.61, 9.58; 9.80 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.19 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.18, 6.48 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.50 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

6.06 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.6–6.8, 6.4; 7.70(suspended sediment, average; algae > 50μm, Oliver 1987a)
4.72, 4.80, 4.77, 3.79 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
4.72, 4.75 (marine humic substances of 5 mg/L DOC, quoted, calculated-MCI χ, Sabljic et al. 1989)
6.32 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.20 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
5.71 (soil, shake flask-GC, Paya-Perez et al. 1991)
6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
5.80 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photodegradation rate constant k = (0.07 ± 0.01) h^{-1} with $t_{½}$ = 9.9 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}-(aq.) = 4.3 × 10^9 dm^3 mol^{-1} s^{-1}, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{½}$ ~ 4–11 d in freshwater systems, $t_{½}$ = 0.1–10 d in cloud water, $t_{½}$ > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.00064\ h^{-1}$; $k_2 = 0.094\ h^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003\ d^{-1}$ with $t_{½} = 204$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{½} \sim 4$–11 d in freshwater systems, $t_{½} = 0.1$–10 d in cloud water, $t_{½} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);
photodegradation $t_{½} = (9.9 \pm 1.6)$ h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½} = 171$ d for high-dose treatment, $t_{½} = 204$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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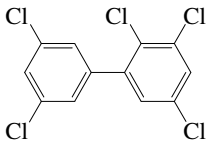
7.1.1.111 2,3,3′,5,5′-Pentachlorobiphenyl (PCB-111)



Common Name: 2,3,3′,5,5′-Pentachlorobiphenyl
Synonym: PCB-111, 2,3,3′,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5,5′-pentachlorobiphenyl
CAS Registry No: 39635-32-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
79 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0315 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
0.00156 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
16.21 (calculated-P/C, Burkhard 1984)
49.45 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
19.89 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (calculated-TSA, Burkhard 1984)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.7224 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.19 (suspended particulate matter, Burkhard 1984)
4.862 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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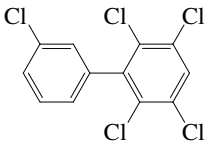
7.1.1.112 2,3,3′,5,6-Pentachlorobiphenyl (PCB-112)



Common Name: 2,3,3′,5,6-Pentachlorobiphenyl
Synonym: PCB-112, 2,3,3′,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5,6-pentachlorobiphenyl
CAS Registry No: 74472-36-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
65 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0463 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00382, 0.00783, 0.00430, 0.00765 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.91×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00316 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.65$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
41.75 (calculated-P/C, Burkhard 1984)
33.34 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
27.02 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.24 (calculated-TSA, Burkhard 1984)
6.40, 6.28, 6.70, 6.25 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.45 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.41 (recommended, Sangster 1993)
6.4916 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.04 (suspended particulate matter, Burkhard 1984)

4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 12 (food lipid mg)/(g worm lipid-d); k_2 = 0.06 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 11 d in earthworm given contaminated food (Wågman et al. 2001)

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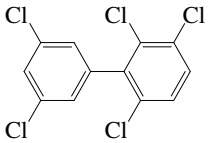
7.1.1.113 2,3,3′,5′,6-Pentachlorobiphenyl (PCB-113)



Common Name: 2,3,3′,5′,6-Pentachlorobiphenyl
Synonym: PCB-113, 2,3,3′,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5′,6-pentachlorobiphenyl
CAS Registry No: 68194-10-5
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
65 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0382 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0036 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.372×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00365, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00306, 0.00368 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00240 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.63$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
28.88 (calculated-P/C, Burkhard 1984)
48.43 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
33.02 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.31 (calculated-TSA, Burkhard 1984)
6.45 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.54 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.45 (recommended, Sangster 1993)
6.3808 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.11 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: measured rate constant $k < 0.05$ M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.3 and 23 ± 2°C, with $t_{½} > 8$ d at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil:

Biota:

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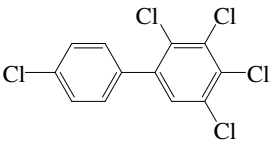
7.1.1.114 2,3,4,4′,5-Pentachlorobiphenyl (PCB-114)



Common Name: 2,3,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-114, 2,3,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′,5-pentachlorobiphenyl
CAS Registry No: 74472-37-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
99 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
109 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.188 (at mp 99°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0121, 0.00879(RP-HPLC-k′ correlation, different mobile phases, Brodsky & Ballschmiter 1988)
0.00146; 0.00246(generator column-GC/ECD; estimated, Hong & Qiao 1995)
0.00263 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
0.000732, 0.00157, 0.00263, 0.00505 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.58×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00136, 0.000881, 0.000352 (calculated-MW, GC-RI correlation, calculated-χ, Burkhard et al. 1985b)
3.45×10^{-4} (20°C, supercooled liquid P_L, Murphy et al. 1987)
0.00124, 0.000115(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
6.92×10^{-4} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4688/(T/K) + 12.82$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
42.56 (calculated-P/C, Burkhard et al. 1985a)
6.99 (20°C, calcd-P/C, Murphy et al. 1987)
11.55 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
14.48 (calculated-QSPR, Dunnivant et al. 1992)
4.96 (calculated-QSPR, Achman et al. 1993)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)

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6.45, 6.78 (RP-HPLC-k′ correlation, different mobile phases, Brodsky & Ballschmiter 1988)
6.65 (calculated, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.72 (recommended, Sangster 1993)
6.5879 (calculated-molecular properties MNDO-AM1, Makino 1998)
6.47 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

9.62 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.34, 6.65 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.09 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.906 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 164 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 187 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: reported biological $t_{½}$ = 155 to > 1000 d for trout, $t_{½}$ = 62–101 d for trout muscle; $t_{½}$ = 73 to > 200 d for carp for pentachlorobiphenyls (Niimi 1987)
depuration $t_{½}$ = 164 d for high-dose treatment, $t_{½}$ = 187 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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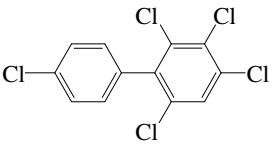
7.1.1.115 2,3,4,4′,6-Pentachlorobiphenyl (PCB-115)



Common Name: 2,3,4,4′,6-Pentachlorobiphenyl
Synonym: PCB-115, 2,3,4,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′,6-pentachlorobiphenyl
CAS Registry No: 74472-38-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
87 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0428 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00342, 0.00517, 0.00142, 0.00494 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0082 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00599, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00224 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.50$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
42.56 (calculated-P/C, Burkhard 1984)
31.11 (calculated-QSAR- MCI χ, Sabljic & Güsten 1989)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.27 (calculated-TSA, Burkhard 1984)
6.43, 6.40, 6.55, 6.38 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.49 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.44 (recommended, Sangster 1993)
6.4654 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.07 (suspended particulate matter, Burkhard 1984)

4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 9 (food lipid mg)/(g worm lipid-d); k_2 = 0.07 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: elimination $t_{½}$ = 11 d in earthworm given contaminated food (Wågman et al. 2001)

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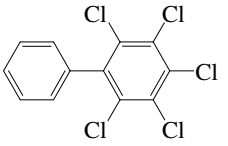
7.1.1.116 2,3,4,5,6-Pentachlorobiphenyl (PCB-116)



Common Name: 2,3,4,5,6-Pentachlorobiphenyl
Synonym: PCB-116, 2,3,4,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4,5,6-pentachlorobiphenyl
CAS Registry No: 18259-05-7
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
123.5 (Lide 2003)
Boiling Point (°C):
381 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3 at 20°C): 1.2803
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.80 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
54.81 (Miller et al. 1984)
54.83, 65.6 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.108 (mp at 123.5°C)
0.105 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0068 (generator column-GC/ECD, Weil et al. 1974)
0.0207 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00548 (generator column-GC/ECD, Miller et al. 1984,1985)
0.00139, 0.00517, 0.00158, 0.00608 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00401 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.0136 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000788, 0.000394, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00341 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.0024 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.53$ (GC-RT correlation, Falconer & Bidleman 1994)
0.00326 (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa m^3/mol at 25°C):
18.34 (calculated-P/C, Burkhard et al. 1985b)
23.41 (calculated-QSPR-MCI χ, Sabljic et al. 1989)
29.97 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.85 (RP-TLC-retention time correlation, Bruggeman et al. 1982)
7.49 (calculated-f const., Yalkowsky et al. 1983)
6.30 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.30; 6.70, 6.40, 6.65, 6.32 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.754 ± 0.015 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
6.25 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.52 (recommended, Sangster 1993)
6.74 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}

9.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Bioaccumulation Factor, log BAF:

5.46 (fish, lipid based-L/kg(Ip), Thomann 1989)

Sorption Partition Coefficient, log K_{OC}:

5.94 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.791 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2: > 0.0007 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ > 1000 d in rainbow trout, and $t_{½}$ = 100 d in its muscle, 100 d (Niimi & Oliver 1983).

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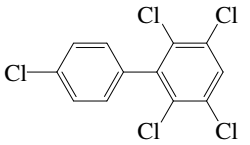
7.1.1.117 2,3,4′,5,6-Pentachlorobiphenyl (PCB-117)



Common Name: 2,3,4′,5,6-Pentachlorobiphenyl
Synonym: PCB-117, 2,3,4′,5,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3,4′,5,6-pentachlorobiphenyl
CAS Registry No: 68194-11-6
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
115 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0457 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0042, 0.00651, 0.0248, 0.00494 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.23×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00561, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
log (P/mmHg) = 11.10 – 4800/(T/K) (GC-RT correlation, Tateya et al. 1988)
0.00257 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 4522/(T/K) + 12.56 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
37.29 (calculated-P/C, Burkhard 1984)
25.13 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
33.02 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.25 (calculated-TSA, Burkhard 1984)
6.37, 6.33, 6.49, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.46 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.39 (recommended, Sangster 1993)
6.4587 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.20 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.05 (suspended particulate matter, Burkhard 1984)

4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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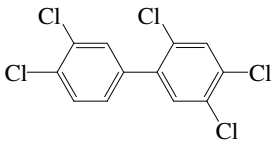
7.1.1.118 2,3′,4,4′,5-Pentachlorobiphenyl (PCB-118)



Common Name: 2,3′,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-118, 2,3′,4,4′,5-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5-pentachlorobiphenyl
CAS Registry No: 31508-00-6
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
106 (Burkhard et al. 1985; Brodsky & Ballschmiter 1988)
109 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
224.5 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.158 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.01344 (20°C, supercooled liquid, Murphy et al. 1987)
0.0153 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00107; 0.00198 (generator column-GC/ECD; estimated, Hong & Qiao 1995)
0.00207* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by Van Noort 2004.
0.0290, 0.0223(supercooled liquid S_L: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_L/(mol m^{-3})] = –1339/(T/K) + 0.32 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00120 (P_L supercooled liquid, GC-RT correlation, Bidleman 1984)
9.62×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000167 (GC-RI correlation, Burkhard et al. 1985b)
0.00123, 0.00104 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.54×10^{-4} (20°C, supercooled liquid P_L, Murphy et al. 1987)
8.32×10^{-4}, 1.12×10^{-3} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4664/(T/K) + 12.72 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
8.91×10^{-4}, 1.0×10^{-4} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = –4853/(T/K) + 13.23 (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
log P_L/Pa = –4627/(T/K) + 12.52 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
40.8 (concn ratio-GC, Murphy et al. 1983)
8.61 (20°C, gas stripping-GC, Murphy et al. 1987)

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11.75 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
3.94 (calculated-QSPR, Achman et al. 1993)
36.12* ± 1.0 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln K_{AW} = 15.877 – 5989.9/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(49.8/kJ{\cdot}mol^{-1})/RT] + (0.132/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where R = 8.314 $J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
36.3 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 50 \pm 6$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
32.36, 14.45 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log H/(Pa m^3/mol) = –2699/(T/K) + 10.56 (LDV linear regression of literature data, Li et al. 2003)
log H/(Pa m^3/mol) = –3289/(T/K) + 12.19 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.42 (HPLC-RT correlation, Shaw & Connell 1982)
6.66, 7.12 (HPLC-k′ correlation, Rapaport & Eisenreich 1984)
6.57 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.74 (calculated-TSA, Hawker & Connell 1988a)
6.24 (generator column-GC, Larsen et al. 1992)
6.57 (recommended, Sangster 1993)
6.49 (generator column-GC/ECD, Yeh & Hong 2002)
6.49, 6.69 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} or as indicated and reported temperature dependence. Additional data at other temperatures designated * are compiled at the end of this section:

10.08* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = –5.92 + 4693/(T/K); temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
11.13, 10.04; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.86 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.80, 9.36 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4646/(T/K) – 6.22 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF or log K_B:

3.60–5.19 (various marine species, mean dry weight, Hope et al. 1998)
5.43 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.88 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-χ, Sabljic et al. 1989)
5.81 (soil from Ispra near Lake Maggiore, Italy, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)
5.20 (colloids and micro-particulates, GC/ECD, Murray & Andren 1992)
5.80 (calculated-K_{OW}, Girvin & Scott 1997)
5.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
4.79–7.42 (range, calculated from sequential desorption of 11 urban soils; Krauss & Wilcke 2001)
5.46; 6.03, 6.67, 6.26 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
6.16–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Sorption Partition Coefficient, log K_P of log K_d:

5.55–5.82 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)
5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_2 = 0.034 d^{-1} with an elimination $t_{½}$ = 20.3 d (earthworm, Belfroid et al. 1995)

k_2 = 0.007 d^{-1} with $t_{½}$ = 103 d and k_2 = 0.013 d^{-1} with $t_{½}$ = 53 d for food concn of 20 ng/g and 133 ng/g respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k_1 = 14 L d^{-1} g^{-1} dry wt.; k_2 = 0.052 d^{-1} (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)

k_2 = 0.052 d^{-1} (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)

k_1 = 6 (food lipid mg)/(g worm lipid-d); k_2 = 0.06 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 180 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.003 d^{-1} with $t_{½}$ = 225 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: reported biological half-lives: $t_{½}$ = 155 to > 1000 d for trout, $t_{½}$ = 62–101 d for trout muscle; $t_{½}$ = 73 to > 200 d for carp for pentachlorobiphenyls (Niimi 1987);

elimination $t_{½}$ = 20.3 d from earthworm (Belfroid et al. 1995)

elimination $t_{½}$ = 95 d in rainbow trout, based on 228 d of elimination (Coristine et al. 1996)

depuration $t_{½}$ = 53–103 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

theoretical half-life to reach 90% steady-state tissue concn 13.3 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);

elimination $t_{½}$ = 12 d in earthworm given contaminated food (predicted, Wågman et al. 2001).

depuration $t_{½}$ = 180 d for high-dose treatment, $t_{½}$ = 225 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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TABLE 7.1.1.118.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,3′,4,4′,5-pentachlorobiphenyl (PCB 118) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	5.85×10^{-4}	4	7.34	–10	11.93
15	1.22×10^{-3}	11	12.81	0	11.23
25	2.07×10^{-3}	18	21.79	10	10.64
35	3.31×10^{-3}	25	36.2	20	10.08
		31	54.8	30	9.57
$\ln x = A - B/(T/K)$					
eq. 1	x	$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		ΔH_{OA}/(kJ mol^{-1}) = 89.86	
A		A	15.8768		
B	$\Delta H_{sol}/R$	B	5989.9	$\log K_{OA} = A + B/T$	
				A	–5.924
mp/°C	111–113	enthalpy, entropy change:		B	4693
ΔH_{sol}/(kJ mol^{-1}) = 37.4		ΔH/(kJ·mol^{-1}) = 49.8 ± 5.8			
		ΔS/(J·mol^{-1}·K^{-1}) = 132 ± 18			

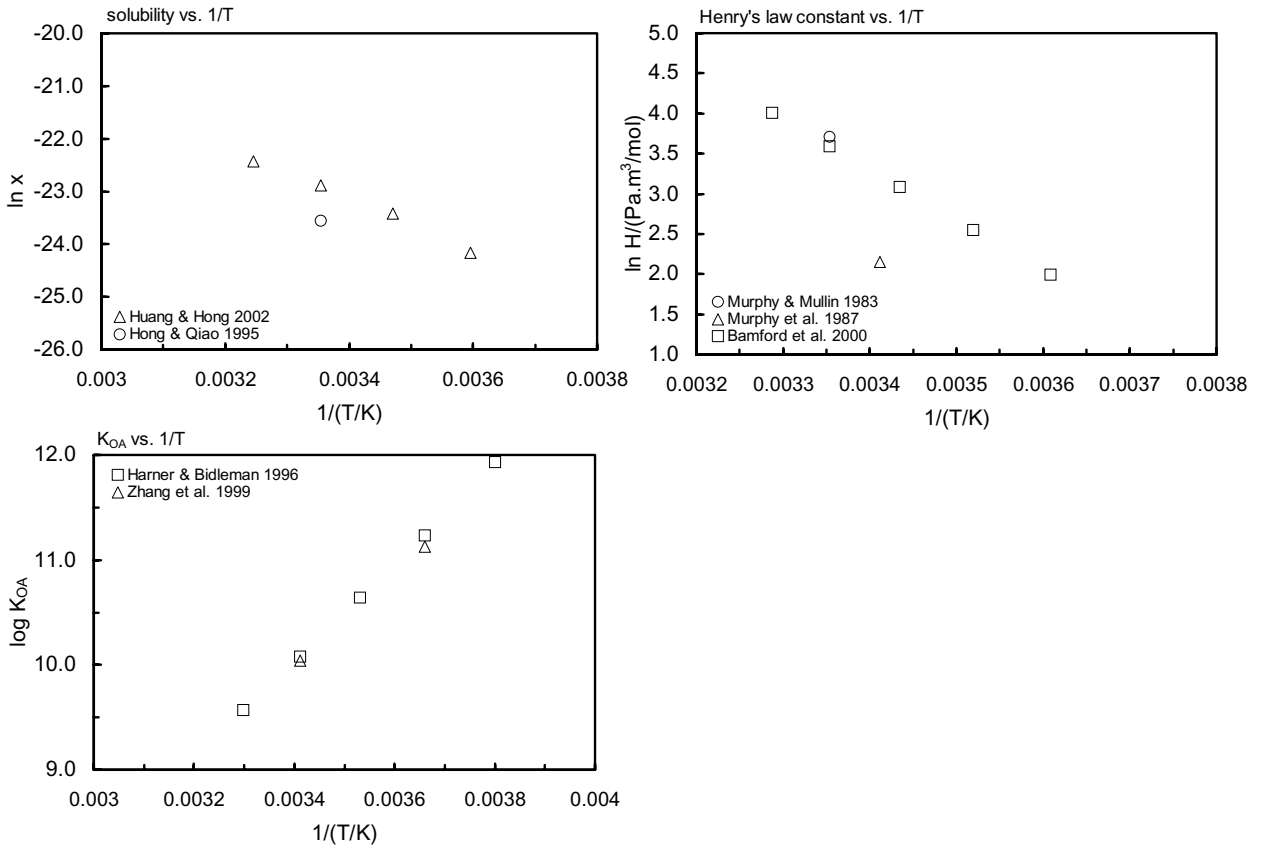

FIGURE 7.1.1.118.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,3′,4,4′,5-pentachlorobiphenyl (PCB-118).

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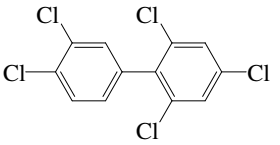
7.1.1.119 2,3′,4,4′,6-Pentachlorobiphenyl (PCB-119)



Common Name: 2,3′,4,4′,6-Pentachlorobiphenyl
Synonym: PCB-119, 2,3′,4,4′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,6-pentachlorobiphenyl
CAS Registry No: 56558-17-9
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0353 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00326, 0.00375, 0.00411, 0.00529 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00651 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.48×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)
0.00735, 0.00269, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00288 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.61$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
22.90 (calculated-P/C, Burkhard 1984)
46.10 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)
5.97 (calculated-QSPR, Achman et al. 1993)
31.46 (calculated-QSPR, Dunnivant et al. 1992)
31.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
50.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 20 \pm 5$ kJ/mol, $\Delta S_H = 0.03 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.36 (calculated-TSA, Burkhard 1984)
6.44, 6.49, 6.33, 6.35 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.58 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.40 (recommended, Sangster 1993)
8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.4124 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, Burkhard 1984)

4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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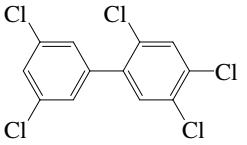
7.1.1.120 2,3′,4,5,5′-Pentachlorobiphenyl (PCB-120)



Common Name: 2,3′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-120, 2,3′,4,5,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 68194-12-7
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
77 (Shiu & Mackay 1986)
77, 93 (exptl., estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.306 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0295 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.42×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)
0.00735, 0.00155, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00197, 0.00203 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
log (P/mmHg) = 11.0 – 4780/(T/K) (GC-RT correlation, Tateya et al. 1988)
log (P_L/Pa) = –4688/(T/K) + 13.02 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
15.71 (calculated-P/C, Burkhard 1984)
40.94 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
6.57 (wetted wall column-GC/ECD, Brunner et al. 1990)
24.87 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.22, 5.68 (HPLC-k′ correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.41 (calculated-TSA, Burkhard 1984)
5.68 (quoted, Sangster 1993)
6.79 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.772 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.87 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.32 (suspended particulate matter, Burkhard 1984)

4.862 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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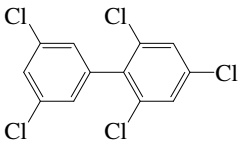
7.1.1.121 2,3′,4,5′,6-Pentachlorobiphenyl (PCB-121)



Common Name: 2,3′,4,5′,6-Pentachlorobiphenyl
Synonym: PCB-121, 2,3′,4,5′,6-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,5′,6-pentachlorobiphenyl
CAS Registry No: 56558-18-0
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
91 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0311 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00411 (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.68×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.00396, 0.000154 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
0.00483, 0.00608(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00501 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4522/(T/K) + 12.85$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
38.50 (calculated-P/C, Burkhard 1984)
75.39 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
56.59 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.39 (calculated-TSA, Burkhard 1984)
6.63, 6.60, 6.19, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.42 (recommended, Sangster 1993)
6.5572 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.84 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.19 (suspended particular matter, Burkhard 1984)

4.704 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d for pentachlorobiphenyls (Atkinson 1987); calculated tropospheric lifetime of 16–48 d for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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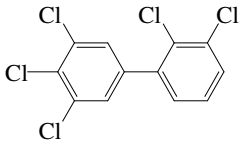
7.1.1.122 2,3,3′,4′,5′-Pentachlorobiphenyl (PCB-122)



Common Name: 2,3,3′,4′,5′-Pentachlorobiphenyl
Synonym: PCB-122
Chemical Name: 2,3,3′,4′,5′-pentachlorobiphenyl
CAS Registry No: 76842-07-4
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
111 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0128 (20°C, supercooled liquid, Murphy et al. 1987)
0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.76×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00735, 0.000854, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
9.93×10^{-4}, 7.23×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.21×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/Pa) = -4688/(T/K) + 12.72$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
6.21 (calculated-P/C, Burkhard 1984)
6.08 (20°C, calculated-P/C, Murphy et al. 1987)
13.88 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.4986 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.09 (suspended particulate matter, Burkhard 1984)

4.906 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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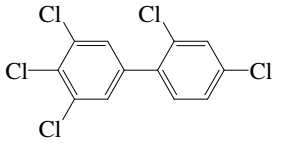
7.1.1.123 2,3′,4,4′,5′-Pentachlorobiphenyl (PCB-123)



Common Name: 2,3′,4,4′,5′-Pentachlorobiphenyl
Synonym: PCB-123, 2,3′,4,4′,5′-pentachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5′-pentachlorobiphenyl
CAS Registry No: 65510-44-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
125 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.000424 (generator column-GC/ECD, Hong & Qiao 1995)
0.000899 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by van Noort 2004.
0.000299, 0.000512, 0.000899, 0.00155 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.08×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00099 (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)
0.0013, 0.00095 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.000933 (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4688/(T/K) + 12.84$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
8.805 (calculated-P/C, Burkhard 1984)
26.55 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
17.65 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.63, 6.60, 6.19, 6.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.74 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.64 (recommended, Sangster 1993)
6.4832 (calculated-molecular properties MNDO-AMI, Makino 1998)
6.50 (generator column-GC/ECD, Yeh & Hong 2002)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.83 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

4.884 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.2–0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = $(0.3–0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 15–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation half-life of 21.2 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).

Ground water:

Sediment:

Soil:

Biota: reported biological half-lives for pentachlorobiphenyls: $t_{½}$ = 155 to > 1000 d for trout, $t_{½}$ = 62–101 d for trout muscle; $t_{½}$ = 73 to > 200 d for carp (Niimi 1987)

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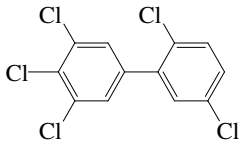
7.1.1.124 2,3′,4′,5,5′-Pentachlorobiphenyl (PCB-124)



Common Name: 2,3′,4′,5,5′-Pentachlorobiphenyl
Synonym: PCB-124, 2′,3,4,5,5′-pentachloro-1,1′-biphenyl, 2′,3,4,5,5′-pentachlorobiphenyl
Chemical Name: 2,3′,4′,5,5′-pentachlorobiphenyl
CAS Registry No: 70424-70-3
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00158 (20°C, supercooled liquid, Murphy et al. 1987)
0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.01×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00112 (GC-RI correlation, Burkhard et al. 1985b)
2.60×10^{-4} (20°C, supercooled liquid P_L, Murphy et al. 1987)
$\log (P_L/Pa) = -4688/(T/K) + 12.62$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
9.84 (calculated-P/C, Burkhard 1984)
5.37 (20°C, calculated-P/C, Murphy et al. 1987)
19.76 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.70 (calculated-QSPR, Achman et al. 1993)
17.65 (calculated-QSPR, Dunnivant et al. 1992)
36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.36 (calculated-TSA, Burkhard 1984)
6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.6178 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.16 (suspended particulate matter, Burkhard 1984)

4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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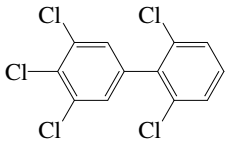
7.1.1.125 2,3′,4′,5′,6-Pentachlorobiphenyl (PCB-125)



Common Name: 2,3′,4′,5′,6-Pentachlorobiphenyl
Synonym: PCB-125
Chemical Name: 2,3′,4′,5′,6-pentachlorobiphenyl
CAS Registry No: 74472-39-2
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
73 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.87×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00204 (GC-RI correlation, Burkhard et al. 1985b)
0.0020 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4255/(T/K) + 12.45$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
14.5 (calculated-P/C, Burkhard 1984)
33.23 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
29.16 (calculated-QSPR, Dunnivant et al. 1992)
44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.29 (calculated-TSA, Burkhard 1984)
6.51 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.2930 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
8.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.09 (suspended particulate matter, Burkhard 1984)

4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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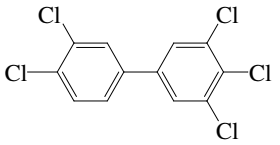
7.1.1.126 3,3′,4,4′,5-Pentachlorobiphenyl (PCB-126)



Common Name: 3,3′,4,4′,5-Pentachlorobiphenyl
Synonym: PCB-126
Chemical Name: 3,3′,4,4′,5-pentachlorobiphenyl
CAS Registry No: 57465-28-8
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
106 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.158 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0321 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.000305 (generator column-GC/ECD, Hong & Qiao 1995)
0.00133* (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see comment by van Noort 2004

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.736×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.05×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
4.86×10^{-4}, 2.86×10^{-4}(supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.09×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4956/(T/K) + 13.31$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
2.51×10^{-4} (P_L, 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.776 (calculated-P/C, Burkhard et al. 1985)
5.471 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
8.39 (calculated-QSAR, Dunnivant et al. 1992)
21.02* ± 0.83 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 35.001 - 11847.5/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(98.5/kJ \cdot mol^{-1})/RT] + (0.291/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
21.3 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 99 ± 9 kJ/mol, ΔS_H = 0.29 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.38 (calculated-TSA, Burkhard 1984)

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6.57 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.89 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.6729 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
6.56; 6.62 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
7.00, 6.67 (calculated-MCI χ, calculated-MNDO-AMI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.61* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = –5.98 + 4870/(T/K); temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
11.77, 10.66; 10.61 (0, 20°C, GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.56 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.81, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor BSAF:

43 (trout, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

6.18 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)
k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 5 (food lipid mg)/(g worm lipid-d); k_2 = 0.05 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.0137 d^{-1} with $t_{½}$ = 51 d (newly contaminated oysters, Gardinali et al. 2004)
k_2 = 0.0116 d^{-1} with $t_{½}$ = 60 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).
Surface water: photodegradation $t_{½}$ = 304 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).
Ground water:
Sediment:
Soil:
Biota: reported biological half-lives for pentachlorobiphenyls: $t_{½}$ = 155 to > 1000 d for trout, $t_{½}$ = 62–101 d for trout muscle; $t_{½}$ = 73 to > 200 d for carp (Niimi 1987);
elimination $t_{½}$ = 13 d in earthworm given contaminated food (Wågman et al. 2001)
Depuration $t_{½}$ = 51 d for newly contaminated oysters, and $t_{½}$ = 60 d for chronically contaminated oysters (Gardinali et al. 2004)

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TABLE 7.1.1.126.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 3,3′,4,4′,5-pentachlorobiphenyl (PCB 126) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
5	6.30×10^{-4}	4	0.958	–10	12.55
15	9.64×10^{-4}	11	2.82	0	11.81
25	1.33×10^{-3}	18	7.88	10	11.24
35	1.60×10^{-3}	25	21.02	20	10.61
		31	47.0	30	10.10
ln x = A –B/(T/K)					
	x	ln K_{AW} = –ΔH/RT + ΔS/R		ΔH_{OA}/(kJ mol^{-1}) = 93.25	
A		ΔS/R	35.012		
B	$\Delta H_{sol}/R$	ΔH/R	11847.5	log K_{OA} = A + B/T	
				A	–5.979
mp/°C	160–161	enthalpy, entropy change:		B	4870
ΔH_{sol}/(kJ mol^{-1}) = 22.3		ΔH/(kJ·mol^{-1}) = 98.5 ± 9.4			
		ΔS/(J·mol^{-1}·K^{-1}) = 291 ± 32			

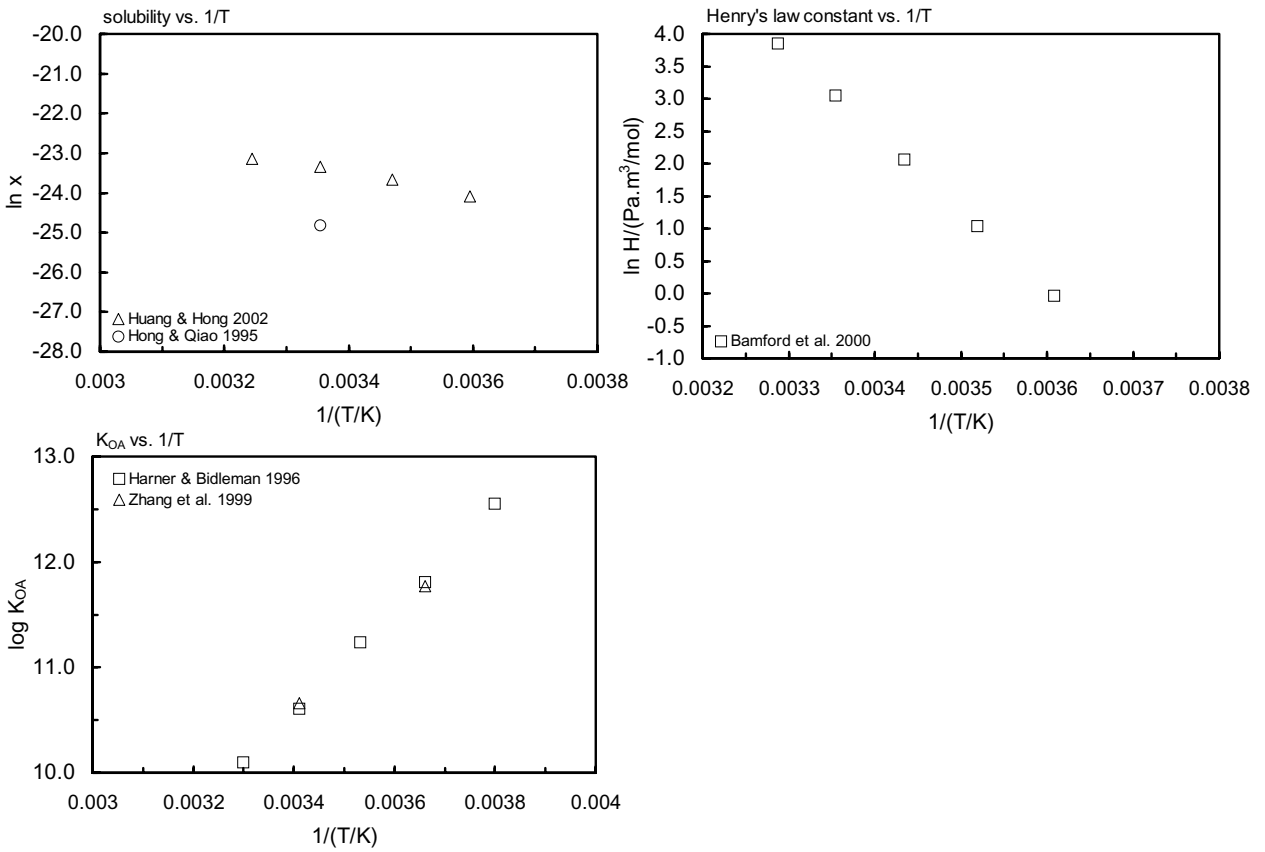

FIGURE 7.1.1.126.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 3,3′,4,4′,5-pentachlorobiphenyl (PCB-126).

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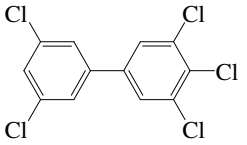
7.1.1.127 3,3′,4,5,5′-Pentachlorobiphenyl (PCB-127)



Common Name: 3,3′,4,5,5′-Pentachlorobiphenyl
Synonym: PCB-127
Chemical Name: 3,3′,4,5,5′-pentachlorobiphenyl
CAS Registry No: 39635-33-1
Molecular Formula: $C_{12}H_5Cl_5$
Molecular Weight: 326.433
Melting Point (°C):
135 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
289.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0285 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.000651 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.04×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000449 (GC-RI correlation, Burkhard et al. 1985b)
7.80×10^{-4}, 5.38×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4956/(T/K) + 13.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
4.64 (calculated-P/C, Burkhard 1984)
34.45 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
21.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 99 \pm 9$ kJ/mol, $\Delta S_H = 0.29 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.42 (calculated-TSA, Burkhard 1984)
6.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.8023 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.53 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.22 (suspended particulate matter, Burkhard 1984)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.2–0.4) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 60–120 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (0.3–0.9) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for pentachlorobiphenyls, and the tropospheric lifetime τ(calc) = 16–48 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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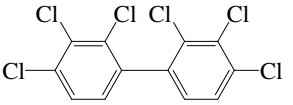
7.1.1.128 2,2′,3,3′,4,4′-Hexachlorobiphenyl (PCB-128)



Common Name: 2,2′,3,3′,4,4′-Hexachlorobiphenyl
Synonym: PCB-128, 2,2′,3,3′,4,4′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′-hexachlorobiphenyl
CAS Registry No: 38380-07-3
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
151 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.83 (Miller et al. 1984)
29.20 (Ruelle et al. 1993; Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
68.62 (Miller et al. 1984; Shiu & Mackay 1986)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0582 (Mackay et al. 1980; Shiu & Mackay 1 986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.40×10^{-4} (generator column-GC/ECD, Weil et al. 1974)
9.90×10^{-4} (shake flask-GC/ECD, Dexter & Pavlou 1978)
2.85×10^{-4} (generator column-GC/ECD, Miller et al. 1984,1985)
0.0067 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
2.74×10^{-3}, 2.17×10^{-3}, 9.07×10^{-4}, 1.54×10^{-3} (RP-HPLC-k′ correlation, different stationary and mobile phase, Brodsky & Ballschmiter 1988)
0.0023 (generator column-GC, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.41×10^{-4} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
3.59×10^{-4} (supercooled liquid P_L, Burkhard 1984)
2.31×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
3.59×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.67×10^{-4}, 2.94×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.83×10^{-5} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
3.67×10^{-4}, 2.94×10^{-4}, 3.41×10^{-4} (supercooled liquid P_L, GC-RT correlation, Foreman & Bidleman 1985)
log (P/mmHg) = 11.40 – 5020/(T/K) (GC-RT correlation, Tateya et al. 1988)
1.78×10^{-4}, 3.31×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4881/(T/K) + 12.91 (GC-RT correlation, Falconer & Bidleman 1994)
$(2.90 – 154.0) \times 10^{-6}$; $(9.80 – 35.9) \times 10^{-5}$ (literature solid P_S range; supercooled liquid P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
50.66 (calculated, Murphy et al. 1983)
6.85 (calculated-P/C, Burkhard et al. 1985b)
11.91 (calculated-P/C, Shiu & Mackay 1986)

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5.78 (20°C, calculated-P/C, Murphy et al. 1987)
3.04 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
50.5 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
1.32 (wetted-wall column-GC/ECD, Brunner et al. 1990)
10.51 (calculated-QSPR, Dunnivant et al. 1992)
0.890, 3.224, 10.99, 35.40 ± 1.5, 92.30 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
ln K_{AW} = 43.30 – 14193/(T/K); temp range 4–31°C (gas stripping-GC, Bamford 2000)
$K_{AW} = \exp[-(118.0/kJ{\cdot}mol^{-1})/ RT] + (0.360/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where R = 8.314 $J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
32.7 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 118 \pm 8$ kJ/mol, $\Delta S_H = 0.36 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

7.44 (RP-TLC-RT correlation, Bruggeman et al. 1982)
6.98 (generator column-GC/ECD, Miller et al. 1984, 1985)
6.14 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.28 (HPLC-RP/MS correlation, Burkhard et al. 1985c)
6.50, 6.67, 6.83, 6.73 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.98 (generator column-GC/ECD, Doucette & Andren 1988)
7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
7.321 ± 0.027(shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
6.98, 6.87; 6.92, 6.87 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.71 (HPLC-k′ correlation, Neogrohati & Hammers 1992)
6.62 (generator column-GC, Larsen et al. 1992)
6.96 (recommended, Sangster 1993)
7.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

9.93 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

1.0 (poultry, Garten & Trabalka 1983)
4.28 (worms, Oliver 1987c)
5.77; 7.30 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.20–5.12 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.90–6.03 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.77, 7.31 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.41, 7.48 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.05 (calculated-MCI, Koch 1983)
6.42 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.06 (calculated-MCI, Bahnick & Doucette 1988)
5.26 (marine humic substance, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)
6.28, 6.17, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.0 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.05 (soil, calculated-MCI, Sabljic et al. 1995)
5.93 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
6.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.00; 5.10 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

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Sorption Partition Coefficient, log K_{OM}:

5.05, 5.09 (quoted, calculated-MCI χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Photooxidation: calculated room temp. rate constant for hexachlorobiphenyls is $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for gas-phase reaction with OH radicals, the tropospheric lifetime is calculated to be 29–60 d (Kwok et al. 1996).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 4970$ d^{-1}; $k_2 = 0.00843$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.009$ d^{-1} with $t_{½} = 75$ d and $k_2 = 0.012$ d^{-1} with $t_{½} = 59$ d for food concn of 8 ng/g and 99 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.005$ d^{-1} with $t_{½} = 146$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003$ d^{-1} with $t_{½} = 205$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{½} > 1000$ d in rainbow trout, and $t_{½} = 89$ d in its muscle (Niimi & Oliver 1983).

Depuration $t_{½} = 59$–75 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½} = 146$ d for high-dose treatment, $t_{½} = 205$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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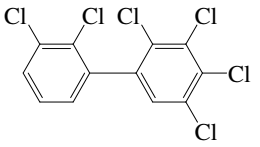
7.1.1.129 2,2′,3,3′,4,5-Hexachlorobiphenyl (PCB-129)



Common Name: 2,2′,3,3′,4,5-Hexachlorobiphenyl
Synonym: PCB-129, 2,2′,3,3′,4,5-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5-hexachlorobiphenyl
CAS Registry No: 55215-18-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
85 (Mackay et al. 1980; Bruggeman et al. 1982; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point,)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.256 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00085 (generator column-GC/ECD, Weil et al. 1974)
0.0117 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00150, 0.00198, 0.000688, 0.00169 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00582 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.76×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
0.00208 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
4.68×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4816/(T/K) + 12.80$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
39.52 (calculated-P/C, Burkhard et al. 1985b)
8.61 (calculated-MCI χ, Sabljic & Güsten 1989)
2.94 (wetted-wall column-GC, Brunner et al. 1990)
14.18 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.50 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
6.71, 6.71, 6.90. 6.71 (RP-HPLC-k′ correlations, Brodsky & Ballschmiter 1988)
6.94, 6.70; 6.81, 6.83 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

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6.76 (recommended, Sangster 1993)
7.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.80 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
6.42 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.259 (marine humic substance, calculated-MCI χ, reported as association coefficient log K_h at 5 mg/L DOC, Sabljic 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.004$ d^{-1} with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 156 d for high-dose treatment, $t_{½}$ = 166 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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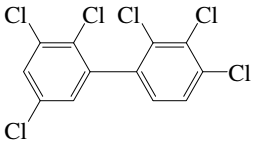
7.1.1.130 2,2′,3,3′,4,5′-Hexachlorobiphenyl (PCB-130)



Common Name: 2,2′,3,3′,4,5′-Hexachlorobiphenyl
Synonym: PCB-130, 2,2′,3,3′,4,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5′-hexachlorobiphenyl
CAS Registry No: 52663-66-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
96 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0168 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00569 (20°C, supercooled liquid, Murphy et al. 1987)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.35×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.92×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.61×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
4.17×10^{-4}, 5.75×10^{-4} (supercooled liquid P_L; GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4816/(T/K) + 12.89$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
11.55 (calculated-P/C, Burkhard 1984)
10.84 (20°C, calculated-P/C, Murphy et al. 1987)
19.45 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
3.75 (wetted wall column-GC/ECD, Brunner et al. 1990)
15.44 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.57, 7.39 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapport & Eisenreich 1984)
6.98, 7.15; 6.79, 6.78 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.12 (recommended, Sangster 1993)
7.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.47 (suspended particulate matter, Burkhard 1984)

5.241 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004$ d^{-1} with $t_{½}$ = 184 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005$ d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 184 d for high-dose treatment, $t_{½}$ = 153 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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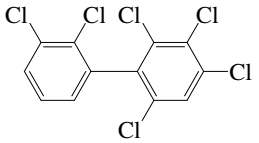
7.1.1.131 2,2′,3,3′,4,6-Hexachlorobiphenyl (PCB-131)



Common Name: 2,2′,3,3′,4,6-Hexachlorobiphenyl
Synonym: PCB-131, 2,2′,3,3′,4,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6-hexachlorobiphenyl
CAS Registry No: 61798-70-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
122 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0151 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01212 (20°C, supercooled liquid, Murphy et al. 1987)
0.00120 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.62×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00285 (GC-RI correlation, Burkhard et al. 1985b)
0.00126, 0.0107 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.63×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
6.92×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.80$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
62.82 (calculated-P/C, Burkhard 1984)
6.59 (20°C, calculated-P/C, Murphy et al. 1987)
26.24 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
3.95 (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)
24.53 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.78 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.97, 6.38; 6.41, 6.44 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.78 (recommended, Sangster 1993)
6.82 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA}:

10.92, 9.83 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.51 (suspended particulate matter, Burkhard 1984)
5.100 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc)$ = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

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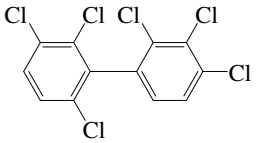
7.1.1.132 2,2′,3,3′,4,6′-Hexachlorobiphenyl (PCB-132)



Common Name: 2,2′,3,3′,4,6′-Hexachlorobiphenyl
Synonym: PCB-132, 2,2′,3,3′,4,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6′-hexachlorobiphenyl
CAS Registry No: 38380-05-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
81 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0149 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00808 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.155×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.27×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
7.58×10^{-4}, 9.08×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.62×10^{-4}, 1.0×10^{-3} (supercooled liquid P_L: GC-RI correlations, different stationary phase, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.5$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
27.97 (calculated-P/C, Burkhard 1984)
16.31 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
4.46 (wetted wall column-GC/ECD, Brunner et al. 1990)
2.42 (calculated-QSPR, Achman et al. 1993)
20.55 (calculated-QSPR, Dunnivant et al. 1992)
16.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
59.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 61 \pm 7$ kJ/mol, $\Delta S_H = 0.17 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.70 (HPLC-RT correlation, Shaw & Connell 1982)
6.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.09. 6.77; 6.63, 6.58 (multi-column-HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.20 (recommended, Sangster 1993)
7.04 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA}:

11.16, 10.07; 9.96 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.52 (suspended particulate matter, Burkhard 1984)
5.10 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.005$ d^{-1} with $t_{½}$ = 136 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½}$ = 147 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 136 d for high-dose treatment, $t_{½}$ = 147 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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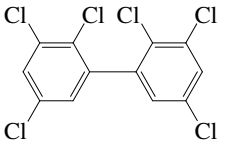
7.1.1.133 2,2′,3,3′,5,5′-Hexachlorobiphenyl (PCB-133)



Common Name: 2,2′,3,3′,5,5′-Hexachlorobiphenyl
Synonym: PCB-133, 2,2′,3,3′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′-hexachlorobiphenyl
CAS Registry No: 35694-04-3
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
129 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0954 (mp at 129°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0149 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
4.37×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.98×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
8.24×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
8.43×10^{-4}, 0.00110 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4816/(T/K) + 13.08$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
19.25 (calculated-P/C, Burkhard 1984)
33.84 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
20.64 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.72 (calculated-TSA, Burkhard 1984)
6.86 (calculated-TSA, Hawker & Connell 1988a)
6.97, 7.02; 6.66, 6.60 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.63, 7.00 (quoted average values of GC-RV and HPLC-k′ correlations of Risby et al. 1990, Sangster 1993)
7.07 (recommended, Hansch et al. 1995)
6.7470 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
7.69 (calculated-CLOGP ver. 4, Ran et al. 2002)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.52 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc)$ = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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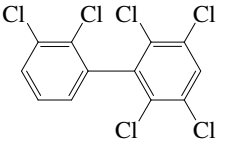
7.1.1.134 2,2′,3,3′,5,6-Hexachlorobiphenyl (PCB-134)



Common Name: 2,2′,3,3′,5,6-Hexachlorobiphenyl
Synonym: PCB-134, 2,2′,3,3′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6-hexachlorobiphenyl
CAS Registry No: 52704-70-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
100 (Mackay et al. 1980; Burkhard et al. 1985a; Kühne et al. 1995; Ruelle & Kesselring 1997)
132 (Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.181 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00091 (generator column-GC/ECD, Weil et al. 1973)
0.0081 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.46×10^{-4} (calculated-S × HLC, Burkhard et al. 1985a)
0.00246 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
4.83×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
0.00127, 0.00185 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.60×10^{-4} (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.30 – 4940/(T/K) (GC-RT correlation, Tateya et al. 1988)
7.41×10^{-4}, 1.32×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4681/(T/K) + 12.79 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
57.76 (Murphy et al. 1983)
55.53 (calculated-P/C, Burkhard et al. 1985b)
9.83 (20°C, calculated-P/C, Murphy et al. 1987)
20.67 (calculated-QSPR MCI χ, Sabljic & Güsten 1989)
4.96 (wetted-wall column-GC/ECD, Brunner et al. 1990)
32.27 (calculated-QSPR, Dunnivant et al. 1992)
25.6 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
68.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 6$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.81 (generator column-GC/ECD,. Doucette & Andren 1987)
6.20 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.22, 6.43; 6.40, 6.44 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.20 (recommended, Sangster 1993)
6.91 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.80, 9.71 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.72 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.49 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.18, 5.16, 5.15, 4.41 (humic substances, in concentrations. of 5, 10, 20, 40 mg C/L, reported as log K_h, Lara & Ernst 1989)
5.18, 5.10 (marine humic substances, quoted, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, and Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:
Biota:

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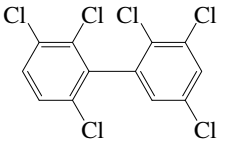
7.1.1.135 2,2′,3,3′,5,6′-Hexachlorobiphenyl (PCB-135)



Common Name: 2,2′,3,3′,5,6′-Hexachlorobiphenyl
Synonym: PCB-135, 2,2′,3,3′,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6′-hexachlorobiphenyl
CAS Registry No: 52744-13-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
102 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0133 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01294 (20°C, supercooled liquid, Murphy et al. 1987)
0.00546 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00361 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00188 (GC-RI correlation, Burkhard et al. 1985b)
0.00115, 0.00184 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.07×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
0.000741, 0.00132 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4861/(T/K) + 12.76$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
46.81 (calculated-P/C, Burkhard 1984)
14.19 (20°C, calculated-P/C, Murphy et al. 1987)
30.8 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
5.67 (wetted wall column-GC/ECD, Brunner et al. 1990)
27.21 (calculated-QSPR, Dunnivant et al. 1992)
26.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
69.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 45 \pm 3$ kJ/mol, $\Delta S_H = 0.12 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
5.94, 7.15 (RP-HPLC-k′ correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
6.32 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.97, 6.95; 6.41, 6.40 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

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6.32 (recommended, Sangster 1993)
7.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.78, 9.69 (0, 20°C, multicolumn GC-k′ correlation, Zhang et al. 1999)
9.71 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.57 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 159 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 192 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 159 d for high-dose treatment, $t_{½}$ = 192 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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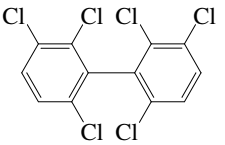
7.1.1.136 2,2′,3,3′,6,6′-Hexachlorobiphenyl (PCB-136)



Common Name: 2,2′,3,3′,6,6′-Hexachlorobiphenyl
Synonym: PCB-136, 2,2′,3,3′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,6,6′-hexachlorobiphenyl
CAS Registry No: 38411-22-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
112.05 (differential scanning calorimetry, Miller et al. 1984)
114.2 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.21 (differential scanning calorimetry, Miller et al. 1984)
21.10 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
54.81 (Miller et al. 1984)
Fugacity Ratio at 25°C, F:
0.138 (calculated, assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00099 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00603 (generator column-GC/ECD, Miller et al. 1984)
0.00451* (generator column-GC/ECD, measured range 4–32°C, Dickhut et al. 1986)
1.10×10^{-3}, 3.25×10^{-3}, 4.51×10^{-3}, 6.68×10^{-3} (4, 20, 25, 32°C, generator column-GC/ECD, Dickhut et al. 1986)
ln x = –5484.72/(T/K) – 3.8682; temp range 4–32°C, ΔH_{ss} = 45.6 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
log x = –2378/(T/K) – 1.679, ΔH_{ss} = 45.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
S/(mol/L) = 2.39×10^{-9} exp(0.065·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
0.0202 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
ln x = –3.880235 – 5471.2/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.000531 (GC-RI correlation, Burkhard et al. 1985a)
0.00374 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00156, 0.00292 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
0.00127 (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00158, 0.00331 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4303/(T/K) + 11.63 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

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Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

93.22 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
22.79 (20°C, calculated-P/C, Murphy et al. 1987)
25.54 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
8.92 (wetted-wall column-GC/ECD, Brunner et al. 1990)
32.64 (calculated-QSPR, Dunnivant et al. 1992)
45.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
81.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

8.35 (Hansch & Leo 1979)
6.81 (generator column-HPLC, Woodburn et al. 1984)
6.63 (generator column-GC/ECD, Miller et al. 1984)
4.91 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
5.48 (HPLC-RP/MS correlation, Burkhard et al. 1985c)
6.81 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
5.76 (generator column-GC/ECD, Hawker & Connell 1988a)
7.118 ± 0.034(shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens)
7.18 (calculated-π const., De Bruijn et al. 1989)
6.63, 6.30; 6.30, 6.24 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.50 (calculated-UNIFAC activity coefficient, Dallos et al. 1993)
6.54 (recommended, Sangster 1993)
7.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.59, 9.53; 9.58 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.51 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

0.86 (poultry, Garten & Trabalka 1983)
5.43; 6.96 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.43, 6.96 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.53 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.53 (suspended solids, 0.7 mg/L, 43.2% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.68 (suspended solids, 6.5 mg/L, 14.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
4.95, 5.05, 4.95, 4.27 (marine humic substances in concentrations of 5, 10, 20, 40 mg L of DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
4.952, 4.942 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h. Observed; calculated-MCI χ, Sabljic et al. 1989)
6.01, 6.06, 5.90 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.04 (5.73–6.35) (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

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Hydrolysis:

Biodegradation: 18% at 24 h and 33% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 4390 d^{-1}; k_2 = 0.0181 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.005 d^{-1} with $t_{½}$ = 132 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 144 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{½}$ = 15.0 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 132 d for high-dose treatment, $t_{½}$ = 144 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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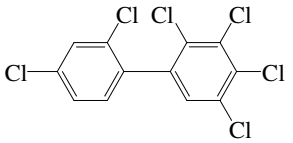
7.1.1.137 2,2′,3,4,4′,5-Hexachlorobiphenyl (PCB-137)



Common Name: 2,2′,3,4,4′,5-Hexachlorobiphenyl
Synonym: PCB-137, 2,2′,3,4,4′,5-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5-hexachlorobiphenyl
CAS Registry No: 35694-06-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
78.0 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.302 (mp at 78°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0158 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0084 (20°C, supercooled liquid, Murphy et al. 1987)
9.94×10^{-4}, 1.12×10^{-3}, 7.54×10^{-4}, 1.69×10^{-3} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.71×10^{-3} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.83×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.50×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
3.80×10^{-4}, 3.02×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phasess, Fischer et al. 1992)
$\log (P_L/Pa) = -4816/(T/K) + 12.61$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
55.02 (calculated-P/C, Burkhard 1984)
6.89 (20°C, calculated-P/C, Murphy et al. 1987)
21.08 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
18.82 (calculated-QSPR, Dunnivant et al. 1992)
3.13 (calculated-QSPR, Achman et al. 1993)
13.0 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
55.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 69 \pm 8$ kJ/mol, $\Delta S_H = 0.20 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
> 6.89, > 7.71 (RP-HPLC-k′ correlation; uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
7.46 (HPLC-RT correlation, De Kock & Lord 1987)

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6.84, 6.87, 6.88, 6.71 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.97, 7.06; 6.82, 6.78 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.83 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
9.89 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.49 (suspended particulate matter, Burkhard 1984)
5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.94 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 186 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 191 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 186 d for high-dose treatment, $t_{½}$ = 191 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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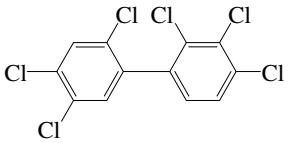
7.1.1.138 2,2′,3,4,4′,5′-Hexachlorobiphenyl (PCB-138)



Common Name: 2,2′,3,4,4′,5′-Hexachlorobiphenyl
Synonym: PCB-138, 2,2′,3,4,4′,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5′-hexachlorobiphenyl
CAS Registry No: 35065-28-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
79 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)
80.5 (Kühne et al.1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)
247.4 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.286 (calculated, assuming ΔS_{fus} = 56 J/mol K, Mackay et al. 1992)
0.285 (calculated-ΔS_{fus} and mp, Passivirta et al. 1995)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0159 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.00729 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00173, 0.00158, 0.00122, 0.0015 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00181 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.0024 (calculated-MCI χ, Patil 1991)
0.00151 (calculated-QSPR, Dunnivant et al. 1992)
0.00268 (calculated-group contribution method, Kühne et al. 1995)
0.00268, 0.0072 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
$\log [S_L/(mol/L)] = -1.12 + 1403/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
6.57×10^{-3} (calculated-mp and K_{OW}, Ran et al. 2002)
7.51×10^{-3}; 6.75×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)
$\log [S_L/(mol\ m^{-3})] = -1437/(T/K) + 0.093$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
5.06×10^{-4}, 5.65×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
1.58×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
4.87×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
5.10×10^{-4}, 4.96×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.33×10^{-4} (quoted average value from Bidleman 1984, Erickson 1986)
1.47×10^{-4} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
$\log (P/mmHg) = 11.60 - 5040/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

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3.31×10^{-4}, 4.90×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4800/(T/K) + 12.81$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
3.63×10^{-4} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
1.47×10^{-4}; 5.14×10^{-4} (solid, supercooled liquid, Passivirta et al. 1999)
$\log (P_S/Pa) = 15.76 - 5842/(T/K)$ (solid, Passivirta et al. 1999)
$\log (P_L/Pa) = 12.81 - 4800/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
5.37×10^{-4}; 5.62×10^{-4} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log (P_L/Pa) = -5034/(T/K) + 13.62$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
$\log (P_L/Pa) = -4770/(T/K) + 12.75$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

48.64 (calculated-P/C, Murphy et al. 1983)
11.04 (calculated-P/C, Burkhard et al. 1985b)
7.60 (20°C, calculated-P/C, Murphy et al. 1987)
10.84 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.13 (wetted-wall column-GC, Brunner et al. 1990)
69.0 (Wittlinger & Ballschmiter 1990)
13.17 (calculated-QSPR, Dunnivant et al. 1992)
$\log [H/(Pa\ m^3/mol)] = 13.93 - 3757/(T/K)$ (Passivirta et al. 1999)
44.6* ± 1.7 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
$\ln K_{AW} = 31.152 - 10476.3/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(87.1/kJ{\cdot}mol^{-1})/RT + (0.259/kJ{\cdot}mol^{-1}{\cdot}K^{-1})/R]$; where $R = 8.314\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
45.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 87 \pm 7$ kJ/mol, $\Delta S_H = 0.26 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
39.81, 30.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -4672/(T/K) + 17.27$ (LDV linear regression of literature data, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -3332/(T/K) + 12.66$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.90 (HPLC-RT correlation, Shaw & Connell 1982)
6.62, 7.44 (RP-HPLC-RT correlation Rapaport & Eisenreich 1984)
6.67, 6.77, 6.73, 6.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.04, 6.80; 6.84, 6.79 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.42 (average, generator column-GC, Larsen et al. 1992)
6.92 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)
7.00, 7.22 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°Cor as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.09* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
$\log K_{OA} = -5.57 + 4584/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
9.51; 9.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -5.17 + 4380/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
10.62 (10°C, estimated, Thomas et al. 1998)
11.34, 10.20; 10.18 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.09 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.76, 9.66 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

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log K_{OA} = 4509/(T/K) – 5.37 (LDV linear regression of literature data, Li et al. 2003)
log K_{OA} = 4510/(T/K) – 5.47 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

5.88; 7.41 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.31–5.47 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.79–5.96 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.88, 7.42 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.42, 7.48 (mussel *Mytilus edilus*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.70 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.52–5.89 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

6.49 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.8–7.3, 6.6 (suspended sediment, average, Oliver 1987a)
7.60 (algae > 50 μm, Oliver 1987a)
6.65 (Lake Michigan water column, Swackhamer & Armstrong 1987)
5.21, 5.22, 5.17, 4.60 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.207, 5.241 (marine humic substances, quoted, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)
5.93 (soil from Ispra, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.50 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.04–7.28; 5.80–7.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.51; 6.28, 6.78, 6.41 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
6.27–7.44 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: photodegradation rate constant k = (0.08 ± 0.01) h^{-1} with $t_{½}$ = 8.2 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16–0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.049 h^{-1}; k_2 = 0.008 h^{-1} (mayfly-sediment model II, Gobas et al. 1989)
k_1 = 4770 d^{-1}; k_2 = 0.00624 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.0344 d^{-1} with an elimination $t_{½}$ = 20.2 d (earthworm, Belfroid et al. 1995)
k_2 = 0.005 d^{-1} with $t_{½}$ = 139 d and k_2 = 0.011 d^{-1} with $t_{½}$ = 64 d for food concn of 31 ng/g and 176 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_1 = 0.00226 h^{-1}; k_2 = 0.145 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)

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k_1(calc) = 5 (food lipid mg)/(g worm lipid-d); k_2(calc) = 0.05 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{½}$ = 186 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 191 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);
$t_{½}$ = 6000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: photodegradation $t_{½}$ = (8.2 ± 0.3) h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995);
$t_{½}$ = 120000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: $t_{½}$ = 19–25 yr (Geyer et al. 2000)
$t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: elimination $t_{½}$ = of 20.d from earthworm (Belfroid et al. 1995)
Depuration $t_{½}$ = 64–139 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$t_{½}$ = 4.8 h in blood plasma (ring doves, Drouillard & Norstrom 2000);
elimination $t_{½}$ = 13 d in earthworm given contaminated food (predicted, Wågman et al. 2001)
depuration $t_{½}$ = 186 d for high-dose treatment, $t_{½}$ = 191 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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TABLE 7.1.1.138.1
Reported Henry's law constants and octanol-air partition coefficients of 2,2′,3,4,4′,5′-hexachlorobiphenyl (PCB-138) at various temperatures and temperature dependence equations

Henry's law constant		log K_{OA}					
Bamford et al. 2000		Harner & Bidleman 1996		Kömp & McLachlan 1997		Zhang et al. 1999	
gas stripping-GC/MS		generator column-GC		fugacity meter-GC/MS		multicolumn-GC-k′ correlation	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}	t/°C	log K_{OA}	t/°C	log K_{OA}
4	2.88	–10	11.81	25	9.51	0	11.34
11	7.50	0	11.27			20	10.20
18	18.68	10	10.61				
25	44.6	20	10.09	log K_{OA} = A + B/T			
31	91.1	30	9.53	A	–5.17		
				B	4380		
		ΔH_{OA}/(kJ mol^{-1}) = 87.77		temp range 10–43°C			
enthalpy, entropy change:							
ΔH/(kJ·mol^{-1}) = 87.1 ± 7.4		log K_{OA} = A + B/T					
ΔS/(J·mol^{-1}·K^{-1}) = 259 ± 26		A	–5.568				
		B	4584				
ln K_{AW} = –ΔH/RT + ΔS/R							
eq. 1	K_{AW}						
A	31.1523						
B	10476						

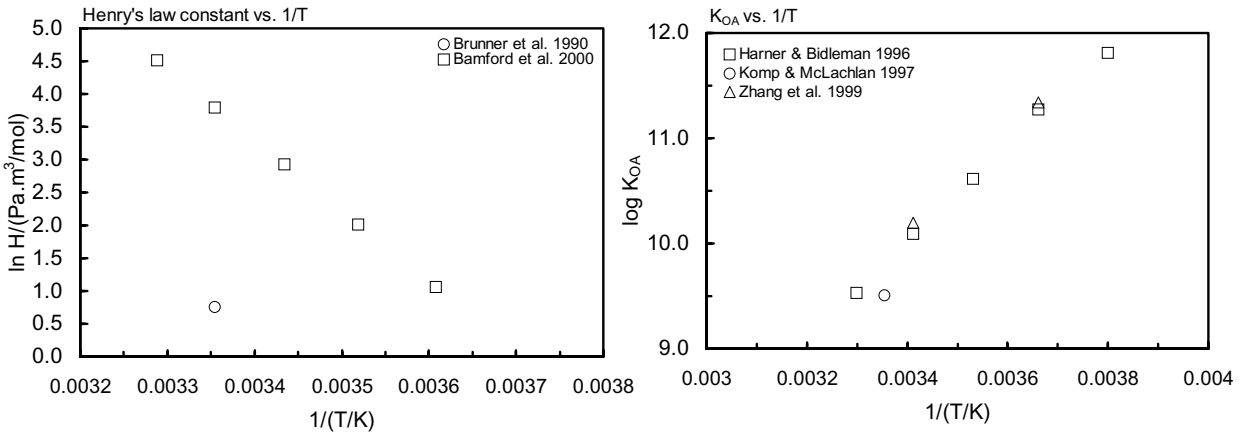

FIGURE 7.1.1.138.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,3,4,4′,5′-hexachlorobiphenyl (PCB-138).

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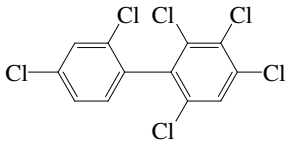
7.1.1.139 2,2′,3,4,4′,6-Hexachlorobiphenyl (PCB-139)



Common Name: 2,2′,3,4,4′,6-Hexachlorobiphenyl
Synonym: PCB-139
Chemical Name: 2,2′,3,4,4′,6-hexachlorobiphenyl
CAS Registry No: 56030-56-9
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
123 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0126 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.05×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.65×10^{-3}, 3.30×10^{-3}, 2.33×10^{-4} (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.26×10^{-3} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.78$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
87.24 (calculated-P/C, Burkhard 1984)
38.60 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
33.32 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.79 (calculated-TSA, Burkhard 1984)
6.67 (calculated-TSA, Hawker & Connell 1988a)
7.12, 6.68; 6.54, 6.50 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.70 (recommended, Sangster 1993)
6.95 (recommended, Hansch et al. 1995)
6.6419 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.59 (suspended particulate matter, Burkhard 1984)

5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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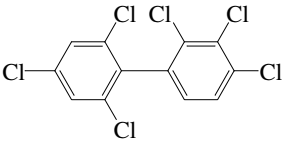
7.1.1.140 2,2′,3,4,4′,6′-Hexachlorobiphenyl (PCB-140)



Common Name: 2,2′,3,4,4′,6′-Hexachlorobiphenyl
Synonym: PCB-140, 2,2′,3,4,4′,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,6′-hexachlorobiphenyl
CAS Registry No: 59291-64-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
123 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0125 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00314, 0.00203, 0.0015, 0.00194 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00325 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
1.26×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00138 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
36.38 (calculated-P/C, Burkhard 1984)
43.06 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
31.17 (calculated-QSAR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.79 (calculated-TSA, Burkhard 1984)
6.48, 6.70, 6.47, 6.66 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.67 (calculated-TSA, Hawker & Connell 1988a)
7.01, 6.86; 6.56, 6.51 (multicolumn HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.58 (recommended, Sangster 1993).
6.97 (recommended, Hansch et al. 1995)
6.4851 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.59 (suspended particulate matter, Burkhard 1984)

5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calc-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH}(calc) = (0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime $\tau(calc)$ = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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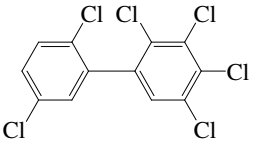
7.1.1.141 2,2′,3,4,5,5′-Hexachlorobiphenyl (PCB-141)



Common Name: 2,2′,3,4,5,5′-Hexachlorobiphenyl
Synonym: PCB-141, 2,2′,3,4,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,5′-hexachlorobiphenyl
CAS Registry No: 52712-04-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
85 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.258 (mp at 85°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0160 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00755 (20°C, supercooled liquid, Murphy et al. 1987)
0.00109, 0.00150, 0.00134, 0.00165 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.0025 (calculated-group contribution method, Kühne et al. 1995)
0.00244, 0.00642 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00295 (GC-RI correlation, Burkhard et al. 1985b)
2.05×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.50 – 5080/(T/K) (GC-RT correlation, Tateya et al. 1988)
5.01×10^{-4}, 6.46×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4816/(T/K) + 12.94 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
61.5 (calculated-P/C, Burkhard 1984)
9.83 (20°C,calculated-P/C, Murphy et al. 1987)
14.49 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
2.33 (wetted wall column-GC/ECD, Brunner et al. 1990)
17.61 (calculated-QSPR, Dunnivant et al. 1992)
6.54 (calculated-QSPR, Achman et al. 1993)
12.7 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
54.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 70 \pm 7$ kJ/mol, $\Delta S_H = 0.20 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.69 (calculated-TSA, Burkhard 1984)
6.80, 6.79, 6.79, 6.71 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.82 (calculated-TSA, Hawker & Connell 1988a)
6.98, 7.02; 6.78, 6.73 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.75 (recommended, Sangster 1993)
9.538 (calculated-UNIFAC group contribution, Chen et al. 1993)
7.19 (recommended, Hansch et al. 1995)
7.10, 6.64–6.89 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
6.70 (estimated, Girvin & Scott 1997)
6.8226 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.55 (10°C, estimated, Thomas et al. 1998)
11.18, 10.07; 10.13 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.87 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.81; 7.34 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC}:

6.49 (suspended particulate matter, Burkhard 1984)
5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.05 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.20 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)
6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 4910 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.00764 d^{-1} (22°C, zebrafish, 30-d clearance, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{½}$ = 171 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 198 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

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Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 171 d for high-dose treatment, $t_{½}$ = 198 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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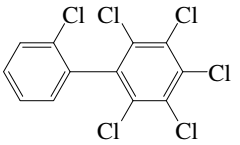
7.1.1.142 2,2′,3,4,5,6-Hexachlorobiphenyl (PCB-142)



Common Name: 2,2′,3,4,5,6-Hexachlorobiphenyl
Synonym: PCB-142, 2,2′,3,4,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,6-hexachlorobiphenyl
CAS Registry No: 41411-61-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
136.0 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0815 (mp at 136°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0171 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00361 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00138 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
3.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000293 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
71.74 (calculated-P/C, Burkhard 1984)
21.18 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
31.89 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
6.66 (calculated-TSA, Burkhard 1984)
6.51 (calculated-TSA, Hawker & Connell 1988)
6.94, 6.75; 6.56, 6.41 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.85 (recommended, Sangster 1993)
6.97 (recommended, Hansch et al. 1995)
6.5729 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.84 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.46 (suspended particulate matter, Burkhard 1984)

5.119 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16–0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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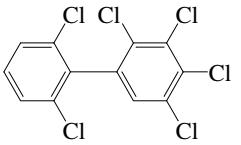
7.1.1.143 2,2′,3,4,5,6′-Hexachlorobiphenyl (PCB-143)



Common Name: 2,2′,3,4,5,6′-Hexachlorobiphenyl
Synonym: PCB-143, 2,2′,3,4,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,6′-hexachlorobiphenyl
CAS Registry No: 68194-15-0
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0143 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00287, 0.00238, 0.00250, 0.00293 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.046×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.41×10^{-3} (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)
9.014×10^{-4}, 9.59×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
7.41×10^{-4}, 1.35×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.65$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
127.7 (calculated-P/C, Burkhard 1984)
25.94 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
3.95 (wetted wall column-GC/ECD, Brunner et al. 1990)
29.83 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 9$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.74 (calculated-TSA, Burkhard 1984)
6.52, 6.65, 6.51, 6.55 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.60 (calculated-TSA, Hawker & Connell 1988)
6.89, 6.63; 6.51, 6.48 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

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6.56 (recommended, Sangster 1993)
6.92 (recommended, Hansch et al. 1995)
6.545 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.54 (suspended particulate matter, Burkhard 1984)
5.100 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 3 (food lipid mg)/(g worm lipid-d); k_2 = 0.07 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 10 d in earthworm given contaminated food (Wågman et al. 2001)

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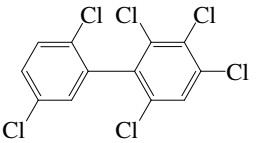
7.1.1.144 2,2′,3,4,5′,6-Hexachlorobiphenyl (PCB-144)



Common Name: 2,2′,3,4,5′,6-Hexachlorobiphenyl
Synonym: PCB-144, 2,2′,3,4,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5′,6-hexachlorobiphenyl
CAS Registry No: 68194-14-9
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
110 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0126 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01294 (20°C, supercooled liquid, Murphy et al. 1987)
0.00353 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.45×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00371 (GC-RI correlation, Burkhard et al. 1985b)
5.07×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
0.00166, 0.00105 (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
98.23 (calculated-P/C, Burkhard 1984)
14.19 (20°C, calculated-P/C, Murphy et al. 1987)
32.22 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
5.70 (calculated-QSPR, Achman et al. 1993)
29.97 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.79 (calculated-TSA, Burkhard 1984)
6.45 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.67 (calculated-TSA, Hawker & Connell 1988a, 1990)
6.96, 6.68; 6.38, 6.29 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.45 (recommended, Sangster 1993)
6.79 (recommended, Hansch et al. 1995)

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6.70 (estimated, Girvin & Scott 1997)
6.6482 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.73, 9.62; 9.62 (0, 20°C, multi-column GC-k′ correlation; calc at 20°C, Zhang et al. 1999)
10.15 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.59 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.20 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.005$ d^{-1} with $t_{½}$ = 137 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½}$ = 184 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 137 d for high-dose treatment, $t_{½}$ = 184 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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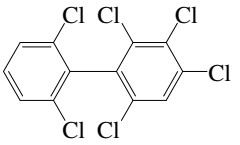
7.1.1.145 2,2′,3,4,6,6′-Hexachlorobiphenyl (PCB-145)



Common Name: 2,2′,3,4,6,6′-Hexachlorobiphenyl
Synonym: PCB-145, 2,2′,3,4,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,6,6′-hexachlorobiphenyl
CAS Registry No: 74472-40-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
84 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0137 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.36×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00681 (GC-RI correlation, Burkhard et al. 1985b)
0.00309 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4303/T + 11.90$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
168.2 (calculated-P/C, Burkhard 1984)
41.34 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
46.61 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
6.25 (calculated-TSA, Hawker & Connell 1988a)
6.92, 6.59; 6.30, 6.26 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phase, Risby et al. 1990)
6.28, 6.78 (quoted average values of Risby et al. 1990, Sangster 1993)
6.71 (recommended, Hansch et al. 1995)
6.2606 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.94 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56 (suspended particulate matter, Burkhard 1984)

4.942 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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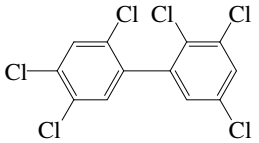
7.1.1.146 2,2′,3,4′,5,5′-Hexachlorobiphenyl (PCB-146)



Common Name: 2,2′,3,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-146, 2,2′,3,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 51908-16-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
90 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00759 (20°C, supercooled liquid, Murphy et al. 1987)
0.00095 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.28×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.000801 (GC-RI correlation, Burkhard et al. 1985b)
7.73×10^{-4}, 9.614×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.87×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
6.31×10^{-4}, 8.51×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4816/(T/K) + 13.04$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
18.54 (calculated-P/C, Burkhard 1984)
8.92 (20°C, calculated-P/C, Murphy et al. 1987)
25.23 (calculated-QSAR- MCI χ, Sabljic & Güsten 1989)
2.53 (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)
19.0 (calculated-QSPR, Dunnivant et al. 1992)
17.8 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
60.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 59 \pm 7$ kJ/mol, $\Delta S_H = 0.17 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.74 (calculated-TSA, Burkhard 1984)
6.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.89 (calculated-TSA, Hawker & Connell 1988a)

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7.02, 7.08; 6.71, 6.71 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.57 (generator column-GC, Larsen et al. 1992)
6.85 (recommended, Sangster 1993)
7.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.96, 9.84 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_P or log K_d

5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

6.54 (suspended particulate matter, Burkhard 1984)
5.40 (Lake Superior suspended solids, GC/ECD, Baker et al. 1986)
5.18, 5.22, 5.14, 4.58 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.18; 5.22 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
5.87 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.20 (colloids and micro-particulates from precipitation events, Murray & Andren 1992)
6.20 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)
6.01 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003$ d^{-1} with $t_{½} = 216$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 166 d for high-dose treatment, $t_{½}$ = 216 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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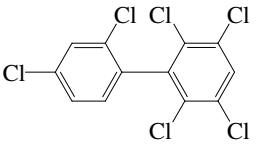
7.1.1.147 2,2′,3,4′,5,6-Hexachlorobiphenyl (PCB-147)



Common Name: 2,2′,3,4′,5,6-Hexachlorobiphenyl
Synonym: PCB-147, 2,2′,3,4′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,6-hexachlorobiphenyl
CAS Registry No: 68194-13-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.86×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00309 (GC-RI correlation, Burkhard et al. 1985b)
log (P/mmHg) = 11.20 – 4910/(T/K) (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant (Pa·m^3/mol at 25°C):
77.21 (calculated-P/C, Burkhard 1984)
32.63 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.17 (wetted wall column-GC/ECD, Brunner et al. 1990)
31.97 (calculated-QSPR, Dunnivant et al. 1992)
5.70 (calculated-QSPR, Achman et al. 1993)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.77 (calculated-TSA, Burkhard 1984)
6.64 (calculated-TSA, Hawker & Connell 1988a)
7.07, 6.73, 6.52, 6.51 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.52, 6.90 (quoted average values of Risby et al. 1990, Sangster 1993)
6.93 (recommended, Hansch et al. 1995)
6.6069 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.79, 9.672 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.70 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.57 (suspended particulate matter, Burkhard 1984)

5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004$ d^{-1} with $t_{½} = 194$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.002$ d^{-1} with $t_{½} = 283$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 194 d for high-dose treatment, $t_{½}$ = 283 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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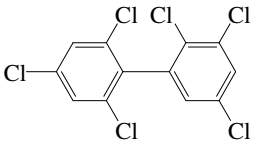
7.1.1.148 2,2′,3,4′,5,6′-Hexachlorobiphenyl (PCB-148)



Common Name: 2,2′,3,4′,5,6′-Hexachlorobiphenyl
Synonym: PCB-148, 2,2′,3,4′,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,6′-hexachlorobiphenyl
CAS Registry No: 74472-42-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
104 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0112 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0369 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.87×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00204 (GC-RI correlation, Burkhard et al. 1985b)
0.00190, 0.00277 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4681/(T/K) + 12.98$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
60.69 (calculated-P/C, Burkhard 1984)
57.65 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
43.52 (calculated-QSPR, Dunnivant et al. 1992)
68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.84 (calculated-TSA, Burkhard 1984)
5.74 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.73 (calculated-TSA, Hawker & Connell 1988a)
7.04, 6.74; 6.46, 6.44 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
5.74 (recommended, Sangster 1993)
6.87 (recommended, Hansch et al. 1995)
6.6291 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

9.51 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.64 (suspended particulate matter, Burkhard 1984)

5.064 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

5.707 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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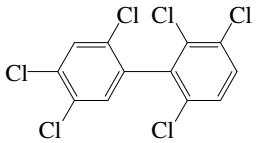
7.1.1.149 2,2′,3,4′,5′,6-Hexachlorobiphenyl (PCB-149)



Common Name: 2,2′,3,4′,5′,6-Hexachlorobiphenyl
Synonym: PCB-149, 2,2′,3,4′,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5′,6-hexachlorobiphenyl
CAS Registry No: 38380-04-0
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 369.9
Melting Point (°C):
oil (Erickson 1986)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0127 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01217 (20°C, supercooled liquid, Murphy et al. 1987)
0.00414 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00454 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.124×10^{-3}, 1.83×10^{-3} (P_L supercooled liquid, GC-RT correlation, different stationary phases, Bidleman 1984)
1.57×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.72×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
0.00105, 0.00158 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.47×10^{-3} (P_L supercooled liquid, quoted average value of Bidleman 1984, Erickson 1986)
4.96×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
8.51×10^{-4}, 1.48×10^{-3} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4689/(T/K) + 12.78$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
44.79 (calculated-P/C, Burkhard 1984)
15.0 (20°C, calculated-P/C, Murphy et al. 1987)
22.09 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
4.32 (calculated-QSPR, Achman et al. 1993)
24.03 (calculated-QSPR, Dunnivant et al. 1992)
0.682; 1.994 (0, 15°C, Hornbuckle et al. 1994)
25.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
68.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 7$ kJ/mol, $\Delta S_H = 0.12 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.70 (HPLC-RT correlation, Shaw & Connell 1982)
6.14, 7.28 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

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6.79 (calculated-TSA, Burkhard 1984)
6.41 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.67 (calculated-TSA, Hawker & Connell 1988a)
7.02, 7.0; 6.45, 6.47 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.54 (generator column-GC, Larsen et al. 1992)
6.41 (recommended, Sangster 1993)
6.86 (recommended, Hansch et al. 1995)
6.4731 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
9.27; 8.68 (generator column; calculated-K_{OW}/K_{AW}, Kömp & McLachlan 1997a)
log K_{OA} = –6.50 + 4700/(T/K), temp range 10–43°C (Kömp & McLachlan 1997a)
9.27 (quoted, Kömp & McLachlan 1997b)
10.83, 9.74; 9.80 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.78 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:
105 (trout, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:
6.59 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
5.79 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.10 (colloids and micro-particulates from precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 0.00097 h^{-1}; k_2 = 0.240 h^{-1} (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_2 = 0.004 d^{-1} with $t_{½}$ = 162 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 199 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 162 d for high-dose treatment, $t_{½}$ = 199 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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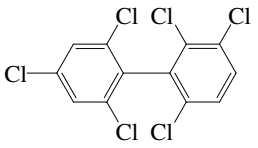
7.1.1.150 2,2′,3,4′,6,6′-Hexachlorobiphenyl (PCB-150)



Common Name: 2,2′,3,4′,6,6′-Hexachlorobiphenyl
Synonym: PCB-150, 2,2′,3,4′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,6,6′-hexachlorobiphenyl
CAS Registry No: 68194-08-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
104 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0121 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00907 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
4.07×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00438 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
121.6 (calculated-P/C, Burkhard 1984)
52.18 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
51.25 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.81 (calculated-TSA, Burkhard 1984)
6.32 (calculated-TSA, Hawker & Connell 1988a)
6.69; 6.59; 6.34, 6.27 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.64, 6.31 (quoted average values of Risby et al. 1990, Sangster 1993)
6.75 (recommended, Hansch et al. 1995)
6.1643 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.61 (suspended particulate matter, Burkhard 1984)

4.924 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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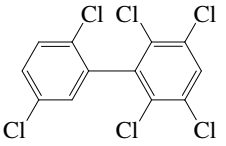
7.1.1.151 2,2′,3,5,5′,6-Hexachlorobiphenyl (PCB-151)



Common Name: 2,2′,3,5,5′,6-Hexachlorobiphenyl
Synonym: PCB-151, 2,2′,3,5,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,5′,6-hexachlorobiphenyl
CAS Registry No: 52663-63-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
101 (Burkhard et al. 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.180 (mp at 101°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.01355 (20°C, supercooled liquid, Murphy et al. 1987)
0.00454, 0.00414, 0.00487, 0.00337 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00223 (calculated-QSPR, Dunnivant et al. 1992)
0.00203 (calculated-group contribution method, Kühne et al. 1995)
0.00173, 0.00454 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
0.00559 (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.32×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.16×10^{-3}, 1.67×10^{-4}, 2.23×10^{-4} (calculated-MW, GC-RI correlation, MCI χ, Burkhard et al. 1985b)
0.00177, 0.00255 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.97×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.30 – 4910/(T/K) (GC-RT correlation, Tateya et al. 1988)
1.91×10^{-3} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = –4681/(T/K) + 12.95 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
86.94 (calculated-P/C, Burkhard 1984)
15.91 (20°C, calculated-P/C, Murphy et al. 1987)
52.18 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
5.98 (wetted wall column-GC/ECD, Brunner et al. 1990)
28.69 (calculated-QSPR, Dunnivant et al. 1992)
33.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)

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73.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 37 \pm 5$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
6.38, 6.49, 6.32, 6.51 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.64 (calculated-TSA, Hawker & Connell 1988a)
6.95, 7.35; 6.44, 6.43 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.45 (generator column-GC, Larsen et al. 1992)
6.43 (recommended, Sangster 1993)
6.85 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
10.08 (10°C, estimated, Thomas et al. 1998)
10.68, 9.58 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.68 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:
5.54; 7.07 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:
6.56 (suspended particulate matter, Burkhard 1984)
5.03, 5.11, 5.09, 4.41 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.031; 5.083 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
6.05, 6.05, 5.93 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.79 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
4.99, 4.82; 4.85 (sediments from Brown's Lake, Helmet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)
6.20 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)
5.75 (4.96–6.18) (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_1 = 4220$ d^{-1}; $k_2 = 0.0121$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.004$ d^{-1} with $t_{½} = 174$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 196$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

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Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 174 d for high-dose treatment, $t_{½}$ = 196 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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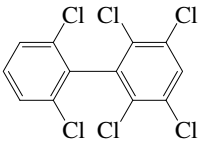
7.1.1.152 2,2′,3,5,6,6′-Hexachlorobiphenyl (PCB-152)



Common Name: 2,2′,3,5,6,6′-Hexachlorobiphenyl
Synonym: PCB-152, 2,2′,3,5,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,5,6,6′-hexachlorobiphenyl
CAS Registry No: 68914-09-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
111 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0145 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.0114 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
5.95×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00638 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
147.9 (calculated-P/C, Burkhard 1984)
35.57 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
43.32 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.73 (calculated-TSA, Burkhard 1984)
6.22 (calculated-TSA, Hawker & Connell 1988a;)
6.86, 6.36; 6.10, 6.09 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.61, 6.10 (average values of Risby et al. 1990, Sangster 1993)
6.51 (recommended, Hansch et al. 1995)
6.2295 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.44 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.53 (suspended particulate matter, Burkhard 1984)

4.942 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16–0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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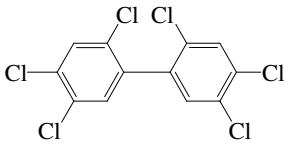
7.1.1.153 2,2′,4,4′,5,5′-Hexachlorobiphenyl (PCB-153)



Common Name: 2,2′,4,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-153, 2,2′,4,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 35065-27-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
103.5 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999; Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.90 (Opperhuizen et al. 1987; Ruelle et al. 1993)
17.50 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C, F:
0.169 (calculated, assuming ΔS_{fus} = 56 J/mol K, Mackay et al. 1980; Shiu & Mackay 1986)
0.167 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0088 (shake flask-GC/ECD, Wallnöfer et al. 1973)
0.0012 (generator column-GC/ECD, Weil et al. 1974)
9.53×10^{-4} (shake flask-GC/ECD, Haque & Schmedding 1975)
9.50×10^{-4} (24°C, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)
0.00105 (16.5°C, shake flask-GC/ECD, Wiese & Griffin 1978)
6.9×10^{-5} (calculated-UNIFAC activity coefficients, Banerjee 1985)
0.00914 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
8.86×10^{-4}, 9.4×10^{-4}, 1.34×10^{-3}, 1.5×10^{-3} (RP-HPLC-k′correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
5.28×10^{-5} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.60×10^{-4} (generator column-GC/ECD, Dunnivant & Elzerman 1988)
8.45×10^{-3}* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988)
4.62×10^{-3}, 8.45×10^{-3}, 1.28×10^{-2} (4, 25, 40°C, generator column-GC/ECD, Doucette & Andren 1988)
S/(mol/L) = 1.15×10^{-8} exp(0.028·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or
log x = –1059/(T/K) – 5.819, temp range 4–40°C, ΔH_{ss} = 20.3 kJ/mol (generator column-GC/ECD, Doucette & Andren 1988a)
0.00115 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
log [S_L/(mol/L)] = –1.20 – 1113/(T/K) (supercooled liquid S_L, Passivirta et al. 1999)
ln x = –13.37313 – 2445.3/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0136, 0.0111 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
log [S_L/(mol m^{-3})] = –1305/(T/K) + 0.14 (supercooled liquid S_L, FAV final adjusted eq., Li et al. 2003)

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Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

6.80×10^{-4}, 7.19×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
6.63×10^{-3} (supercooled liquid P_L, GC-RT correlation Burkhard 1984)
1.24×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
6.63×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
7.08×10^{-4}, 8.13×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.57×10^{-4} (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985b)
1.19×10^{-4}; 7.0×10^{-4} (selected values: solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
2.53×10^{-4} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
log (P/mmHg) = 11.40 – 5040/(T/K) (GC-RT correlation, Tateya et al. 1988)
7.0×10^{-4} (supercooled liquid P_L, Dunnivant & Elzerman 1988)
5.60×10^{-4} (Wittlinger & Ballschmiter 1990)
5.62×10^{-4}, 7.24×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = – 4775/(T/K) + 12.85 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
3.63×10^{-4} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
1.39×10^{-4}; 8.34×10^{-4} (solid; supercooled liquid, Passivirta et al. 1999)
log (P_S/Pa) = 15.80 – 5887/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 12.85 – 4775/(T/K) (supercooled liquid, Passivirta et al. 1999)
$(3.20 – 124.0) \times 10^{-5}$; $(1.80 – 66.3) \times 10^{-4}$ (literature P_S range; literature P_L range, Delle Site 1997)
7.75×10^{-5} (estimated-EPIWIN v3.04, Hardy 2002)
5.25×10^{-4}; 6.03×10^{-4} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log P_L/Pa = –4923/(T/K) + 13.24 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log P_L/Pa = –4712/(T/K) + 12.59 (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):

35.46 (calculated, Murphy et al. 1983)
12.46 (gas stripping-GC, Coates 1984)
17.93 (calculated-P/C, Burkhard et al. 1985b)
6.08 (20°C, batch stripping-GC, Oliver 1985)
42.9 (calculated-P/C, Shiu & Mackay 1986)
10.03 (20°C, calculated-P/C, Murphy et al. 1987)
13.37 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
50.34 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
2.33 (wetted-wall column-GC/ECD, Brunner et al. 1990)
16.70 (calculated-QSPR, Dunnivant et al. 1992)
13.98 ± 1.5, 13.48 ± 1.2 (gas stripping-GC/ECD, purge vessel's height at 26-cm; 67-cm; Girvin et al. 1997)
log [H/(Pa m^3/mol)] = 14.05 – 3662/(T/K) (Passivirta et al. 1999)
52.8* ± 1.6 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
ln K_{AW} = 22.853 – 7950.45/(T/K); temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp\{-[66.1/(\text{kJ mol}^{-1})]/ RT\} + [0.190/(\text{kJ mol}^{-1}\ \text{K}^{-1})/R]$; where R = 8.314 J K^{-1} mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
54.0 (exptl. data, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 66 \pm 5$ kJ/mol, $\Delta S_H = 0.19 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
6.94 (estimated-bond method EPIWIN v.3.04, Hardy 2002)
25.12, 19.95 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log H/(Pa m^3/mol) = –2584/(T/K) + 10.07 (LDV linear regression of literature data, Li et al. 2003)
log H/(Pa m^3/mol) = –3407/(T/K) + 12.72 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

6.72 (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)
8.35 (Hansch & Leo 1979)

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6.34 (shake flask-GC/ECD, Karickhoff et al. 1979)
7.44 (RP-TLC-k′ correlation, Bruggeman et al. 1982; 1984)
6.93, 7.75 (RP-HPLC-RT correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.90 (generator column-HPLC, Woodburn et al. 1984)
6.68 (HPLC/MS correlation, Burkhard et al. 1985c)
7.69, 7.71 (HPLC-k′ correlation, calculated, De Kock & Lord 1987)
6.90 (generator column-GC/ECD, Doucette & Andren 1987,1988)
7.69 (HPLC-RT correlation, De Kock & Lord 1987)
7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
6.84, 6.90, 6.71, 6.74 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.82, 6.85 (RP-HPLC-k′ correlation, different stationary phases, Sherbolm & Eganhouse 1988)
7.00 (RP-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
7.07, 7.12; 6.75, 6.72 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.81 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
6.51 (average, generator column-GC, Larsen et al. 1992)
6.80 (recommended, Sangster 1993)
7.50 (recommended, Hansch et al. 1995)
6.58 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)
6.71, 6.87 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
10.04* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = –6.02 + 4696/(T/K); temp range –10 to +30°C (generator column-GC, Harner & Bidleman 1996)
9.37; 9.09 (fugacity meter/generator column-GC; measured range 10–43°C, calculated, Kömp & McLachlan 1997a)
log K_{OA} = –5.49 + 4430/(T/K) ; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
10.50 (10°C, estimated, Thomas et al. 1998)
11.03, 9.99; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
9.80; 9.65 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
9.52, 9.44 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4966/(T/K) – 7.14 (LDV linear regression of literature data, Li et al. 2003)
log K_{OA} = 3785/(T/K) – 7.00 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:

4.68 (oyster, Vreeland 1974)
4.66 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
4.48, 5.23 (calculated-S, K_{OC}, Kenaga 1980)
5.23, 3.76 (amphipods, clams, Lynch et al. 1982)
5.03, 4.88, 4.65 (algae, snail, aquatic earthworm, Lynch et al. 1982)
4.82, 4.63 (crayfish, fish, Lynch et at. 1982)
4.00, 4.72, 3.77 (calculated-S, calculated-C, calculated-K_{OW}, Lynch et al. 1982)
0.99 (poultry, Garten & Trabalka 1983)
6.78 (guppy, 3.5% lipid, Bruggeman et al. 1982, 1984)
4.84 (rainbow trout, ratio of uptake and depuration rate constants, Muir et al. 1985)
5.87; 6.00 (rainbow trout: laboratory studies; Lake Ontario field data, Oliver & Niimi 1985)
2.60, 2.48 (human fat of lipid, wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
5.32 (guppy, Gobas et al. 1987)
4.57 (*Selenastrum capricornutum*, Mailhot 1987)
4.48 (worms, Oliver 1987c)
4.84, 5.32 (fish, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)

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3.85 (*Hexagenia limbata*, 4°C, rate const. ratio: uptake and depuration k_1/k_2, Landrum & Poore 1988)
4.94–5.28 (*Hexagenia limbata*, May-November, calculated-lipid-normalized, Landrum & Poore 1988)
5.01 (*Pontoporeia hoyi*, calculated, Evans & Landrum 1989)
5.06 (guppy, estimated, Banerjee & Baughman 1991)
5.65; 7.18 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
3.31–5.57 (various marine species, mean dry wt. BCF, Hope et al. 1998)
5.11–6.96 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
5.32 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
4.68, 5.93 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.48, 7.40 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.63, 6.99 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.65, 7.19 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.95; 3.95 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)
4.40 (estimated-EPIWIN v3.04, Hardy 2002)

Sorption Partition Coefficient, log K_P:

3.95–4.17 (Saginaw Bay sediment, sorption isotherm, Horzempa & Di Toro 1983)
4.12–4.55 (Saginaw Bay suspended solids, sorption isotherm, Horzempa & Di Toro 1983)
5.30 (Lake Superior suspended solids, field measurement-GC/ECD, Baker et al. 1986)
5.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.65–5.91 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

5.62 (soil/sediment, batch equilibrium-sorption isotherm, Haque & Schmedding 1976)
5.34 (soil, batch equilibrium-sorption isotherm measurement, Chiou et al. 1979)
6.51 (soil, calculated-K_{OW}, Karickhoff et al. 1979)
6.08 (soil, quoted experimental value, Kenaga 1980)
5.33 (calculated-K_{OW}, Schwarzenbach & Westall 1981)
6.51 (calculated-K_{OW}, Schwarzenbach & Westall 1981 from Karickhoff 1981)
6.43, 6.42, 5.33 (calculated-K_{OW}, calculated-C_L, calculated-C_S, Karickhoff 1981)
6.51 (sediment, calculated-K_{OW}, Lynch et al. 1982)
6.57 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.60; 5.50; 7.30 (field data of sediment trap material; Niagara River-org. matter; calculated-K_{OW}, Oliver & Charlton 1984)
6.61 (sediment/pore water-Saginaw Bay, dual radio-tag experiment, Di Toro et al. 1985)
5.51 (Aldrich humic acid, reversed phase separation, Landrum et al. 1985)
5.40, 5.70, 6.10 (Offshore Grand Haven sediment, nearshore Grand Haven sediment, Benton Harbor sediment, by batch equilibrium-sorption isotherm, Voice & Weber 1985)
7.56, 7.68 (river sediment, Coates & Elzerman 1986)
5.575 (correlated literature values in soils, Sklarew & Girvin 1987)
5.8–7.3, 6.60; 7.20 (suspended sediment, average; algae > 50 μm, Oliver 1987a)
6.60 (river sediment 7–13% OC, batch equilibrium, Oliver 1987)
6.48 (Lake Michigan water column, Swackhamer & Armstrong 1987)
4.75 (12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans 1988)
5.26, 5.25, 5.19, 4.62 (humic substances, in concentration of 5, 10, 20, 40 mg/L DOC, reported as log K_h, Lara & Ernst 1989)
5.258, 5.222 (marine humic substances, calculated-MCI χ, reported as log K_h at concentration of 5 mg/L DOC, Sabljic et al. 1989)
6.76, 4.42 (Great Lake suspended matter, Great Lake DOC: reversed phase separation, Eadie et al. 1990)
6.18, 6.13, 5.99 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.86 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
5.54 (Red Hood sediment, batch equilibrium, Brannon et al. 1995)

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5.65 (soil, calculated-MCI χ, Sabljic et al. 1995)
6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
6.42–6.48 (Catlin silt loam, f_{OC} = 0.0226, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.77–6.84 (Cloudland loam, f_{OC} = 0.0024, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997
6.43–6.52 (Kenoma silt loam, f_{OC} = 0.0153, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.51–6.57 (Kenoma silt loam, f_{OC} = 0.0092, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.19–6.28 (Norborne silt loam, f_{OC} = 0.0137, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.55 (Norborne silt loam, f_{OC} = 0.009, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.41–6.59 (Norborne silt loam, f_{OC} = 0.0057, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
6.40 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.20; 5.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
5.86, 5.81 (sediments: organic carbon OC –0.1%, OC –0.5%, average, Delle Site 2001)
6.05–7.27; 5.30–7.60 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.55; 6.17, 6.96, 6.50 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
5.088 (estimated-EPIWIN v3.04, Hardy 2002)
6.20–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Sorption Partition Coefficient, log K_{OM}:
4.42 (natural sediment, Eadie et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: depletion rate constant k = 17 d^{-1} from a 26-cm or 67-cm high purge vessel (Girvin et al. 1997); $t_{½}$ = 2.096 d from river, $t_{½}$ = 29.5 d from lake (estimated-EPIWIN v3.04, Hardy 2002).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16–0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 29.5 d^{-1} in pond, k_1 = 14.6 d^{-1} in river, k_1 = 36.8 d^{-1} in sand by *Chironomus tentans* larvae (Muir et al. 1983)
k_2 = 0.0029 d^{-1} with elimination $t_{½}$ = 241 h in pond-sediment, k_2 = 0.0059 d^{-1} with $t_{½}$ = 117 h in river water, k_2 = 0.0034 d^{-1} with $t_{½}$ = 203 h in river sediment and k_2 = 0.0030 d^{-1} with $t_{½}$ = 230 h in sand-sediment by *Chironomus tentans* larvae (Muir et al. 1983)
k_2 > 0.0007 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 800 d^{-1}; k_2 = 0.004 d^{-1} (guppy, Bruggeman et al. 1984)
k_1 = 461 d^{-1}; k_2 = 0.008 d^{-1} (rainbow trout, total ^{14}C in whole fish-wet weight, Muir et al. 1985)
k_1 = 1100 d^{-1} (guppy, Opperhuizen 1986)
k_1 = 63.2 h^{-1}; k_2 = 0.009 h^{-1} (10–20°C, *Hexagenia limbata*, Landrum & Poore 1988)
k_s = 0.049 h^{-1}; k_t = 0.009 h^{-1} (uptake, depuration of mayfly-sediment model II, Gobas et al. 1989)
log k_1 = 2.90, 2.66 d^{-1}; log $1/k_2$ = 2.39, 2.10 d (fish, quoted, Connell & Hawker 1990)
k_1 = 4660 d^{-1}; k_2 = 0.0104 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.044 d^{-1} with an elimination half-life of 15.9 d (earthworm, Belfroid et al. 1995)
k_2 = 0.003 d^{-1} with $t_{½}$ = 224 d and k_2 = 0.010 d^{-1} with $t_{½}$ = 69 d for food concn of 22 ng/g and 124 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_1 = 5.7 L d^{-1} g^{-1}; k_2 = 0.027 d^{-1} (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)
k_1 = 0.00231 h^{-1}; k_2 = 0.137 h^{-1} (in blood plasma of ring doves, Drouillard & Norstrom 2000)

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k_1 = 5 (food lipid mg)/(g worm lipid-d); k_2 = 0.04 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.004 d^{-1} with $t_{½}$ = 177 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.003 d^{-1} with $t_{½}$ = 219 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
k_2 = 0.015 d^{-1} with $t_{½}$ = 46.2 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radical for hexachlorobiphenyls (Kwok et al. 1995);
$t_{½}$ = 6000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: 25–53 min in aqueous solution purged at a flow rate of 1 L/min (Coates 1984);
$t_{½}$ = 123000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000;
volatilization $t_{½}$ = 2.096 d from river, 29.5 d from lake (estimated-EPIWIN v3.04, Hardy 2002).
Groundwater:
Sediment: uptake clearance from sediment was (0.0021 ± 0.001) g of dry sediment·g^{-1} of organism·h^{-1} for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C (Landrum 1989);
k(exptl) < 0.9 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.3, with $t_{½}$ > 7 h at pH 7 and 23 ± 2°C (Yao & Haag 1991).
$t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: half-life in rainbow trout, > 1000 d and its muscle, 77 d (Niimi & Oliver 1983);
$t_{½}$ = 170 d in worms at 8°C (Oliver 1987c);
$t_{½}$ = 175 d in guppy (Bruggeman et al. 1984);
$t_{½}$ = 45.6 d in *Pontoporeia hoyi* (Evans & Landrum 1989);
elimination $t_{½}$ = 15.9 d from earthworm (Belfroid et al. 1995)
Depuration $t_{½}$ = 69–224 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
theoretical $t_{½}$ = 25.7 d to reach 90% steady-state tissue concn (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);
$t_{½}$ = 5.1 h in blood plasma (ring doves, Drouillard & Norstrom 2000);
elimination $t_{½}$ = 18 d in earthworm given contaminated food (Wågman et al. 2001).
depuration $t_{½}$ = 177 d for high-dose treatment, $t_{½}$ = 219 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
depuration $t_{½}$ = 46.2 d (juvenile carp in 100-d experiment Stapleton et al. 2004)

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TABLE 7.1.1.153.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,2′,4,4′,5,5′-hexachlorobiphenyl (PCB-153) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Doucette & Andren 1988		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	H/(Pa m^3/mol)	t/°C	log K_{OA}
4	0.00462	4	6.50	–10	11.73
25	0.00845	11	13.52	0	11.25
40	0.0128	18	27.2	10	10.62
		25	52.8	20	10.04
S/(mol/L) = A·exp[B·(t/°C)]		31	91.2	30	9.39
A	1.15×10^{-8}				
B	0.028	ln K_{AW} = –ΔH/RT + ΔS/R		ΔH_{OA}/(kJ mol^{-1}) = 89.90	
		A	22.8530		
ΔH_{sol}/(kJ mol^{-1}) = 20.3		B	7950.45	log K_{OA} = A + B/T	
for 4–40°C				A	–6.015
		enthalpy, entropy change:		B	4695
		ΔH/(kJ·mol^{-1}) = 66.1 ± 5.4			
		ΔS/(J·mol^{-1}·K^{-1}) = 190 ± 18			

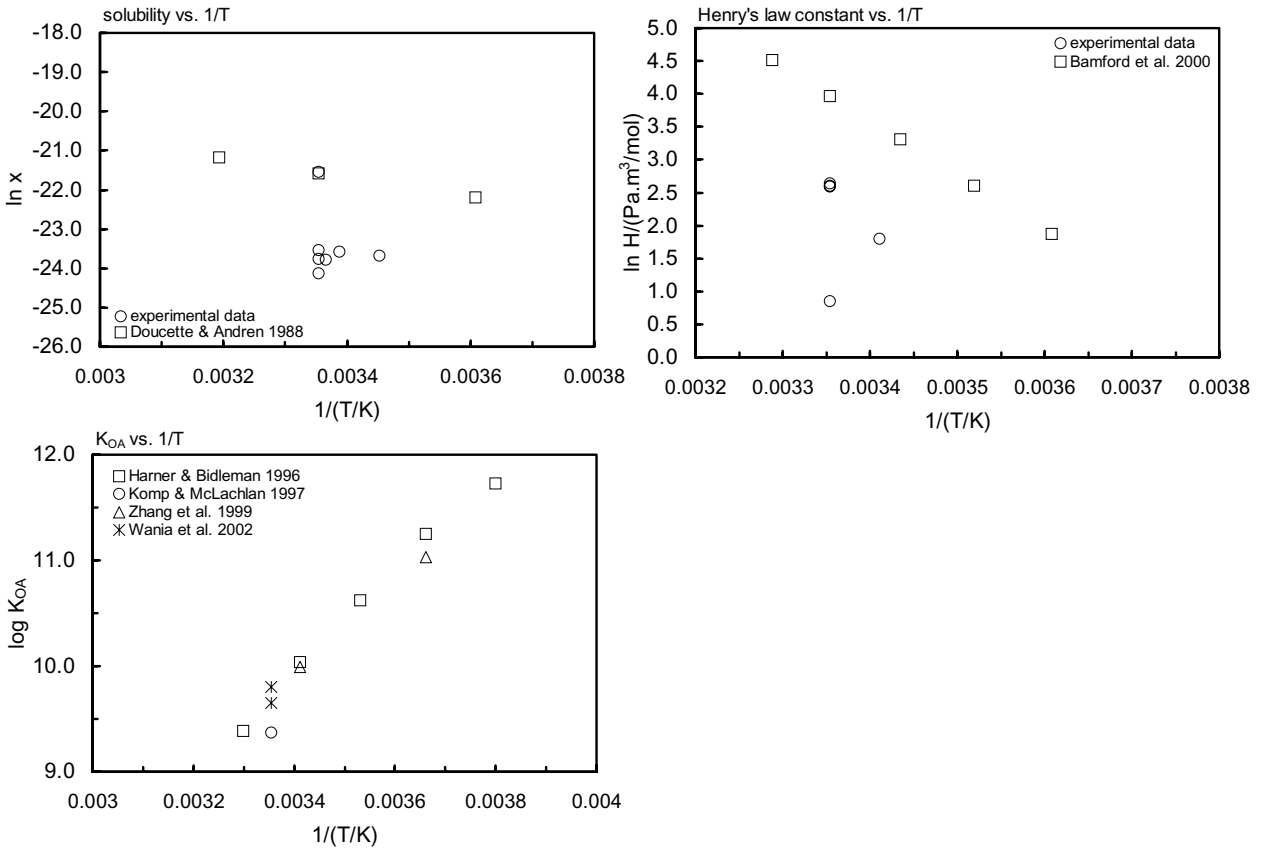

FIGURE 7.1.1.153.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,4,4′,5,5′-hexachlorobiphenyl (PCB-153).

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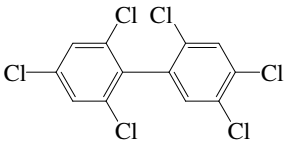
7.1.1.154 2,2′,4,4′,5,6′-Hexachlorobiphenyl (PCB-154)



Common Name: 2,2′,4,4′,5,6′-Hexachlorobiphenyl
Synonym: PCB-154, 2,2′,4,4′,5,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,5,6′-hexachlorobiphenyl
CAS Registry No: 60145-22-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
oil (Erickson 1986)
117 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
0.0106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00173, 0.00137, 0.00293, 0.00213 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.71×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.86×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
0.00182 (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4681/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
58.46 (calculated-P/C, Burkhard 1984)
48.84 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
38.7 (calculated-QSPR, Dunnivant et al. 1992)
17.34, 29.16, 47.85, 76.7 ± 2.2, 113.7 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 15.155 - 5556.89/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(46.2/kJ \cdot mol^{-1})/RT] + (0.126/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
75.4 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 5$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.87 (calculated-TSA, Burkhard 1984)
6.67, 6.81, 6.47, 6.64 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
6.76 (calculated-TSA, Hawker & Connell 1988a)
7.05, 7.03; 6.48, 6.43 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

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6.65 (recommended, Sangster 1993)
6.89 (recommended, Hansch et al. 1995)
6.6326 (molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.66 (suspended particulate matter, Burkhard 1984)
5.064 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = (0.16–0.5) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota:

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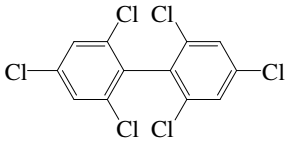
7.1.1.155 2,2′,4,4′,6,6′-Hexachlorobiphenyl (PCB-155)



Common Name: 2,2′,4,4′,6,6′-Hexachlorobiphenyl
Synonym: PCB-155, 2,2′,4,4′,6,6′-hexachloro-1,1′-biphenyl
Chemical Name: 2,2′,4,4′,6,6′-hexachlorobiphenyl
CAS Registry No: 33979-03-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
112.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3482
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.5 (differential scanning calorimetry, Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)
20.30 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
45.19 (Miller et al. 1984)
45.25, 66.9 (exptl., calculated, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.139 (mp at 112.5°C)
0.131 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00090 (generator column-GC/ECD, Weil et al. 1974)
0.00041 (generator column-GC/ECD, Miller et al. 1984,1985)
0.0000528 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
2.50×10^{-3}, 1.34×10^{-3}, 6.27×10^{-3}, 2.68×10^{-3} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0023 (generator column-GC/ECD, Dunnivant & Elzerman 1988)
0.00109 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
0.0033 (generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)
0.00284 (shake flask-GC/ECD, Li & Andren 1994)
0.0028* ± 0.00013 (generator column-GC/ECD, Shiu et al. 1997)
1.89×10^{-3}, 0.0050 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
ln x = –8.9206 – 4112.07/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0142, 0.0138 (supercooled liquid S_L: derivation of literature-derived value LDV, final-adjusted value FAV, Li et al. 2003)
log [S_L/(mol m^{-3})] = –861/(T/K) – 1.52 (supercooled liquid, linear regression of literature data, Li et al. 2003)
log [S_L/(mol m^{-3})] = –1268/(T/K) – 0.16 (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0016 (GC-RT, Westcott et al. 1981)
0.0122 (P_L calculated from P_S using fugacity ratio F, Westcott et al. 1981)
0.00173 (gas saturation, Westcott & Bidleman 1981)
0.00443 (supercooled liquid P_L, Burkhard 1984)

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3.57×10^{-4}, 6.41×10^{-4}, 8.04×10^{-4} (calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985a)
0.00443 (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
0.00159, 0.012(selected P_S, P_L, Shiu & Mackay 1986)
4.76×10^{-4} (calculated-S × HLC, Dunnivant & Elzerman 1988)
3.54×10^{-4} (supercooled liquid P_L, calculated-mp, Dunnivant & Elzerman 1988)
$\log (P_L/Pa) = -4303/(T/K) + 12.02$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
3.25×10^{-4}* (gas saturation-GC/ECD, measured range –10 to 30°C, Wania et al. 1994)
$\log (P_S/Pa) = 14.84 - 5399/(T/K)$; temp range –10 to 30°C (gas saturation-GC, Wania et al. 1994)
2.188×10^{-3} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
0.000285–0.0016; 0.00344–0.00443 (exptl. solid P_S range; exptl. liquid P_L range, Delle Site 1997)
3.42×10^{-4} (supercooled P_L: calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)
3.31×10^{-3}; 3.47×10^{-3} (supercooled P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/Pa = -4697/(T/K) + 13.27$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
$\log P_L/Pa = -4562/(T/K) + 12.85$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

11.65 (gas stripping-GC, Coates 1984)
157.0 (calculated-P/C, Burkhard et al. 1985b)
12.46 (calculated, Coates & Elzerman 1986)
817.9 (calculated-P/C, Shiu & Mackay 1986)
76.5 (gas stripping-GC, Dunnivant et al. 1988, Dunnivant & Elzerman 1988)
60.8 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
85.25 (calculated-QSPR, Dunnivant et al. 1992)
81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
75.86, 91.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
$\log [H/(Pa\ m^3/mol)] = -3294/(T/K) + 13.01$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.70 (shake flask-GC, Chiou et al. 1977)
6.34 (shake flask-GC, Karickhoff et al. 1979)
6.37 (HPLC-k′ correlation, McDuffie 1981)
7.12 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
6.88 (calculated-TSA, Burkhard 1984)
7.55 (generator column-GC/ECD, Miller et al. 1984,1985)
6.39 (HPLC-RT/MS correlation, Burkhard et al. 1985c)
6.01 (HPLC-k′ correlation, Tomlinson & Hafkenscheid 1986)
7.24 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
6.54, 6.81, 6.24, 6.57 (RP-HPLC-RI correlations, Brodsky & Ballschmiter 1988)
7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
7.287 ± 0.065(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
7.08, 7.03; 6.24, 6.22 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.83 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
7.24 (shake flask-GC/ECD, Li & Doucette 1993)
6.54 (recommended, Sangster 1993)
7.29 (recommended, Hansch et al. 1995)
7.36, 7.19 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.99* (generator column-GC/ECD; measured range –10 to +20°C; Harner & Mackay 1995)
$\log K_{OA} = -2.20 + 3954/(T/K)$; (temp range –10 to +20°C, generator column-GC, Harner & Mackay 1995)

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9.15 (20°C, generator column-GC, Harner & Bidleman 1996)
log K_{OA} = –2.21 + 3954/(T/K); temp range –10 to +20°C (generator column-GC, Harner & Bidleman 1996)
10.19, 9.13; 9.16 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
9.24 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
8.89, 9.14 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4357/(T/K) – 5.47 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:

1.02 (poultry, Garten & Trabalka 1983)
2.79–3.68 highest value 3.68, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7-d to 96-d laboratory study, Oliver & Niimi 1985)
> 4.94; 3.68 (rainbow trout, laboratory data: kinetic BCF (k_1/k_2), steady-state BCF (C_F/C_W), Oliver & Niimi 1985)
4.53 (worms, Oliver 1987c)
3.68 (fish, Isnard & Lambert 1988)
5.99, 7.29 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.08 (natural sediment, sorption isotherm by batch equilibrium technique-GC, Karickhoff et al. 1979)
5.95, 7.28, 5.95(calculated-K_{OW}, calculated-C_L, calculated-C_S, Karickhoff 1981)
6.68 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
4.905 (calculated-MCI χ, marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, Sabljic et al. 1989)
6.08; 6.17 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 8.6–29.5 h^{-1} in pond-sediment system, k_1 = 22.9–14.6 h^{-1} in river-water system, k_1 = 29.6–39.8 h^{-1} in river-send system, k_1 = 26.7–47.0 h^{-1} in sand-sediment system (*Chironomus tentans* larvae, Muir et al. 1983)
k_2 = 0.0029 h^{-1} with $t_{½}$ = 241 h in pond-sediment system, k_2 = 0.0059 h^{-1} with $t_{½}$ = 117 h in river-water system, k_2 = 0.0034 h^{-1} with $t_{½}$ = 203 h in river-send system, k_2 = 0.0030 h^{-1} with $t_{½}$ = 230 h in sand-sediment system (*Chironomus tentans* larvae, Muir et al. 1983)
k_2 > 0.0007 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
k_1 = 60 d^{-1}; k_2 > 0.0007 d^{-1} (rainbow trout, Oliver & Niimi 1985; Thomann 1989)
log $1/k_2$ = 3.1, 3.6 h (fish, quoted, calculated-K_{OW}, Hawker & Connell 1988b)
$1/k_2$ = 141 d (guppy, Gobas et al. 1989; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil:

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Biota: $t_{½}$ = 117–241 h in sediment-water systems (*Chironomus tentans* larvae, Muir et al. 1983)
$t_{½}$ > 1000 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{½}$ = 77 d in its muscle (Niimi & Oliver 1983).

TABLE 7.1.1.155.1
Reported aqueous solubilities and octanol-air partition coefficients log of 2,2′,4,4′,6,6′-hexachlorobiphenyl (PCB-155) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1997		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		gas saturation-GC		generator column-GC	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	log K_{OA}
5	1.0×10^{-3}	–10	1.634×10^{-6}	–10	10.49
15	1.70×10^{-3}	0	1.185×10^{-5}	0	9.97
25	2.80×10^{-3}	10	8.039×10^{-5}	10	9.635
35	4.30×10^{-3}	20	3.250×10^{-4}	20	9.158
45	6.40×10^{-3}	30	7.739×10^{-4}	25	8.99
ΔH_{sol}/(kJ mol^{-1}) = 34.2 for 5–45°C		log (P/Pa) = A – B/(T/K)		ΔH_{OA}/(kJ mol^{-1}) = 63.9	
		A	14.84		
		B	5399	log K_{OA} = A + B/RT	
				A	–2.2
		ΔH_{subl}/(kJ mol^{-1}) = 103.4		B	3337.4

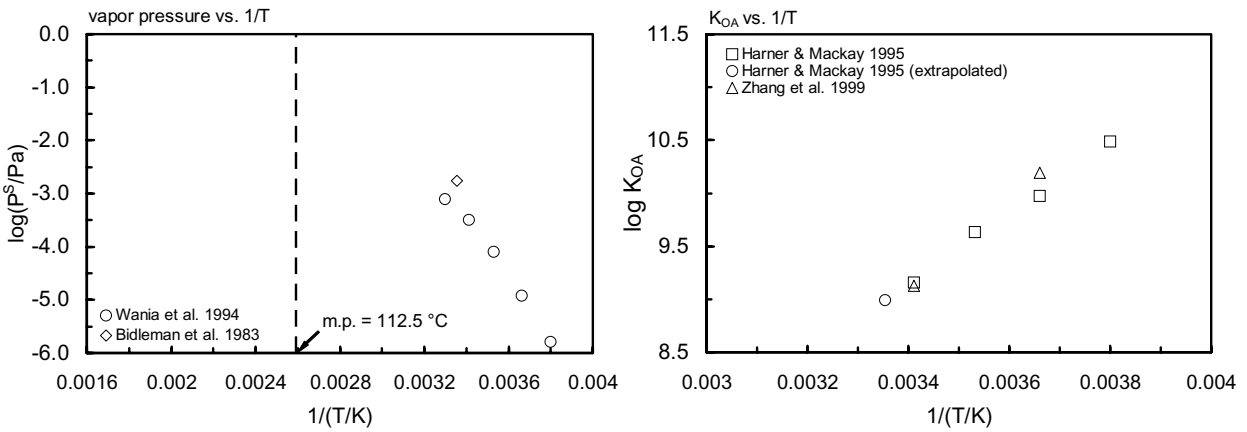

FIGURE 7.1.1.155.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 2,2′,4,4′,6,6′-hexachlorobiphenyl (PCB-155).

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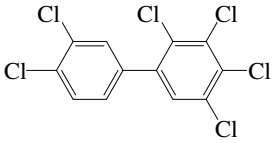
7.1.1.156 2,3,3′,4,4′,5-Hexachlorobiphenyl (PCB-156)



Common Name: 2,3,3′,4,4′,5-Hexachlorobiphenyl
Synonym: PCB-156, 2,3,3′,4,4′,5-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5-hexachlorobiphenyl
CAS Registry No: 38380-08-4
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
127 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F: 0.100 (mp at 127°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.00533 (20°C, supercooled liquid S_L, Murphy et al. 1987)
0.00361, 0.00244, 0.00112, 0.00102 (RP-HPLC-k′ correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)
0.000397 (generator column-GC/ECD, Hong & Qiao 1995)
0.0011 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000513, 0.000711, 0.00110, 0.00153 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.000215 (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
7.34×10^{-4} (supercooled liquid P_L, GC-RT correlation, Burkhard et al. 1985a)
0.000809 (GC-RI correlation, Burkhard et al. 1985b)
0.00021, 0.00016 (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.26×10^{-4}, 1.62×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4949/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
88.14 (concn ratio-GC, Murphy & Mullin 1983)
17.53 (calculated-P/C, Burkhard et al. 1985)
2.23 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
8.97 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)
3.72 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
37.0 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 112 \pm 10$ kJ/mol, $\Delta S_H = 0.34 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

7.13, 7,26, 7.84, 7.53 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.14, 7.12; 7.16, 7.13 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.70 (generator column-GC, Larsen et al. 1992)
7.11 (recommended, Sangster 1993)
7.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.07, 10.87; 10.87 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.36 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.88, 7.18 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.51 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.40 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.024 d^{-1} with an elimination $t_{½}$ = 29 d (earthworm, Belfroid et al. 1995)
k_2 = 0.004 d^{-1} with $t_{½}$ = 163 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 182 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: clearance $t_{½}$ = 50–100 d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);
reported biological half-lives for hexachlorobiphenyls: $t_{½}$ = 87 to > 850 d for trout, $t_{½}$ = 77–91 d for trout muscle; $t_{½}$ > 200 d for carp; $t_{½}$ = 75–175 d for guppy (Niimi 1987);
elimination $t_{½}$ = 29 d from earthworm (Belfroid et al. 1995)
depuration $t_{½}$ = 163 d for high-dose treatment, $t_{½}$ = 182 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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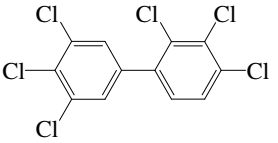
7.1.1.157 2,3,3′,4,4′,5′-Hexachlorobiphenyl (PCB-157)



Common Name: 2,3,3′,4,4′,5′-Hexachlorobiphenyl
Synonym: PCB-157, 2,3,3′,4,4′,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5′-hexachlorobiphenyl
CAS Registry No: 69782-90-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
141 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0152 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.000119 (generator column-GC/ECD, Hong & Qiao 1995)
0.000296 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000084, 0.000139, 0.000296, 0.000540 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.39×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
8.09×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
2.02×10^{-4}, 1.27×10^{-4} (supercooled liquid P_L, GC-RT correlation; different stationary phases, Foreman & Bidleman 1985)
1.17×10^{-4}, 1.58×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4994/(T/K) + 13.05$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.30 (calculated-P/C, Burkhard et al. 1985a)
58.76 (concn ratio-GC, Murphy & Mullin 1983)
6.69 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
8.56 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)
2.27 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
31.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 129 \pm 10$ kJ/mol, $\Delta S_H = 0.40 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.18 (calculated-TSA, Hawker & Connell 1988a)
7.26, 7.14; 7.19, 7.04 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.20 (quoted average values of Risby et al. 1990: GC-RV and HPLC-k′ correlations, Sangster 1993)

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7.60 (recommended, Hansch et al. 1995)
6.9661 (calculated-molecular properties MNDO-AM1, Makino 1998)
6.73; 6.90 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
7.37, 6.97 (calculated-MCI χ, calculated-MNDO-AMI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.28, 11.07; 10.76 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.51 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.40 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: clearance $t_{½}$ = 50–100 d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);
reported biological half-lives for hexachlorobiphenyls: $t_{½}$ = 87 to > 850 d for trout, $t_{½}$ = 77–91 d for trout muscle; $t_{½}$ > 200 d for carp; $t_{½}$ = 75–175 d for guppy (Niimi 1987)

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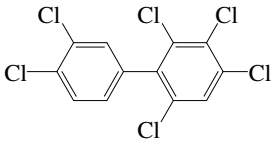
7.1.1.158 2,3,3′,4,4′,6-Hexachlorobiphenyl (PCB-158)



Common Name: 2,3,3′,4,4′,6-Hexachlorobiphenyl
Synonym: PCB-158, 2,3,3′,4,4′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,6-hexachlorobiphenyl
CAS Registry No: 74472-42-7
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
107 (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.157 (mp at 107°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.0159 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00807 (20°C, supercooled liquid, Murphy et al. 1987)
0.00120 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00114 (TSA and mp, Abramowitz & Yalkowsky 1990)
0.00185 (calculated-group contribution method, Kühne et al. 1995)
0.00147, 0.00396 (molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
9.26×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.02×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
6.19×10^{-4}, 4.486×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.73×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
3.09×10^{-4}, 4.57×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4816/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
20.97 (calculated-P/C, Burkhard 1984)
4.37 (20°C, calculated-P/C, Murphy et al. 1987)
21.89 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.86 (calculated-QSPR, Achman et al. 1993)
16.74 (calculated-QSPR, Dunnivant et al. 1992)
9.64 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 80 \pm 7$ kJ/mol, $\Delta S_H = 0.24 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

6.69 (calculated-TSA, Burkhard 1984)
6.78 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.02 (calculated-TSA, Hawker & Connell 1988a)
7.10, 6.87; 6.84, 6.82 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.78 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)
6.8874 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
7.69 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

9.51; 9.12 (generator column-GC.; K_{OW}/K_{AW}, Kömp & McLachlan 1997a)
$K_{OA} = -5.17 + 4380/(T/K)$, temp range 10–43°C (Kömp & McLachlan 1997a)
10.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.49 (suspended particulate matter, Burkhard 1984)
5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 - 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.006$ d^{-1} with $t_{½} = 124$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003$ d^{-1} with $t_{½} = 241$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 124 d for high-dose treatment, $t_{½}$ = 241 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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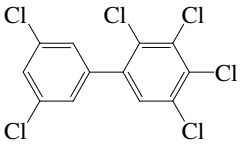
7.1.1.159 2,3,3′,4,5,5′-Hexachlorobiphenyl (PCB-159)



Common Name: 2,3,3′,4,5,5′-Hexachlorobiphenyl
Synonym: PCB-159, 2,3,3′,4,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5,5′-hexachlorobiphenyl
CAS Registry No: 39635-35-3
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
116 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0135 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
5.72×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.084×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00119 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
29.08 (calculated-P/C, Burkhard 1984)
31.41 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.027 (wetted wall column-GC/ECD, Brunner et al. 1990)
15.77 (calculated-QSPR, Dunnivant et al. 1992)
35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 116 \pm 12$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
7.24 (calculated-TSA, Hawker & Connell 1988a)
7.09, 7.24; 7.02, 7.00 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.17, 7.01 (quoted average values of Risby et al. 1990, Sangster 1993)
7.43 (recommended, Hansch et al. 1995)
7.2038 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.37 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56 (suspended particulate matter, Burkhard 1984)

5.381 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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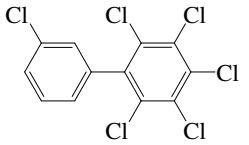
7.1.1.160 2,3,3′,4,5,6-Hexachlorobiphenyl (PCB-160)



Common Name: 2,3,3′,4,5,6-Hexachlorobiphenyl
Synonym: PCB-160, 2,3,3′,4,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5,6-hexachlorobiphenyl
CAS Registry No: 41411-62-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
99 (Burkhard et al. 1985b)
97–100 (Erickson 1986)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.188 (mp at 99°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0191 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00158 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
1.33×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00027 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
25.13 (calculated-P/C, Burkhard 1984)
25.74 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.027 (wetted wall column-GC/ECD, Brunner et al. 1990)
21.66 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.62 (calculated-TSA, Burkhard 1984)
6.93 (calculated-TSA, Hawker & Connell 1988a)
6.88, 6.79; 6.89, 6.87 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.84, 6.88 (quoted average values of Risby et al. 1990, Sangster 1993)
7.30 (recommended, Hansch et al. 1995)
6.9006 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.42 (suspended particulate matter, Burkhard 1984)

5.259 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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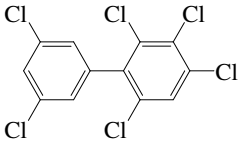
7.1.1.161 2,3,3′,4,5′,6-Hexachlorobiphenyl (PCB-161)



Common Name: 2,3,3′,4,5′,6-Hexachlorobiphenyl
Synonym: PCB-161, 2,3,3′,4,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5′,6-hexachlorobiphenyl
CAS Registry No: 74472-43-8
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
84.0 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.37×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00150 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
34.96 (calculated-P/C, Burkhard 1984)
51.27 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
28.89 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
7.08 (calculated-TSA, Hawker & Connell 1988a)
7.16, 6.94; 6.69, 6.66 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.05, 6.68 (quoted average values of Risby et al. 1990, Sangster 1993)
7.10 (recommended, Hansch et al. 1995)
7.0318 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.33 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.56 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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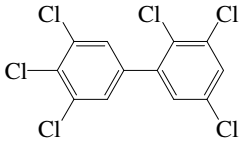
7.1.1.162 2,3,3′,4′,5,5′-Hexachlorobiphenyl (PCB-162)



Common Name: 2,3,3′,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-162, 2,3,3′,4,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 39635-34-2
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
84.0 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.37×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00150 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
34.96 (calculated-P/C, Burkhard 1984)
51.27 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
28.89 (calculated-QSPR, Dunnivant et al. 1992)
35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 116 \pm 12$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
7.08 (calculated-TSA, Hawker & Connell 1988a)
7.16, 6.94; 6.69, 6.66 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.05, 6.68 (quoted average values of Risby et al. 1990, Sangster 1993)
7.10 (recommended, Hansch et al. 1995)
7.0318 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.42 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.56 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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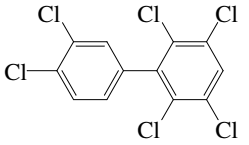
7.1.1.163 2,3,3′,4′,5,6-Hexachlorobiphenyl (PCB-163)



Common Name: 2,3,3′,4′,5,6-Hexachlorobiphenyl
Synonym: PCB-163, 2,3,3′,4′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5,6-hexachlorobiphenyl
CAS Registry No: 74472-44-9
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
88.2 (Shiu & Mackay 1986)
122 (Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F:
0.237 (assuming ΔS_{fus} = 56 J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.00531 (generator column-HPLC/UV, Huang 1983)
0.0053 (generator column-HPLC/UV, Billington et al. 1988)
0.0012 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8.67×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.54×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
6.01×10^{-4}, 4.92×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.31×10^{-4}, 5.25×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4816/(T/K) + 12.93$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
18.54 (calculated-P/C, Burkhard 1984)
11.75 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
1.52 (wetted wall column-GC/ECD, Brunner et al. 1990)
12.73 (calculated-QSPR, Dunnivant et al. 1992)
9.37 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 81 \pm 7$ kJ/mol, $\Delta S_H = 0.24 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.78 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.08; 6.99; 6.84, 6.79 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.39 (generator column-GC, average, Larsen et al. 1992)
6.78 (recommended, Sangster 1993)
7.25 (recommended, Hansch et al. 1995)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.26, 10.16 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
9.90 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.47 (suspended particulate matter, Burkhard 1984)
5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004$ d^{-1} with $t_{½} = 170$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003$ d^{-1} with $t_{½} = 198$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 170 d for high-dose treatment, $t_{½}$ = 198 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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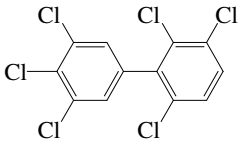
7.1.1.164 2,3,3′,4′,5′,6-Hexachlorobiphenyl (PCB-164)



Common Name: 2,3,3′,4′,5′,6-Hexachlorobiphenyl
Synonym: PCB-164, 2,3,3′,4′,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5′,6-hexachlorobiphenyl
CAS Registry No: 74472-45-0
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
96 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0161 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00194 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00144 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
4.478×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
4.97×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
10.04 (calculated-P/C, Burkhard 1984)
19.96 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
17.41 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.69 (calculated-TSA, Burkhard 1984)
6.63 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.02 (calculated-TSA, Hawker & Connell 1988a)
7.22, 7.32; 6.79, 6.73 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
6.63 (recommended, Sangster 1993)
7.20 (recommended, Hansch et al. 1995)
6.6712 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.35 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.49 (suspended particulate matter, Burkhard 1984)

5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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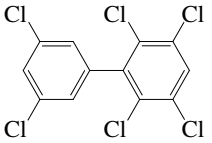
7.1.1.165 2,3,3′,5,5′,6-Hexachlorobiphenyl (PCB-165)



Common Name: 2,3,3′,5,5′,6-Hexachlorobiphenyl
Synonym: PCB-165, 2,3,3′,5,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,5,5′,6-hexachlorobiphenyl
CAS Registry No: 74472-46-1
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
101 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0150 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00114 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.292×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00140 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
30.9 (calculated-P/C, Burkhard 1984)
45.19 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
2.94 (wetted wall column-GC/ECD, Brunner et al. 1990)
27.91 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.57, 7.37 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
6.72 (calculated-TSA, Burkhard 1984)
7.05 (calculated-TSA, Hawker & Connell 1988a)
7.17, 6.90; 6.70, 6,65 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.37, 6.68, 7.04 (quoted literature values, Sangster 1993)
7.37 (recommended, Hansch et al. 1995)
7.0191 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
9.88 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

6.52 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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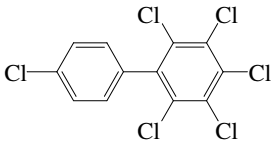
7.1.1.166 2,3,4,4′,5,6-Hexachlorobiphenyl (PCB-166)



Common Name: 2,3,4,4′,5,6-Hexachlorobiphenyl
Synonym: PCB-166, 2,3,4,4′,5,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3,4,4′,5,6-hexachlorobiphenyl
CAS Registry No: 41411-63-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
163.0 (Burkhard et al. 1985b)
160–165 (Erickson 1986)
145 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0443 (mp at 163°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0189 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
7.20×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
2.46×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C):
1.175×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
0.00140 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
22.49 (calculated-P/C, Burkhard 1984)
17.43 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
18.65 (calculated-QSPR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.62 (calculated-TSA, Burkhard 1984)
6.93 (calculated-TSA, Hawker & Connell 1988a)
7.13, 7.18; 6.90, 6.83 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.17, 6.87 (quoted average values of Risby et al. 1990, Sangster 1993)
7.31 (recommended, Hansch et al. 1995)
6.8501 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.42 (suspended particulate matter, Burkhard 1984)

5.259 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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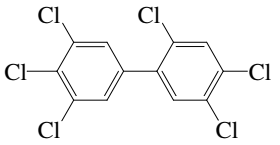
7.1.1.167 2,3′,4,4′,5,5′-Hexachlorobiphenyl (PCB-167)



Common Name: 2,3′,4,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-167, 2,3′,4,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 52663-72-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
135 (calculated-molecular properties, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0128 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00223 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.000531 (generator column-GC/ECD, Hong & Qiao 1995)
0.000107 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000442, 0.000682, 0.00107, 0.00161 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.88×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.12×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
2.80×10^{-4}, 2.39×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.34×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4994/(T/K) + 13.20$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.33 (calculated-P/C, Burkhard et al. 1985a)
12.46 (calculated-QSPR-MCIχ, Sabljic & Güsten 1989)
20.55 (calculated-QSPR, Dunnivant et al. 1992)
4.47 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
39.28 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 106 \pm 8$ kJ/mol, $\Delta S_H = 0.32 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.29 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.24, 7.30; 7.00, 7.03 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.29 (recommended, Sangster 1993)
7.50 (recommended, Hansch et al. 1995)
6.82 (generator column-GC/ECD, Yeh & Hong 2002)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or indicated:

12.07, 10.77; 10.76 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.59 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.97, 7.27 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.58 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.381 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-MCI χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_2 = 0.0263 d^{-1} with an elimination $t_{½}$ = 26 4 d (earthworm, Belfroid et al. 1995)
k_2 = 0.005 d^{-1} with $t_{½}$ = 134 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.005 d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).
Surface water: photodegradation $t_{½}$ = 38 min when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW Xenon lamp (De Felip et al. 1996)
Ground water:
Sediment:
Soil:
Biota: clearance $t_{½}$ = 50–100 d in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);
reported biological half-lives for hexachlorobiphenyls: $t_{½}$ = 87 to > 850 d for trout, $t_{½}$ = 77–91 d for trout muscle; $t_{½}$ > 200 d for carp; $t_{½}$ = 75–175 d for guppy (Niimi 1987);
elimination $t_{½}$ = 26.4 d from earthworm (Belfroid et al. 1995)
depuration $t_{½}$ = 134 d for high-dose treatment, $t_{½}$ = 153 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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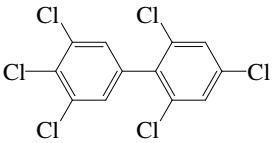
7.1.1.168 2,3′,4,4′,5′,6-Hexachlorobiphenyl (PCB-168)



Common Name: 2,3′,4,4′,5′,6-Hexachlorobiphenyl
Synonym: PCB-168, 2,3′,4,4′,5′,6-hexachloro-1,1′-biphenyl
Chemical Name: 2,3′,4,4′,5′,6-hexachlorobiphenyl
CAS Registry No: 59291-65-5
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
110–111 (Erickson 1986)
133 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
5.72×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
9.76×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.87×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.40×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
6.88×10^{-4}, 6.24×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4816/(T/K) + 12.99$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
13.07 (calculated-P/C, Burkhard 1984)
46.91 (calculated-QSAR-MCI χ, Sabljic & Güsten 1989)
27.97 (calculated-QSAR, Dunnivant et al. 1992)
49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.76 (calculated-TSA, Burkhard 1984)
7.11 (calculated-TSA, Hawker & Connell 1988a)
7.23, 7.13; 6.76, 6.71 (multi-column HPLC-k′ correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
7.18, 6.74 (quoted average values from Risby et al. 1990, Sangster 1993)
7.17 (recommended, Hansch et al. 1995)
6.8539 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

10.39 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.56 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calc-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

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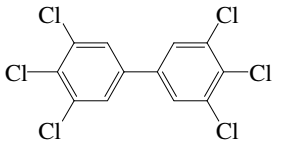
7.1.1.169 3,3′,4,4′,5,5′-Hexachlorobiphenyl (PCB-169)



Common Name: 3,3′,4,4′,5,5′-Hexachlorobiphenyl
Synonym: PCB-169, 3,3′,4,4′,5,5′-hexachloro-1,1′-biphenyl
Chemical Name: 3,3′,4,4′,5,5′-hexachlorobiphenyl
CAS Registry No: 32774-16-6
Molecular Formula: $C_{12}H_4Cl_6$
Molecular Weight: 360.878
Melting Point (°C):
201–202.0 (Hutzinger et al. 1974)
201 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
310.0 (calculated-Le Bas method at normal boiling point)
237.4 (Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0178 (calculated, Mackay et al. 1992; Passivirta et al. 1999)
0.0177 (Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
4.54×10^{-4}, 3.0×10^{-4}, 5.22×10^{-4}, 9.07×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.0000219; 0.000116 (generator column-GC, ECD; estimated, Hong & Qiao 1995)
log (S_L/(mol/L)) = –1.12 + 1403/(T/K) (supercooled liquid, Passivirta et al. 1999)
0.000130 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000053, 0.000083, 0.000130, 0.000215 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.08×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)
5.36×10^{-5} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
6.76×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = – 5313/(T/K) + 13.64 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
1.03×10^{-4}, 1.82×10^{-6} (supercooled liquid P_L, solid P_S, Passivirta et al. 1999)
log (P_S/Pa) = 16.59 – 6715/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 13.64 – 5313/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa m^3/mol at 25°C):
1.57 (calculated-P/C, Burkhard et al. 1985b)
5.98 (calculated-QSPR-MCI χ, Sabljic & Güsten 1989)
6.60 (calculated-QSPR, Dunnivant et al. 1992)
0.85 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
23.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 162 \pm 20$ kJ/mol, $\Delta S_H = 0.51 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

7.42, 7.54, 7.62, 7.61 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.408 ± 0.005 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
7.39, 7.55; 7.46, 7.42 (multi-column HPLC-k′ correlation; capillary GC-RT correlation, different stationary phases, Risby et al. 1990)
7.55 (recommended, Sangster 1993)
7.41 (recommended, Hansch et al. 1995)
7.01 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or indicated:

12.51, 11.32; 11.19 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.27 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.97; 7.50 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.97, 7.51 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.60 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 7200 d^{-1}; k_2 = 0.00766 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_1 = 2 (food lipid mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)
k_2 = 0.0065 d^{-1} with $t_{½}$ = 107 d (newly contaminated oysters, Gardinali et al. 2004)
k_2 = 0.0082 d^{-1} with $t_{½}$ = 85 d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);
$t_{½}$ = 6000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: photodegradation $t_{½}$ = 548 min when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);
$t_{½}$ = 120000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)
Groundwater:
Sediment: $t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{½}$ = 165000 h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: elimination $t_{½}$ = 24 d in earthworm given contaminated food (Wågman et al. 2001)
Depuration $t_{½}$ = 107 d for newly contaminated oysters, and $t_{½}$ = 85 d for chronically contaminated oysters (Gardinali et al. 2004)

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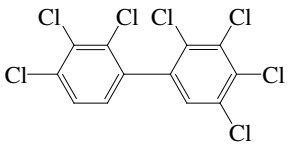
7.1.1.170 2,2′,3,3′,4,4′,5-Heptachlorobiphenyl (PCB-170)



Common Name: 2,2′,3,3′,4,4′,5-Heptachlorobiphenyl
Synonym: PCB-170, 2,2′,3,3′,4,4′,5-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5-heptachlorobiphenyl
CAS Registry No: 35065-30-6
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
135 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0833 (mp at 135°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.00767 (supercooled liquid S_L, Burkhard et al. 1985b)
0.00347 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.000504 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.000395 (calculated-TSA, Abramowitz & Yalkowsky 1990)
0.00052 (calculated-MCI χ, Patil 1991)
0.000130 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.37×10^{-5} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
3.37×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
3.72×10^{-4} (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)
8.37×10^{-5}, 8.11×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.32×10^{-5} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
5.13×10^{-5}, 7.76×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5139/(T/K) + 13.07$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
19.25 (calculated-P/C, Burkhard 1985b)
1.52 (20°C, calculated-P/C, Murphy et al. 1987)
0.912 (wetted-wall column-GC, Brunner et al. 1990)
8.85 (calculated-QSPR, Dunnivant et al. 1992)
0.128, 0.760, 4.139, 20.84* ± 0.80, 78.50 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 61.342 - 19725.76/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(164.0/kJ \cdot mol^{-1})/ RT] + (0.510/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 $J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
19.4 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 164 \pm 9$ kJ/mol, $\Delta S_H = 0.51 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

7.05 (calculated-TSA, Burkhard 1984)
7.08 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.27 (calculated-TSA, Hawker & Connell 1988a)
7.03 (calculated-MCI χ, Patil 1991)
7.30 (calculated-TSA, Murray & Andren 1992)
6.83 (generator column-GC, Larsen et al. 1992)
6.96 (recommended, Sangster 1993)
7.10 (estimated, Girvin & Scott 1997)
7.0639 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.42 (10°C, estimated, Thomas et al. 1998)
12.34, 11.07; 11.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.69 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

2.43–4.76 (various marine species, mean dry wt. BCF, Hope et al. 1998)
3.75–4.61 (Various marine species, mean lipid-normalized BCF, Hope et al. 1999)

Sorption Partition Coefficient, log K_{OC}:

6.85 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.63, 5.48, 5.42, 4.99 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.632, 5.675 (marine humic substances of 5 mg/L DOC, quoted; calculated-MCI χ, reported as association coefficient log K_h, Sabljic et al. 1989)
6.10 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.60 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 164$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 180$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 164 d for high-dose treatment, $t_{½}$ = 180 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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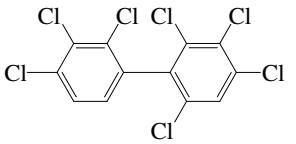
7.1.1.171 2,2′,3,3′,4,4′,6-Heptachlorobiphenyl (PCB-171)



Common Name: 2,2′,3,3′,4,4′,6-Heptachlorobiphenyl
Synonym: PCB-171, 2,2′,3,3′,4,4′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,6-heptachlorobiphenyl
CAS Registry No: 52663-71-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
117.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.29 (Miller et al. 1984; Ruelle et al. 1993)
22.80 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
51.04 (Miller et al. 1984; Shiu & Mackay 1986)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.124 (mp at 117.5°C)
0.109 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00624 (shake flask-GC/ECD, Dexter & Pavlou 1978)
0.00217 (generator column-GC/ECD, Miller et al. 1984,1985)
0.00412 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
9.81×10^{-6} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
0.00102, 0.000687, 0.000521 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.87×10^{-4}, 2.98×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
5.71×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
4.69×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
2.57×10^{-4}, 3.17×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases**,** Foreman & Bidleman 1985)
2.73×10^{-5}, 2.50×10^{-4} (selected, solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
1.26×10^{-4}, 2.09×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5008/(T/K) + 13.07$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
9.77×10^{-5} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa m^3/mol at 25°C):
29.79 (calculated-P/C, Burkhard et al. 1985b)
5.40 (calculated-P/C, Shiu & Mackay 1986)
17.49 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)

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59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
6.68 (generator column-GC/ECD, Miller et al. 1984,1985)
7.85 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
7.04, 7.06 (RP-HPLC-k′ correlation, different mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.99 (recommended, Sangster 1993)
6.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:
9.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
10.51 (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
12.31, 11.78, 11.14, 10.51, 9.96 (–10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
log $K_{OA} = -5.71 + 4757/(T/K)$; (temp range –10 to 30°C, Harner & Bidleman 1996)
11.76, 10.51; 10.50 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
6.94 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.516 (marine humic substances of 5 mg/L DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.004$ d^{-1} with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004$ d^{-1} with $t_{½} = 182$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:
Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 260 d in worms at 8°C (Oliver 1987c).
depuration $t_{½} = 156$ d for high-dose treatment, $t_{½} = 182$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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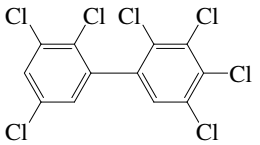
7.1.1.172 2,2′,3,3′,4,5,5′-Heptachlorobiphenyl (PCB-172)



Common Name: 2,2′,3,3′,4,5,5′-Heptachlorobiphenyl
Synonym: PCB-172, 2,2′,3,3′,4,5,5′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′-heptachlorobiphenyl
CAS Registry No: 52663-74-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
113 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00688 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00430 (20°C, supercooled liquid, Murphy et al. 1987)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
4.98×10^{-4} (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.55×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.14×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.41×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5109/(T/K) + 12.28$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
31.82 (calculated-P/C, Burkhard 1984)
1.317 (wetted wall column-GC/ECD, Brunner et al. 1990)
12.07 (calculated-QSPR, Dunnivant et al. 1992)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.10 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.85 (generator column-GC, Larsen et al. 1992)
7.33 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.03 (recommended, Sangster 1993)
7.2349 (molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.84, 10.67 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.50 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.89 (suspended particulate matter, Burkhard 1984)

5.71, 5.44, 5.38, 4.97 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)

5.711; 5.66 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 165$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 179$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 165 d for high-dose treatment, $t_{½}$ = 179 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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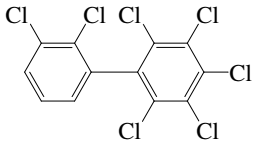
7.1.1.173 2,2′,3,3′,4,5,6-Heptachlorobiphenyl (PCB-173)



Common Name: 2,2′,3,3′,4,5,6-Heptachlorobiphenyl
Synonym: PCB-173, 2,2′,3,3′,4,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6-heptachlorobiphenyl
CAS Registry No: 68194-16-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
145 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00731 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00416 (20°C, supercooled liquid, Murphy et al. 1987)
6.265×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
5.55×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.14×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
29.89 (calculated-P/C, Burkhard 1984)
1.42 (wetted wall column-GC/ECD, Brunner et al. 1990)
18.48 (calculated-QSPR, Dunnivant et al. 1992)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.07 (calculated-TSA, Burkhard 1984)
7.02 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.30 (calculated-TSA, Murray & Andren 1992)
6.9556 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.79, 10.60 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.48 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.87 (suspended particulate matter, Burkhard 1984)

5.532 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 2 (food lipid mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 162 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 186 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 20 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{½}$ = 162 d for high-dose treatment, $t_{½}$ = 186 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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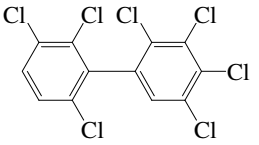
7.1.1.174 2,2′,3,3′,4,5,6′-Heptachlorobiphenyl (PCB-174)



Common Name: 2,2′,3,3′,4,5,6′-Heptachlorobiphenyl
Synonym: PCB-174, 2,2′,3,3′,4,5,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6′-heptachlorobiphenyl
CAS Registry No: 38411-25-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
130.6 (Burkhard 1985b)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (KJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.092 (mp at 130.6°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00625 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00525 (20°C, supercooled liquid, Murphy et al. 1987)
0.001016 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.687×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
3.191×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.206×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.19×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.80×10^{-4}, 2.43×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
6.69×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
2.75×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 12.90$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
93.53 (calculated-P/C, Burkhard 1984)
4.96 (20°C, calculated-P/C, Murphy et al. 1987)
1.419 (wetted wall column-GC/ECD, Brunner et al. 1990;)
17.13 (calculated-QSPR, Dunnivant et al. 1992)
4.91 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
49.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 113 \pm 11$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
6.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

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6.85 (recommended, Sangster 1993)
7.10 (estimated, Girvin & Scott 1997)
6.9132 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.67, 10.51; 10.64 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.38 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

89 (trout in Lake Ontario, Niimi 1996)
0.29, 2.8, 1.4(grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:

6.94 (suspended particulate matter, Burkhard 1984)
5.52 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
5.82 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.60 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1979)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 194$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 160 d for high-dose treatment, $t_{½}$ = 194 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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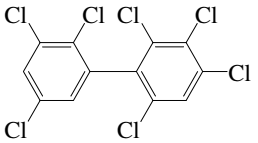
7.1.1.175 2,2′,3,3′,4,5′,6-Heptachlorobiphenyl (PCB-175)



Common Name: 2,2′,3,3′,4,5′,6-Heptachlorobiphenyl
Synonym: PCB-175, 2,2′,3,3′,4,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5′,6-heptachlorobiphenyl
CAS Registry No: 40186-70-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
133 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00557 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00894 (20°C, supercooled liquid, Murphy et al. 1987)
0.00104 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
4.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7.00×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.72×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
3.98×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 12.22$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
49.55 (calculated-P/C, Burkhard 1984)
22.63 (calculated-QSPR, Dunnivant et al. 1992)
2.069 (calculated-QSPR, Achman et al. 1993)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.19 (calculated-TSA, Burkhard 1984)
6.92 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988a)
7.17 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
6.92 (recommended, Sangster 1993)
7.10 (estimated, Girvin & Scott 1997)
7.0957 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.35, 10.17 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

144 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

6.99 (suspended particulate matter, Burkhard 1984)

5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

6.60 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005\ d^{-1}$ with $t_{½} = 154$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 169$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 154 d for high-dose treatment, $t_{½}$ = 169 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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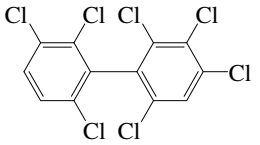
7.1.1.176 2,2′,3,3′,4,6,6′-Heptachlorobiphenyl (PCB-176)



Common Name: 2,2′,3,3′,4,6,6′-Heptachlorobiphenyl
Synonym: PCB-176, 2,2′,3,3′,4,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,6,6′-heptachlorobiphenyl
CAS Registry No: 52663-65-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
101 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00601 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00585 (20°C, supercooled liquid, Murphy et al. 1987)
0.00280 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00314 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.66×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
5.31×10^{-4}, 8.83×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.35×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.50 – 5080/(T/K) (GC-RT correlation, Tateya et al. 1988)
4.17×10^{-4}, 7.24×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –4579/(T/K) + 12.07 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
100 (calculated-P/C, Burkhard 1984)
9.12 (20°C, calculated-P/C, Murphy et al. 1987)
30.11 (calculated-QSPR, Dunnivant et al. 1992)
3.13 (calculated-QSPR, Achman et al. 1993)
107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.16 (calculated-TSA, Burkhard 1984)
6.55 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.76 (generator column-GC, Larsen et al. 1992)
6.65 (recommended, Sangster 1993)
6.6653 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.22, 10.06; 10.13 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.96 (suspended particulate matter, Burkhard 1984)
5.358 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 184$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005\ d^{-1}$ with $t_{½} = 153$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 184 d for high-dose treatment, $t_{½}$ = 153 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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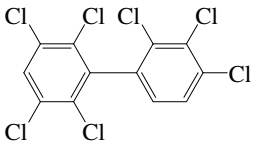
7.1.1.177 2,2′,3,3′,4,5′,6′-Heptachlorobiphenyl (PCB-177)



Common Name: 2,2′,3,3′,4,5′,6′-Heptachlorobiphenyl
Synonym: PCB-177, 2,2′,3,3′,4,5′,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5′,6′-heptachlorobiphenyl
CAS Registry No: 52663-70-4
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
145 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00656 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00482 (20°C, supercooled liquid, Murphy et al. 1987)
0.00150 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
4.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
4.40×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
4.88×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
2.50×10^{-4}, 3.38×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
4.15×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
1.38×10^{-4}, 2.51×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 13.04$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
26.45 (calculated-P/C, Burkhard 1984)
3.34 (20°C, calculated-P/C, Murphy et al. 1987)
15.55 (calculated-QSPR, Dunnivant et al. 1992)
2.069 (calculated-QSPR, Achman et al. 1993)
5.12 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
50.6 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 112 \pm 11$ kJ/mol, $\Delta S_H = 0.34 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.12 (calculated-TSA, Burkhard 1984)
6.73 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.73 (recommended, Sangster 1993)

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7.10 (estimated, Girvin & Scott 1997)
6.9207 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.74, 10.58 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.92 (suspended particulate matter, Burkhard 1984)
5.54, 5.39, 5.35, 4.90 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.359; 5.52 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
5.82 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.60 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005\ d^{-1}$ with $t_{½} = 147$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 186$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 147 d for high-dose treatment, $t_{½}$ = 186 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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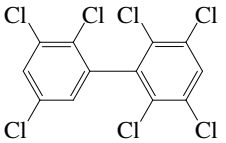
7.1.1.178 2,2′,3,3′,5,5′,6-Heptachlorobiphenyl (PCB-178)



Common Name: 2,2′,3,3′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-178, 2,2′,3,3′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-67-9
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
125 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00588 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00884 (20°C, supercooled liquid, Murphy et al. 1987)
0.001016 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.000627 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.57×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.24×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.47×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
log (P/mmHg) = 11.70 – 5220/(T/K) (GC-RT correlation, Tateya et al. 1988)
4.57×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
log (P_L/Pa) = –4962/(T/K) + 13.28 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
44.08 (calculated-P/C, Burkhard 1984)
6.586 (20°C, calculated-P/C, Murphy et al. 1987)
2.33 (wetted wall column-GC/ECD, Brunner et al. 1990)
21.61 (calculated-QSPR, Dunnivant et al. 1992)
11.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
71.4 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 90 \pm 10$ kJ/mol, $\Delta S_H = 0.27 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.17 (calculated-TSA, Burkhard 1984)
6.85 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.14 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.85 (recommended, Sangster 1993)
7.0564 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.28, 10.12 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.33 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.97 (suspended particulate matter, Burkhard 1984)
5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 156 d for high-dose treatment, $t_{½}$ = 166 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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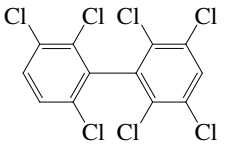
7.1.1.179 2,2′,3,3′,5,6,6′-Heptachlorobiphenyl (PCB-179)



Common Name: 2,2′,3,3′,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-179, 2,2′,3,3′,5,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,6,6′-heptachlorobiphenyl
CAS Registry No: 52663-64-6
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
99 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00632 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00454 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.0039 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.42×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.55×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
5.15×10^{-4}, 1.004×10^{-3} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.01×10^{-4}, 8.71×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4579/(T/K) + 12.07$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
88.96 (calculated-P/C, Burkhard 1984)
2.432 (wetted wall column-GC/ECD, Brunner et al. 1990)
27.91 (calculated-QSPR, Dunnivant et al. 1992)
37.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 144 \pm 7$ kJ/mol, $\Delta S_H = 0.45 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
6.77, 8.13 (RP-HPLC-k′ correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
7.14 (calculated-TSA, Burkhard 1984)
6.41 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.41 (recommended, Sangster 1993)
6.6366 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.26, 10.10 (0, 20°C, multi-column k′ correlation, Zhang et al. 1999)
10.34 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.94 (suspended particulate matter, Burkhard 1984)
5.358 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 198$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 171 d for high-dose treatment, $t_{½}$ = 198 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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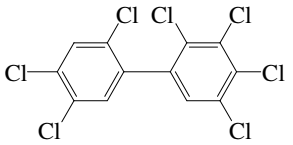
7.1.1.180 2,2′,3,4,4′,5,5′-Heptachlorobiphenyl (PCB-180)



Common Name: 2,2′,3,4,4′,5,5′-Heptachlorobiphenyl
Synonym: PCB-180, 2,2′,3,4,4′,5,5′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,5′-heptachlorobiphenyl
CAS Registry No: 35065-29-3
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
109–110 (Hutzinger et al. 1974)
Boiling Point (°C): 240–280 (20mm Hg)
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.144 (calculated-Mackay et al. 1992; Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):
0.00656 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
0.00385 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.00031 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00063 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.00053 (calculated-MCI χ, Patil 1991)
2.45×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)
$\log S_L$ (mol/L) = –1.676 + 1132/(T/K) (supercooled liquid, Passivirta et al. 1999)
3.17×10^{-3}; 5.22×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3})$ = –1356/(T/K) – 0.33 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8.10×10^{-5} (Verlag Chemie 1983)
1.30×10^{-4}, 1.29×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Bidleman 1984)
8.07×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
5.06×10^{-4} (supercooled liquid P_L, calculated-GC-RI correlation, Burkhard 1985b)
1.21×10^{-4}, 1.43×10^{-4} (supercooled liquid. P_L, GC-RT correlation, different stationary phases Foreman & Bidleman 1985)
3.14×10^{-5} (20°C, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
8.13×10^{-5}, 1.20×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/\text{Pa})$ = – 5042/(T/K) + 13.03 (GC-RT correlation, Falconer & Bidleman 1994)
1.45×10^{-4}, 2.09×10^{-5} (supercooled liquid P_L, solid P_S, Passivirta et al. 1999)
$\log (P_S/\text{Pa})$ = 15.98 – 6173/(T/K) (solid, Passivirta et al. 1999)
$\log (P_L/\text{Pa})$ = 13.03 – 5042/(T/K) (supercooled liquid, Passivirta et al. 1999)
1.32×10^{-4}; 1.072×10^{-4} (supercooled P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/\text{Pa}$ = –4809/(T/K) + 12.16 (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

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Henry's Law Constant (Pa m^3/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

30.40 (calculated-P/C, Burkhard et al. 1985b)
3.24 (20°C, calculated-P/C, Murphy et al. 1987)
1.013 (wetted-wall column-GC/ECD, Brunner et al. 1990)
10.88 (calculated-QSPR, Dunnivant et al. 1992)
7.10 (estimated, Girvin & Scott 1997)
log H/(Pa m^3/mol) = 14.71 – 3910/(T/K) (Passivirta et al. 1999)
37.0* ± 0.20 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
K_{AW} = exp[–(143.6/kJ·mol^{-1})/ RT] + (0.447/kJ·mol^{-1}·K^{-1})/R]; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
37.3 (exptl. data, Bamford et al. 2002)—see Comment by Goss et al. 2004
ln K_{AW} = $-\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 144 ± 7 kJ/mol, ΔS_H = 0.45 ± 0.03 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
5.89, 8.51 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log H/(Pa m^3/mol) = –3453/(T/K) + 12.49 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

7.12 (calculated-TSA, Burkhard 1984)
6.70 (calculated-chlorine substituents, Oliver 1987a)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.36 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.02 (calculated-MCI χ, Patil 1991)
7.40 (calculated-TSA, Murray & Andren 1992)
6.56 (average, generator column-GC, Larsen et al. 1992)
6.89 (recommended, Sangster 1993)
7.2506 (calculated-molecular properties MNDO-AM1, Makino 1998)
7.20 (calculated, Passivirta et al. 1999)
7.29, 7.16 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

10.75* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
log K_{OA} = –4.70 + 4535/(T/K); (temp range –10 to 30°C, Harner & Bidleman 1996)
9.88; 9.72 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = –3.31 + 3930/(T/K); (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
11.22 (10°C, estimated, Thomas et al. 1998)
9.88 (quoted, Kömp & McLachlan 1997b; Kaupp & McLachlan 1999)
11.94, 10.72; 10.86 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
10.12, 10.16 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4975/(T/K) – 6.55 (LDV linear regression of literature data, Li et al. 2003)
log K_{OA} = 4845/(T/K) – 6.09 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.99–5.68 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.22–6.41 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
4.45, 6.45 (*Daphnia magna*, 21-d exposure: wet wt basis, lipid wt basis, Geyer et al. 2000)
6.06, 7.36 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

6.92 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.2–7.4, 6.9; 7.30 (suspended sediments, range; average, algae > 50 μm, Oliver 1987a)
6.51 (Lake Michigan water column, Swackhamer & Armstrong 1987)

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5.73, 5.54, 5.50, 5.09 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.73; 5.66 (marine humic substances at 5 mg/L DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.36, 6.23, 6.10 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
5.78 (Ispra soil, shake flask-GC/ECD, Paya-Perez et al. 1991)
6.60 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.60 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.53–7.76; 5.80–7.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.42; 6.56, 7.42, 6.83 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
6.31–6.98 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 0.049\ h^{-1}$; $k_1 = 0.008\ h^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)
$k_2 = 0.0246\ d^{-1}$ with an elimination $t_{½} = 282$ d (earthworm, Belfroid et al. 1995)
$k_1 = 0.00348\ h^{-1}$; $k_2 = 0.111\ h^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
k_1(calc) = 2 (food lipid mg)/(g worm lipid-d); k_2(calc) = $0.03\ d^{-1}$ (earthworm, Wågman et al. 2001)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 162$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 186$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
$k_2 = 0.021\ d^{-1}$ with $t_{½} = 33.0$ d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: $t_{½} = 12000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Surface water: $t_{½} = 240000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Groundwater:
Sediment: very persistent, $t_{½} = 25$ yr (Geyer et al. 2000)
$t_{½} = 330000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Soil: $t_{½} = 333000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
Biota: elimination $t_{½} = 28.3$ d from earthworm (Belfroid et al. 1995);
elimination $t_{½} = 22$ d in earthworm given contaminated food (predicted, Wågman et al. 2001)
depuration $t_{½} = 162$ d for high-dose treatment, $t_{½} = 186$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)
depuration $t_{½} = 33.0$ d (juvenile carp in 100-d experiment Stapleton et al. 2004)

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TABLE 7.1.1.180.1
Reported Henry's law constants and octanol-air partition coefficients of 2,2′,3,4,4′,5,5′-heptachlorobiphenyl (PCB-180) at various temperatures and temperature dependence equations

Henry's law constant		log K_{OA}	
Bamford et al. 2000		Harner & Bidleman 1996	
gas stripping-GC/MS		generator column-GC	
t/°C	H/(Pa m³/mol)	t/°C	log K_{OA}
4	0.425	–10	12.46
11	2.025	0	12.00
18	8.96	10	11.38
25	37.0	20	10.75
31	118.5	30	10.23
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 86.83$	
A	53.7647		
B	17272	$\log K_{OA} = A + B/T$	
		A	–4.695
enthalpy, entropy change:		B	4535
$\Delta H/(kJ \cdot mol^{-1}) = 143.6 \pm 7.4$			
$\Delta S/(J \cdot mol^{-1} \cdot K^{-1}) = 447 \pm 26$			

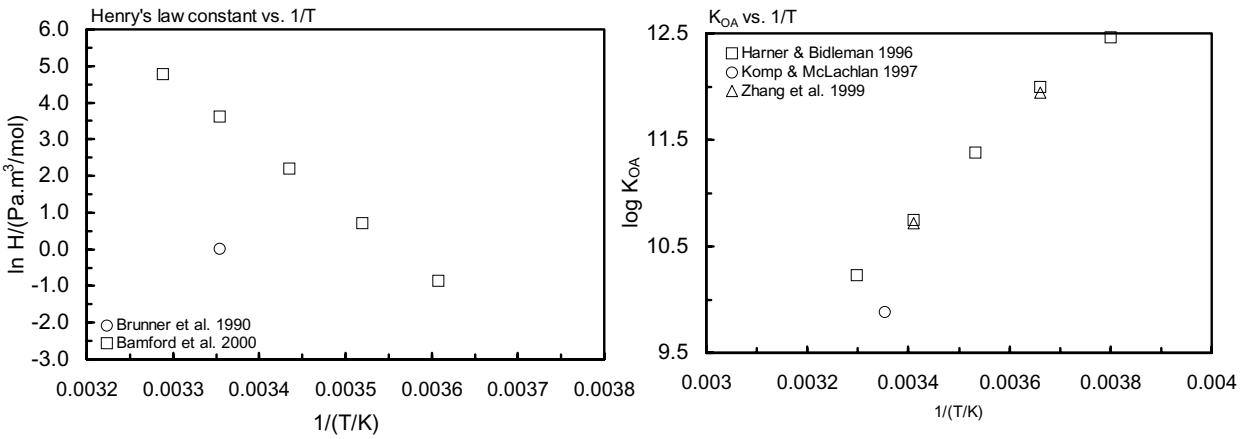

FIGURE 7.1.1.180.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,2′,3,4,4′,5,5′-heptachlorobiphenyl (PCB-180).

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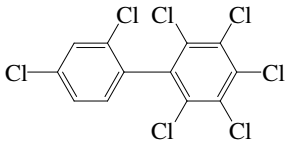
7.1.1.181 2,2′,3,4,4′,5,6-Heptachlorobiphenyl (PCB-181)



Common Name: 2,2′,3,4,4′,5,6-Heptachlorobiphenyl
Synonym: PCB-181, 2,2′,3,4,4′,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6-heptachlorobiphenyl
CAS Registry No: 74472-47-2
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
140 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00625 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.44×10^{-4}, 5.21×10^{-4}; 2.30×10^{-4}, 4.54×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)
3.95×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.44×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.11×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
2.92×10^{-4}, 4.206×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.54×10^{-4} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/Pa) = -4962/(T/K) + 13.11$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
40.83 (calculated-P/C, Burkhard 1984)
23.31 (calculated-QSPR, Dunnivant et al. 1992)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
7.11, 7.12, 7.19, 7.11 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.13 (recommended, Sangster 1993)
7.0558 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.61 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log K_B or log BCF:

Sorption Partition Coefficient, log K_{OC}:

6.94	(suspended particulate matter, Burkhard 1984)
5.516	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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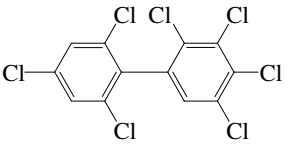
7.1.1.182 2,2′,3,4,4′,5,6′-Heptachlorobiphenyl (PCB-182)



Common Name: 2,2′,3,4,4′,5,6′-Heptachlorobiphenyl
Synonym: PCB-182, 2,2′,3,4,4′,5,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6′-heptachlorobiphenyl
CAS Registry No: 60145-23-5
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
152 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0567 (mp at 152°C)

Water Solubility (g/m^3 or mg/L at 25°C):
5.34×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
8.26×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
3.95×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.36×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.31×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.43×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
3.66×10^{-4}, 3.56×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.14×10^{-4}, 3.72×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 13.11$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
97.07 (calculated-P/C, Burkhard 1984)
26.04 (calculated-QSPR, Dunnivant et al. 1992)
2.07 (calculated-QSPR, Achman et al. 1993)
8.71 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
63.8 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 97 \pm 10$ kJ/mol, $\Delta S_H = 0.30 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.22 (calculated-TSA, Burkhard 1984)
6.92 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.92 (recommended, Sangster 1993)
7.0964 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA}:

10.42 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.02 (suspended particulate matter, Burkhard 1984)

5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calc-molecular connectivity indices, Sabljic et al. 1989)

6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 159$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 182$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 159 d for high-dose treatment, $t_{½}$ = 182 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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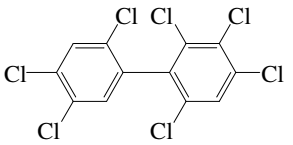
7.1.1.183 2,2′,3,4,4′,5′,6-Heptachlorobiphenyl (PCB-183)



Common Name: 2,2′,3,4,4′,5′,6-Heptachlorobiphenyl
Synonym: PCB-183, 2,2′,3,4,4′,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-69-1
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
152 (estimated, Abramowitz & Yalkowsky 1990)
83 (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.270 (mp at 83°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00534 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00490 (20°C, supercooled liquid, Murphy et al. 1987)
3.14×10^{-4}, 4.98×10^{-4}, 6.27×10^{-4}, 5.09×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
3.14×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
0.000641 (calculated-group contribution method, Kühne et al. 1995)
9.27×10^{-4}, 2.49×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
1.77×10^{-3} (calculated-mp and K_{OW}, Ran et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.38×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
7.05×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
3.57×10^{-4}, 5.09×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
8.61×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
2.0×10^{-4}, 3.24×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 13.19$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
47.32 (calculated-P/C, Burkhard 1984)
6.89 (20°C, calculated-P/C, Murphy et al. 1987)
20.40 (calculated-QSPR, Dunnivant et al. 1992)
2.069 (calculated-QSPR, Achman et al. 1993)
0.326, 0.954 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
8.02 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
61.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 100 \pm 10$ kJ/mol, $\Delta S_H = 0.30 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

7.22 (calculated-TSA, Burkhard 1984)
7.02, 7.13, 6.96, 7.07 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.78 (generator column-GC, Larsen et al. 1992)
6.92 (recommended, Sangster 1993)
7.0868 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
8.27 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

10.80 (10°C, estimated, Thomas et al. 1998)
11.44, 10.26; 10.35 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.84, 7.37 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:

220 (trout in Lake Ontario, Niimi 1996)
0.52, 4.2, 0.84 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:

7.02 (suspended particulate matter, Burkhard 1984)
5.53, 5.40, 5.35, 4.92 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.53; 5.50 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
6.36, 6.25, 6.09 (North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
5.82 (Ispra soil, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 165$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.003\ d^{-1}$ with $t_{½} = 206$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 165 d for high-dose treatment, $t_{½}$ = 206 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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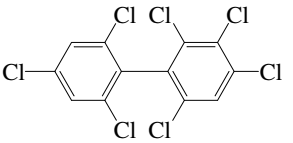
7.1.1.184 2,2′,3,4,4′,6,6′-Heptachlorobiphenyl (PCB-184)



Common Name: 2,2′,3,4,4′,6,6′-Heptachlorobiphenyl
Synonym: PCB-184, 2,2′,3,4,4′,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,6,6′-heptachlorobiphenyl
CAS Registry No: 74472-48-3
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
108 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00514 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00198 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C):
1.65×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.80×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m^3/mol at 25°C):
126.7 (calculated-P/C, Burkhard 1984)
46.42 (calculated-QSPR, Dunnivant et al. 1992)
3.94 (calculated-QSPR, Achman et al. 1993)
107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.23 (calculated-TSA, Burkhard 1984)
6.85 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.76 (generator column-GC, Larsen et al. 1992)
6.65 (recommended, Sangster 1993)
6.8203 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
7.03 (suspended particulate matter, Burkhard 1984)
5.342 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 2 (food lipid mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 20 d in earthworm given contaminated food (Wågman et al. 2001)

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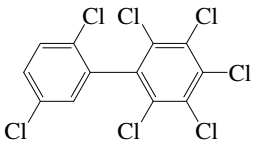
7.1.1.185 2,2′,3,4,5,5′,6-Heptachlorobiphenyl (PCB-185)



Common Name: 2,2′,3,4,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-185, 2,2,3,4,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52712-05-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
149 (Bruggeman et al. 1982; Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.3702
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0607 (mp at 149°C)
0.0595 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00047 (generator column-GC/ECD, Weil et al. 1974)
0.00546 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
5.71×10^{-4}, 8.26×10^{-4}, 6.27×10^{-4}, 6.56×10^{-4} (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.75×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
7.28×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.21×10^{-4}, 4.78×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.70×10^{-4}, 2.95×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4962/(T/K) + 13.15$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
46.0 (calculated-P/C, Burkhard et al. 1985b)
1.62 (wetted-wall column-GC, Brunner et al. 1990)
21.71 (calculated-QSPR, Dunnivant et al. 1992)
2.67 (calculated-QSPR, Achman et al. 1993)
59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.93 (TLC-RT correlation, Bruggeman et al. 1982)
7.01, 6.98, 6.96, 7.00 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.99 (recommended, Sangster 1993)

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Octanol/Air Partition Coefficient, log K_{OA}:

10.58 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

4.36 (*Picea omorika*, Reischl et al. 1989 from Reischl 1988)
5.93; 7.46 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.93, 7.47 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.95 (Koch 1983)
6.94 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.52 (marine humic substances of 5 mg/L DOC, calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
5.33 (calculated-K_{OW}, Bahnick & Doucette 1988)
6.43 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
5.28 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
6.29. 6.08, 6.13 (North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
5.80 (calculated-MCI, Park & Lee 1993)
6.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.40 (soil, calculated-universal solvation model; Winglet et al. 2000)

Sorption Partition Coefficient, log K_{OM}:

5.95, 5.31 (selected, calculated-molecular connectivity indices χ, Sabljic 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 5810 d^{-1}; k_2 = 0.00677 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{½}$ = 156 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 184 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ = 48 d in *Picea omorika* (Reischl et al. 1989 from Reischl 1988).
depuration $t_{½}$ = 156 d for high-dose treatment, $t_{½}$ = 184 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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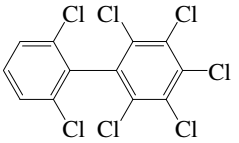
7.1.1.186 2,2′,3,4,5,6,6′-Heptachlorobiphenyl (PCB-186)



Common Name: 2,2′,3,4,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-186
Chemical Name: 2,2′,3,4,5,6,6′-heptachlorobiphenyl
CAS Registry No: 74472-49-4
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
142 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00672 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00157 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.35×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.47×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)
4.68×10^{-4}, 7.55×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -4579/(T/K) + 12.03$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
79.13 (calculated-P/C, Burkhard 1984)
37.3 (calculated-QSPR, Dunnivant et al. 1992)
107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.11 (calculated-TSA, Burkhard 1984)
6.69 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.7069 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.36 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
6.91 (suspended particulate matter, Burkhard 1984)
5.383 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

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Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota:

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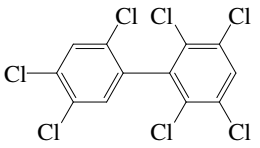
7.1.1.187 2,2′,3,4′,5,5′,6-Heptachlorobiphenyl (PCB-187)



Common Name: 2,2′,3,4′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-187, 2,2′,3,4′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 52663-68-0
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
149.0 (Mackay et al. 1980; Burkhard et al. 1985a)
147 (Ruelle & Kesselring 1997)
Boiling Point (°C):
417 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
250.3 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0607 (mp at 149°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.70×10^{-4} (generator column-GC/ECD, Weil et al. 1974)
0.00451 (20°C, supercooled liquid S_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
0.0826 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.05×10^{-4} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
3.92×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
5.98×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.47×10^{-4}, 5.74×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.42×10^{-5} (20°C, supercooled liquid P_L, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
2.14×10^{-4}, 3.72×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -4977/(T/K) + 12.96$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
42.15 (calculated-P/C, Burkhard et al. 1985b)
8.41 (20°C, calculated-P/C, Murphy et al. 1987)
20.55 (calculated-QSPR, Dunnivant et al. 1992)
2.07 (calculated-QSPR, Achman et al. 1993)
3.304, 8.72, 23.84, 82.20 ± 2.2, 136.7 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 35.242 - 11582.87/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(96.3/kJ \cdot mol^{-1})/RT] + (0.293/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
65.9 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 96 \pm 7$ kJ/mol, $\Delta S_H = 0.29 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

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Octanol/Water Partition Coefficient, log K_{OW}:

7.19 (calculated-TSA, Burkhard 1984)
6.92 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
7.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.40 (calculated-TSA, Murray & Andren 1992)
6.76 (generator column-GC, Larsen et al. 1992)
6.84 (recommended, Sangster 1993)
7.10 (estimated, Girvin & Scott 1997)
7.0464 (calculated-molar properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

9.87; 9.25 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
log K_{OA} = –5.20 + 4490/(T/K); (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
10.85 (10°C, estimated, Thomas et al. 1998)
11.36, 10.22 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.54 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

3.51–5.48 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.94–6.05 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Biota Sediment Accumulation Factor, BSAF:

244 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC}:

6.99 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.51, 5.40, 5.33, 4.90 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.51; 5.50 (marine humic substances of 5 mg/L DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.60 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.60 (soil, calculated-K_{OW}, Girvin & Scott 1997)
6.40; 6.00 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.005 d^{-1} with $t_{½}$ = 131 d and k_2 = 0.010 d^{-1} with $t_{½}$ = 71 d for food concn of 22 ng/g and 125 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_2 = 0.004 d^{-1} with $t_{½}$ = 159 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 190 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

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Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 71–131 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{½}$ = 159 d for high-dose treatment, $t_{½}$ = 190 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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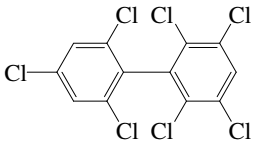
7.1.1.188 2,2′,3,4′,5,6,6′-Heptachlorobiphenyl (PCB-188)



Common Name: 2,2′,3,4′,5,6,6′-Heptachlorobiphenyl
Synonym: PCB-188, 2,2′,3,4′,5,6,6′-heptachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4′,5,6,6′-heptachlorobiphenyl
CAS Registry No: 74487-85-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
130 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.00538 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
0.00451 (20°C, supercooled liquid, Murphy et al. 1987)
0.00128 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00125 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.55×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55×10^{-4}, 1.69×10^{-3}, 2.96×10^{-5} (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
8.51×10^{-4}, 1.50×10^{-3} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.42×10^{-5} (20°C, supercooled liquid, Murphy et al. 1987)
$\log (P_L/Pa) = -4579/(T/K) + 13.29$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
113.5 (calculated-P/C, Burkhard 1984)
8.41 (20°C, calculated-P/C, Murphy et al. 1987)
44.95 (calculated-QSPR, Dunnivant et al. 1992)
15.77, 31.39, 60.5, 113.1 ± 4.0, 188.6 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 21.891 - 7457.3/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(62.0/kJ \cdot mol^{-1})/RT] + (0.182/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 J·K^{-1}·mol^{-1} and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
107.9 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, ΔH_H = 62 ± 5 kJ/mol, ΔS_H = 0.18 ± 0.02 kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.21 (calculated-TSA, Burkhard 1984)
6.78 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

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6.82 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.78 (recommended, Sangster 1993)
6.7947 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.22 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
7.01 (suspended particulate matter, Burkhard 1984)
5.342 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 2 (food lipid mg)/(g worm lipid-d); $k_{2.}$ = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 21 d in earthworm given contaminated food (Wågman et al. 2001)

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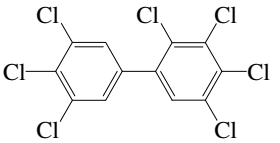
7.1.1.189 2,3,3′,4,4′,5,5′-Heptachlorobiphenyl (PCB-189)



Common Name: 2,3,3′,4,4′,5,5′-Heptachlorobiphenyl
Synonym: PCB-189, 2,3,3′,4,4′,5,5′-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5,5′-heptachlorobiphenyl
CAS Registry No: 39635-31-9
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
170 (Burkhard et al. 1985b)
163 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0378 (mp at 170°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0063 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
7.53×10^{-5} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.26×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.30×10^{-4}; 4.47×10^{-5} (generator column-GC/ECD, estimated, Hong & Qiao 1995)
4.05×10^{-4} (calculated-mp and K_{OW}, Ran et al. 2002)
0.000063 (generator column-GC/ECD, measured range 5–35°C, Huang & Hong 2002)—see Comment by van Noort 2004
0.000029, 0.000044, 0.000063, 0.000136 (5, 15, 25, 35°C, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.44×10^{-4} (P_L supercooled liquid GC-RT correlation, Burkhard et al. 1985a)
5.95×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
4.77×10^{-5}, 3.30×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.69×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5300/(T/K) + 13.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
9.18 (calculated-P/C, Burkhard et al. 1985a)
6.74 (calculated-QSPR, Dunnivant et al. 1992)
0.903 (calculated-QSPR, Achman et al. 1993)
28.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.14 (calculated-TSA, Burkhard 1984)
7.72 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

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6.75 (generator column-GC, Larsen et al. 1992)
7.24 (recommended, Sangster 1993)
7.15 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.81, 11.54; 11.45 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.15 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

6.41, 7.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.94 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.817 (as log $K_{h,}$ association coefficient with marine humic substance, calculated-χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.011\ d^{-1}$ with $t_{½} = 64$ d and $k_2 = 0.012\ d^{-1}$ with $t_{½} = 58$ d for food concn of 19 ng/g and 138 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 176$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 171$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: reported biological $t_{½} > 200$ d for heptachlorobiphenyls in carp (Niimi 1987)

Depuration $t_{½} = 58$–64 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{½} = 176$ d for high-dose treatment, $t_{½} = 171$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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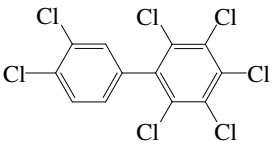
7.1.1.190 2,3,3′,4,4′,5,6-Heptachlorobiphenyl (PCB-190)



Common Name: 2,3,3′,4,4′,5,6-Heptachlorobiphenyl
Synonym: PCB-190, 2,3,3′,4,4′,5,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5,6-heptachlorobiphenyl
CAS Registry No: 41411-64-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
117.0 (Burkhard et al. 1985b)
116 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.125 (mp at 117°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.00767 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.98×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
2.20×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.96×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
2.70×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
1.09×10^{-4}, 1.47×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.13×10^{-5}, 7.08×10^{-5} (supercooled liquid P_L: GC-RI correlation, different stationary phases, Fischer et al. 1992)
log (P_L/Pa) = –5109/(T/K) + 13.17 (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
10.06 (calculated-P/C, Burkhard 1984)
11.37 (calculated-QSPR, Dunnivant et al. 1992)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.05 (calculated-TSA, Burkhard 1984)
7.08 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.46 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.08 (recommended, Sangster 1993)
7.2887 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.09, 10.87 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.90 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.84 (suspended particulate matter, Burkhard 1984)

5.675 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 2 (food lipid (mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

k_2 = 0.004 d^{-1} with $t_{½}$ = 160 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.004 d^{-1} with $t_{½}$ = 184 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 25 d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{½}$ = 160 d for high-dose treatment, $t_{½}$ = 184 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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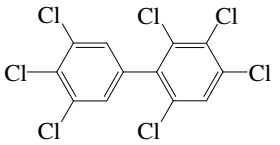
7.1.1.191 2,3,3′,4,4′,5′,6-Heptachlorobiphenyl (PCB-191)



Common Name: 2,3,3′,4,4′,5′,6-Heptachlorobiphenyl
Synonym: PCB-191, 2,3,3′,4,4′,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5′,6-heptachlorobiphenyl
CAS Registry No: 74472-50-7
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
126 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
6.60×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.89×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55×10^{-4}, 2.04×10^{-4}, 5.68×10^{-6} (supercooled liquid P_L, calculated- MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.05×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5109/(T/K) + 13.15$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
17.33 (calculated-P/C, Burkhard 1984)
13.48 (calculated-QSAR, Dunnivant et al. 1992)
1.367 (calculated-QSPR, Achman et al. 1993)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.12 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.55 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.3254 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.07, 10.91; 10.93 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.10 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.92	(suspended particulate matter, Burkhard 1984)
5.659	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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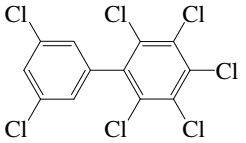
7.1.1.192 2,3,3′,4,5,5′,6-Heptachlorobiphenyl (PCB-192)



Common Name: 2,3,3′,4,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-192, 2,3,3′,4,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,5,5′,6-heptachlorobiphenyl
CAS Registry No: 74472-51-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
142 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
6.92×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.57×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.89×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
9.55×10^{-4}, 3.23×10^{-4}, 2.96×10^{-5} (P_L, calculated-MW, GC-RI correlation, calculated-MCI χ, Burkhard et al. 1985b)
1.75×10^{-4}, 2.49×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.12×10^{-5}, 1.41×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5109/(T/K) + 13.38$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
16.52 (calculated-P/C, Burkhard 1984)
19.40 (calculated-QSPR, Dunnivant et al. 1992)
1.37 (calculated-QSPR, Achman et al. 1993)
28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.09 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.52 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.409 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA}:
10.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.89	(suspended particulate matter, Burkhard 1984)
5.659	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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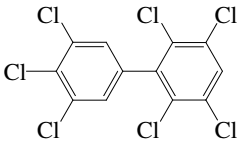
7.1.1.193 2,3,3′,4′,5,5′,6-Heptachlorobiphenyl (PCB-193)



Common Name: 2,3,3′,4′,5,5′,6-Heptachlorobiphenyl
Synonym: PCB-193, 2,3,3′,4′,5,5′,6-heptachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4′,5,5′,6-heptachlorobiphenyl
CAS Registry No: 69782-91-8
Molecular Formula: $C_{12}H_3Cl_7$
Molecular Weight: 395.323
Melting Point (°C):
154 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
330.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
6.96×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.14×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.25×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.70×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.91×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.37×10^{-4}, 8.79×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
7.59×10^{-5}, 1.20×10^{-4} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5109/(T/K) + 13.27$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
9.70 (calculated-P/C, Burkhard 1984)
13.61 (calculated-QSPR, Dunnivant et al. 1992)
1.37 (calculated-QSPR, Achman et al. 1993)
1.93 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
32.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 140 \pm 13$ kJ/mol, $\Delta S_H = 0.43 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.09 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.52 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.409 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.99, 10.82; 10.02 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
10.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

6.89 (suspended particulate matter, Burkhard 1984)
5.659 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 5 (food lipid mg)/(g worm lipid-d); k_2 = 0.03 d^{-1} (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: elimination $t_{½}$ = 21 d in earthworm given contaminated food (Wågman et al. 2001)

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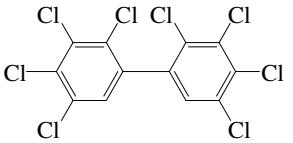
7.1.1.194 2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl (PCB-194)



Common Name: 2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl
Synonym: PCB-194, 2,2′,3,3′,4,4′,5,5′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,5′-octachlorobiphenyl
CAS Registry No: 35694-08-7
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
159–160 (Binns & Suschitzky 1971)
156 (Kühne et al. 1995; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm^3): 1.507 (at 22°C)
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
263.2 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0484 (mp at 159°C)
0.0474 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.0072 (shake flask-GC/ECD, Wallnöfer et al. 1973)
0.000272 (generator column-GC/ECD, Weil et al. 1974)
8.58×10^{-5} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
0.00124 (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
3.79×10^{-3}; 2.40×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)
$\log S_L/(\text{mol m}^{-3}) = -1533/(T/K) - 0.11$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.03×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)
3.86×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
2.07×10^{-5}, 1.79×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.29×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/\text{Pa}) = -5402/(T/K) + 13.43$ (GC-RT correlation, Falconer & Bidleman 1994)
2.04×10^{-5}; 2.45×10^{-5} (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Li et al. 2003)
$\log P_L/\text{Pa} = -5099/(T/K) + 12.49$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):
47.52 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
10.13 (wetted-wall column-GC, Brunner et al. 1990)
6.79 (calculated-QSPR, Dunnivant et al. 1992)
1.01 (calculated-QSPR, Achman et al. 1993)
0.34 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
10.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

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ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 169 \pm 6$ kJ/mol, $\Delta S_H = 0.52 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
6.76, 4.37 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
log [H/(Pa m^3/mol)] = –3566/(T/K) + 12.60 (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

8.68 (RP-TLC-RT correlation, Bruggeman et al. 1982)
9.35 (HPLC-RT correlation, Shaw & Connell 1982)
7.62 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.67 (generator column-GC, Hawker & Connell 1988a)
6.94 (generator column-GC, Larsen et al. 1992)
7.65 (recommended, Sangster 1993)
7.67, 7.80, 9.35 (quoted lit. values, Hansch et al. 1995)
7.67, 7.76 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

10.50 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
12.83, 11.59; 11.71 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
11.31, 11.13 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
log K_{OA} = 4906/(T/K) – 5.33 (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:

5.81 (guppy, 3.5% lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)
4.35 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)
4.18 (worms, Oliver 1987c)
4.35 (guppy, calculated-C_B/C_W, or k_1/k_2, Connell & Hawker 1988; Hawker 1990)
4.81 (guppy, estimated, Banerjee & Baughman 1991)
5.81; 7.34 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.81, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

7.27 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.5–7.1, 6.8; 7.80 (suspended sediment, average; algae > 50 μm, Oliver 1987a)
5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.943, 6.016 (marine humic substances or 5 mg/L DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.41, 6.20, 6.06 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
6.96 (soil, calculated-Characteristic Root Index CRI model, Saçan & Balcioğlu 1996)
7.30 (soil, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 150$ d^{-1}; $k_2 = 0.007$ d^{-1} (guppy, Bruggeman et al. 1984)
$k_1 = 1000$ d^{-1} (guppy, Opperhuizen 1986)

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log k_1 = 2.18 d^{-1}; log $1/k_2$ = 2.15 d (fish, quoted, Connell & Hawker 1988)
k_1 = 5640 d^{-1}; k_2 = 0.00865 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.004 d^{-1} with $t_{½}$ = 158 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 174 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ > 1000 d in rainbow trout and $t_{½}$ = 78 d in its muscle (Niimi & Oliver 1983);
$t_{½}$ = 100 d in guppy (Bruggeman et al. 1984);
$t_{½}$ = 220 d in worms at 8°C (Oliver 1987c).
depuration $t_{½}$ = 158 d for high-dose treatment, $t_{½}$ = 174 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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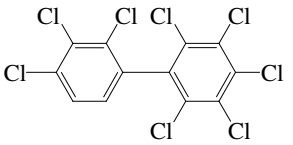
7.1.1.195 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl (PCB-195)



Common Name: 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl
Synonym: PCB-195, 2,2′,3,3′,4,4′,5,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,6-Octachlorobiphenyl
CAS Registry No: 52663-78-2
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
176 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00334 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
2.204×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
9.92×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.12×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
4.53×10^{-5}, 7.46×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.19×10^{-5}, 3.63×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5244/(T/K) + 13.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
12.77 (calculated-P/C, Burkhard 1984)
1.115 (wetted-wall column-GC/ECD, Brunner et al. 1990)
12.01 (calculated-QSPR, Dunnivant et al. 1992)
14.13 ± 0.78 (gas stripping-GC/ECD, measured range 4–31°C, Bamford et al. 2000)
0.079, 0.485, 2.724, 14.13, 54.5 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$\ln K_{AW} = 62.305 - 20086.6/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(167.0/kJ \cdot mol^{-1})/ RT] + (0.518/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 $J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
15.1 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.49 (calculated-TSA, Burkhard 1984)
7.35 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.56 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

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6.95 (generator column-GC, Larsen et al. 1992)
7.15 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.13, 10.04; 10.02 (0, 20°C, GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.26 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.92; 7.45 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:

7.29 (suspended particulate matter, Burkhard 1984)
5.78, 5.59, 5.55, 5.32 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.78; 5.87 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
6.42, 6.26, 6.14 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 5930 d^{-1}; k_2 = 0.00711 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.010 d^{-1} with $t_{½}$ = 67 d and k_2 = 0.011 d^{-1} with $t_{½}$ = 61 d for food concn of 24 ng/g and 126 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
k_2 = 0.005 d^{-1} with $t_{½}$ = 143 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 158 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 61–67 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{½}$ = 143 d for high-dose treatment, $t_{½}$ = 158 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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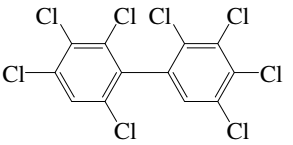
7.1.1.196 2,2′,3,3′,4,4′,5,6′-Octachlorobiphenyl (PCB-196)



Common Name: 2,2′,3,3′,4,4′,5,6′-Octachlorobiphenyl
Synonym: PCB-196, 2,2′,3,3′,4,4′,5,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,6′-Octachlorobiphenyl
CAS Registry No: 42740-50-1
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.91×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.63×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.87×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.40×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
6.11×10^{-5}, 8.41×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.47×10^{-5}, 5.89×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5244/(T/K) + 13.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
71.94 (calculated-P/C, Burkhard 1984)
1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)
13.23 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.57 (calculated-TSA, Burkhard 1984)
7.43 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.43 (recommended, Sangster 1993)
7.70 (estimated, Girvin & Scott 1997)
7.4190 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.27, 11.03; 11.19 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.37 (suspended particulate matter, Burkhard 1984)
5.857 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
7.30 (soil-organic carbon, calculated-K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 168$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 156 d for high-dose treatment, $t_{½}$ = 168 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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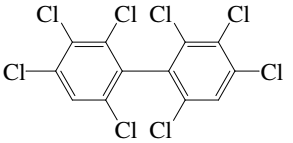
7.1.1.197 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl (PCB-197)



Common Name: 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl
Synonym: PCB-197, 2,2′,3,3′,4,4′,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,6,6′-Octachlorobiphenyl
CAS Registry No: 33091-17-7
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
132 (Brodsky & Ballschmiter 1988)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0892 (mp at 132°C)

Water Solubility (g/m^3 or mg/L at 25°C):
2.81×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.41×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
1.71×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)
1.03×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
6.79×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.93×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
1.90×10^{-4}, 1.22×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
9.12×10^{-5} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4581/(T/K) + 12.52$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
94.03 (calculated-P/C, Burkhard 1984)
25.69 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.59 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.30 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
11.74, 10.52; 10.68 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.30 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.39	(suspended particulate matter, Burkhard 1984)
5.699	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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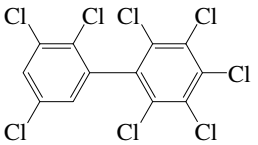
7.1.1.198 2,2′,3,3′,4,5,5′,6-Octachlorobiphenyl (PCB-198)



Common Name: 2,2′,3,3′,4,5,5′,6-Octachlorobiphenyl
Synonym: PCB-198, 2,2′,3,3′,4,5,5′,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6-Octachlorobiphenyl
CAS Registry No: 68194-17-2
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
162 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.03×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.63×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
8.58×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
1.48×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.44×10^{-4}, 1.67×10^{-4}, 5.68×10^{-6} (GC-RI correlation, Burkhard et al. 1985b)
6.85×10^{-5}, 1.224×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.01×10^{-5}, 7.08×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5244/(T/K) + 13.42$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
20.97 (calculated-P/C, Burkhard 1984)
1.419 (wetted wall column-GC/ECD, Brunner et al. 1990)
15.62 (calculated-QSPR, Dunnivant et al. 1992)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.55 (calculated-TSA, Burkhard 1984)
7.43 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.62 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.43 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.32, 11.05; 10.02 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
11.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

7.35 (suspended particulate matter, Burkhard 1984)

5.91, 5.63, 5.56, 5.23 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)

5.91; 5.86 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 158$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 185$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 158 d for high-dose treatment, $t_{½}$ = 185 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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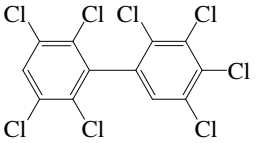
7.1.1.199 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl (PCB-199)



Common Name: 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl
Synonym: PCB-199, 2,2′,3,3′,4,5,5′,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6′-Octachlorobiphenyl
CAS Registry No: 52663-75-9
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.23×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
3.41×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
5.41×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.20×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.57×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
9.35×10^{-5}, 1.67×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.05×10^{-4}, 2.04×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, reported as the revised order PCB-200-2,2′,3,3′,4,5,6,6′- Fischer et al. 1992)
$\log (P_L/Pa) = -5244/(T/K) + 13.36$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
42.66 (calculated-P/C, Burkhard 1984)
1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)
23.0 (calculated-QSPR, Dunnivant et al. 1992)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.51 (calculated-TSA, Burkhard 1984)
7.21 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.21 (recommended, Sangster 1993)
7.28 (quoted lit., Maruya & Lee 1998-reported as revised order PCB-200: 2,2′,3,3′,4,5,6,6′-PCB)
7.21 (revised previously quoted value; Maruya & Lee 2000)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.28, 11.05; 10.02 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Biota Sediment Accumulation Factor, BSAF:

96 (trout in Lake Ontario, Niimi 1996)
0.26, 7.1, 1.1(grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:

7.31 (suspended particulate matter, Burkhard 1984)
5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.711 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.44, 6.18, 6.02 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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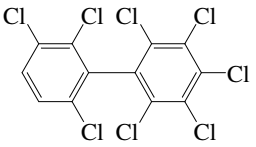
7.1.1.200 2,2′,3,3′,4,5,6,6′-Octachlorobiphenyl (PCB-200)



Common Name: 2,2′,3,3′,4,5,6,6′-Octachlorobiphenyl
Synonym: PCB-200, 2,2′,3,3′,4′,5,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,6,6′-Octachlorobiphenyl
CAS Registry No: 52663-73-7
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
130 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.93×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
4.105×10^{-4}, 1.79×10^{-4}, 1.08×10^{-4}, 2.01×10^{-4} (RP-HPLC-k′ correlation, different and mobile stationary phases, Brodsky & Ballschmiter 1988)
4.30×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.56×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
6.37×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.75×10^{-4}, 3.32×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.89×10^{-5}, 5.89×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, reported in revised order as PCB-201-2,2′,3,3′,4,5′,6,6′-, Fischer et al. 1992)
$\log (P_L/Pa) = -4851/(T/K) + 12.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
2.34×10^{-5} (P_L, calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)

Henry's Law Constant (Pa·m^3/mol at 25°C):
66.98 (calculated-P/C, Burkhard 1984)
1.50 (calculated-QSPR, Achman et al. 1993)
24.36 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.57 (calculated-TSA, Burkhard 1984)
7.16, 7.54, 7.16, 7.36; 7.35 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.35 (recommended, Sangster 1993)
7.27 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

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8.16; 7.27–7.30 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
7.63; 7.28 (previously quoted; revised value, Maruya & Lee 2000)
7.32 (calculated-QSPR, Yeh & Hong 2002- reported as PCB-201 for 2,2′,3,3′,4,5,6,6′-octachlorobiphenyl)

Octanol/Air Partition Coefficient, log K_{OA} at 25°Cor as indicated:
12.05, 10.82 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
7.36 (suspended particulate matter, Burkhard 1984)
5.50, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.68; 5.70 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
7.05 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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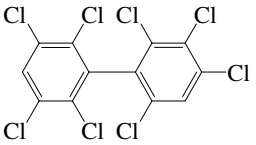
7.1.1.201 2,2′,3,3′,4,5′,6,6′-Octachlorobiphenyl (PCB-201)



Common Name: 2,2′,3,3′,4,5′,6,6′-Octachlorobiphenyl
Synonym: PCB-201, 2,2′,3,3′,4,5,5′,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3′,3′,4,5′,6,6′-Octachlorobiphenyl
CAS Registry No: 40186-71-8
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
162 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.06×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
2.204×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
8.58×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
4.56×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
5.06×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
5.94×10^{-5}, 1.0×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.41×10^{-4} (supercooled liquid P_L: GC-RI correlation, different stationary phases, reported as revised order PCB-199, 2,2′,3,3′,4,5,5′,6′-octachlorobiphenyl, Fischer et al. 1992)
$\log (P_L/Pa) = -4581/(T/K) + 12.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
64.54 (calculated-P/C, Burkhard 1984)
1.72 (wetted wall column-GC/ECD, Brunner et al. 1990)
13.23 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
0.156, 0.457 (0, 15°C, from modified two-film exchange model, Hornbuckle et al. 1994)
95.8 ± 4.4 (gas stripping-GC/ECD, measured range 4–31°C, Bamford et al. 2000)
1.069, 5.14, 22.98, 95.8, 308 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
$K_{AW} = \exp[-(144.5/kJ \cdot mol^{-1})/ RT] + (0.458/kJ \cdot mol^{-1} \cdot K^{-1})/R]$; where R = 8.314 $J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
97.5 (exptl. data, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.54 (calculated-TSA, Burkhard 1984)
7.35 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)

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7.21 (generator column-GC, Hawker & Connell 1988)
7.62 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.80 (calculated-TSA, Murray & Andren 1992)
7.31 (recommended, Sangster 1993)
7.70 (estimated, Girvin & Scott 1997)
7.21 (quoted lit., Maruya & Lee 1998, reported as the revised order PCB-199, 2,2′,3,3′,4′,5,5′,6-octachlorobiphenyl)
7.62 (revised previously quoted value, Maruya & Lee 2000)
7.21; 7.32 (quoted exptl.-generator column method; calculated-QSPR, Yeh & Hong 2002, reported as PCB-201 for 2,2′3,3′,4,5,6,6′-octachlorobiphenyl-should be PCB-200 in B&Z/IUPAC numbering system for 2,2′,3,3′,4,5,5′,6-octachlorobiphenyl)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.22, 10.98 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.30 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

5.88; 7.41 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, log K_{OC}:

7.34 (suspended particulate matter, Burkhard 1984)
5.913; 5.857 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
6.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
7.30 (soil, estimated-log K_{OW}, Girvin & Scott 1997)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

k_1 = 5950 d^{-1}; k_2 = 0.00776 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
k_2 = 0.005 d^{-1} with $t_{½}$ = 153 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
k_2 = 0.004 d^{-1} with $t_{½}$ = 172 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 153 d for high-dose treatment, $t_{½}$ = 172 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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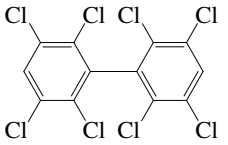
7.1.1.202 2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl (PCB-202)



Common Name: 2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl
Synonym: PCB-202, 2,2′,3,3′,5,5′,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl
CAS Registry No: 2136-99-4
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
161 (Van Roosmalen 1934; Burkhard et al. 1985a; Erickson 1986; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.507
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
263.2 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.80 (Miller et al. 1984; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
52.72 (Miller et al. 1984; Shiu & Mackay 1986; selected, Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0463 (mp at 161°C)
0.0443 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.80×10^{-4} (generator column-GC/ECD, Weil et al. 1974;)
3.93×10^{-4} (generator column-GC/ECD, Miller et al. 1984,1985)
1.47×10^{-4}* (generator column-GC/ECD, measured range 20–50°C, Dickhut et al. 1986)
1.14×10^{-4}, 1.47×10^{-4}, 2.12×10^{-4}, 4.66×10^{-4} (4. 20, 25, 32°C, generator column-GC/ECD, Dickhut et al. 1986)
ln x = –6098/(T/K) – 5.333, temp range 4–32°C, ΔH_{ss} = 50.7 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
log x = –2652/(T/K) – 2.308, ΔH_{ss} = 50.6 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
S/(mol/L) = 6.91×10^{-11} exp(0.064·t/°C) (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
2.53×10^{-4}, 5.93×10^{-4}, 6.51×10^{-4}, 2.36×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
ln x = –5.34 – 6100/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.90×10^{-5}* (extrapolated gas saturation-GC, measured range 29–61.2°C, Burkhard et al. 1984)
log (P/Pa) = 13.262 – 5307.3/(T/K); temp range 29–61.2°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)
2.89×10^{-5}, 6.43×10^{-4} (solid P_S, P_L calculated from P_S using fugacity ratio F, Burkhard et al. 1985a)
5.40×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
1.70×10^{-4}, 3.91×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
6.59×10^{-4}, 5.26×10^{-4} (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
2.22×10^{-4} (P_{GC} by GC-RT correlation with *p,p′*-DDT as reference standard, Hinckley et al. 1990)

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$\log P_L/Pa = 12.99 - 4851/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
2.40×10^{-4} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4851/(T/K) + 12.99$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
$(2.41 - 29.5) \times 10^{-6}$; $(1.73 - 5.40) \times 10^{-4}$ (literature solid P_S range; literature liquid P_L range, Delle Site 1997)
$\log (P/Pa) = 13.282 - 5307.3/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m^3/mol at 25°C):

75.79 (calculated-P/C, Burkhard et al. 1985b)
38.08 (calculated-P/C, Shiu & Mackay 1986)
1.82 (wetted-wall column-GC, Brunner et al. 1990)
22.63 (calculated-QSPR, Dunnivant et al. 1992)
1.50 (calculated-QSPR, Achman et al. 1993)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

9.77 (Hansch & Leo 1979)
8.42 (TLC-RT correlation, Bruggeman et al. 1982)
7.11 (generator column-GC/ECD, Miller et al. 1984, 1985)
7.14 (generator column-HPLC, Woodburn et al. 1984)
7.12 (generator column-GC/ECD, Doucette & Andren 1987,1988)
7.01, 7.35, 6.98, 7.31 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.21 (generator column-GC, Hawker & Connell 1988a)
7.67 (HPLC-RT correlation, Hawker & Connell 1988)
7.729 ± 0.031 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
7.54 (HPLC-k′ correlation, Noegrohati & Hammers 1992)
7.15 (recommended, Sangster 1993)
7.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

11.57, 10.38 (0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)
10.77 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.82; 7.35 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
5.82, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

7.34 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.61, 5.46, 5.41, 4.99 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.610, 5.699 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, observed; calculated-MCI χ, Sabljic et al. 1989)
6.36, 6.13, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
7.04 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:

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Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 5070 d^{-1}; k_2 = 0.0077 d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k_2 = 0.006 d^{-1} with $t_{½}$ = 119 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

k_2 = 0.005 d^{-1} with $t_{½}$ = 145 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 110 d for high-dose treatment, $t_{½}$ = 145 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.202.1
Reported aqueous solubilities and vapor pressures of 2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl (PCB-202) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure	
Dickhut et al. 1986		Burkhard et al. 1984	
generator column-GC/ECD		gas saturation-GC/ECD	
t/°C	S/g·m^{-3}	t/°C	P/Pa
20	1.29×10^{-4}	29.0	4.95×10^{-5}
25	1.29×10^{-4}	39.9	2.24×10^{-4}
32	2.15×10^{-4}	50.0	5.83×10^{-4}
50	7.73×10^{-4}	61.2	2.65×10^{-3}
		25.0	2.90×10^{-5}
ln x = A – B/(T/K)			
A	–5.333	log (P/Pa) = A – B/(T/K)	
B	6098.15	A	13.262
		B	5307.3
ΔH_{sol}/(kJ mol^{-1}) = 50.7 ± 3.8 for 25–50°C		temp range 29–61.2°C	
		ΔH_{subl}/(kJ mol^{-1}) = 101.7	

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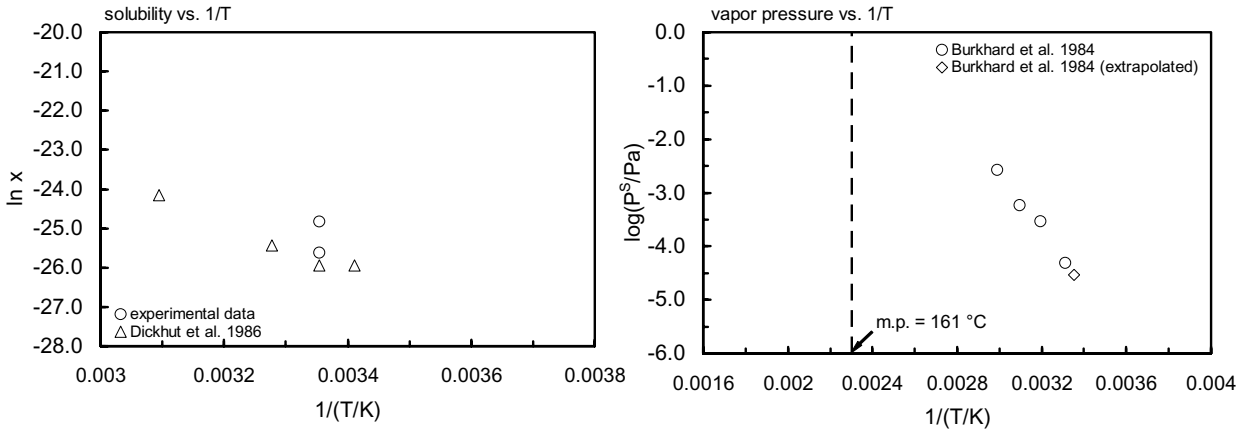

FIGURE 7.1.1.202.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl (PCB-202).

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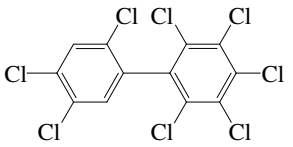
7.1.1.203 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl (PCB-203)



Common Name: 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl
Synonym: PCB-203, 2,2′,3,4,4′,5,5′,6-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,5′,6-Octachlorobiphenyl
CAS Registry No: 52663-76-0
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
170 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.91×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.36×10^{-4} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):
1.35×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
1.52×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
9.29×10^{-5}, 1.047×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
3.47×10^{-5}, 5.62×10^{-5} (supercooled liquid P_L, GC-RI correlation, different stationary phases, Fischer et al. 1992)
$\log (P_L/Pa) = -5244/(T/K) + 13.39$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.252 (calculated-P/C, Burkhard 1984)
14.21 (calculated-QSPR, Dunnivant et al. 1992)
0.990 (calculated-QSPR, Achman et al. 1993)
15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.57 (calculated-TSA, Burkhard 1984)
7.49 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.93 (generator column-GC, Larsen et al. 1992)
7.21 (recommended, Sangster 1993)
7.4825 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated :

12.36, 11.10 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.37 (suspended particulate matter, Burkhard 1984)
5.857 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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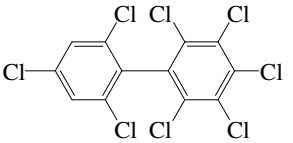
7.1.1.204 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl (PCB-204)



Common Name: 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl
Synonym: PCB-204, 2,2′,3,4,4′,5,6,6′-octachloro-1,1′-biphenyl
Chemical Name: 2,2′,3,4,4′,5,6,6′-Octachlorobiphenyl
CAS Registry No: 74472-52-9
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
132 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
2.81×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
1.49×10^{-4}, 9.85×10^{-5}, 1.83×10^{-4}, 1.49×10^{-4} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
4.30×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
3.49×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
3.88×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)
1.54×10^{-4}, 2.76×10^{-4} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
1.38×10^{-4} (supercooled liquid P_L, GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -4851/(T/K) + 12.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
53.3 (calculated-P/C, Burkhard 1984)
34.89 (calculated-QSAR, Dunnivant et al. 1992)
97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.59 (calculated-TSA, Burkhard 1984)
7.46, 7.63, 7.37, 7.45 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.30 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.48 (recommended, Sangster 1993)
7.2632 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:
11.15 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

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Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

7.39	(suspended particulate matter, Burkhard 1984)
5.699	(marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

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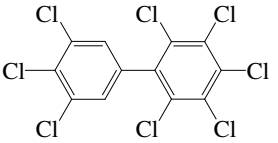
7.1.1.205 2,3,3′,4,4′,5,5′,6-Octachlorobiphenyl (PCB-205)



Common Name: 2,3,3′,4,4′,5,5′,6-Octachlorobiphenyl
Synonym: PCB-205, 2,3,3′,4,4′,5,5′,6-octachloro-1,1′-biphenyl
Chemical Name: 2,3,3′,4,4′,5,5′,6-Octachlorobiphenyl
CAS Registry No: 74472-53-0
Molecular Formula: $C_{12}H_2Cl_8$
Molecular Weight: 429.768
Melting Point (°C):
150 (estimated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
351.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
3.50×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)
8.58×10^{-5} (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
3.41×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.84×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)
4.40×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)
2.49×10^{-5}, 2.91×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -5402/(T/K) + 13.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
4.70 (calculated-P/C, Burkhard 1984)
8.644 (calculated-QSPR, Dunnivant et al. 1992)
10.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 169 \pm 6$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.47 (calculated-TSA, Burkhard 1984)
7.62 (RP-HPLC-k′ correlation, Brodsky & Ballschmiter 1988)
8.00 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.62 (recommended, Sangster 1993)
7.7326 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:
12.86, 11.62 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.34 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

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Sorption Partition Coefficient, log K_{OC}:

7.27 (suspended particulate matter, Burkhard 1984)

6.016 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 166$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004\ d^{-1}$ with $t_{½} = 168$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{½}$ = 166 d for high-dose treatment, $t_{½}$ = 168 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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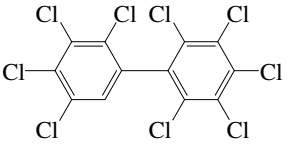
7.1.1.206 2,2′,3,3′,4,4′,5,5′,6-Nonachlorobiphenyl (PCB-206)



Common Name: 2,2′,3,3′,4,4′,5,5′,6-Nonachlorobiphenyl
Synonym: PCB-206, 2,2′,3,3′,4,4′,5,5′,6-nonochloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,5′,6-nonachlorobiphenyl
CAS Registry No: 40186-72-9
Molecular Formula: $C_{12}HCl_9$
Molecular Weight: 464.213
Melting Point (°C):
204.5–206.5 (Hutzinger et al. 1974)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.507
Molar Volume (cm^3/mol):
372.7 (calculated-Le Bas method at normal boiling point)
276.1 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.70 (Opperhuizen et al. 1988; Ruelle et al. 1993)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.016 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
0.000112 (generator column-GC/ECD, Weil et al. 1974)
2.55×10^{-5} (generator column-GC/ECD, measured range 25–50°C, Dickhut et al. 1986)
2.55×10^{-5}, 5.117×10^{-5}, 6.59×10^{-5}, 1.32×10^{-4} (25, 32, 40, 50°C, generator column-GC/ECD, Dickhut et al. 1986)
$\ln x = -5990/(T/K) - 7.427$, temp range 25–50°C, ΔH_{ss} = 49.8 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
$\log x = -2609/(T/K) - 3.222$, ΔH_{ss} = 50.0 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
$S/(mol/L) = 1.27 \times 10^{-11} \exp(0.062 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
0.00011 (selected, Shiu & Mackay 1986)
3.07×10^{-5}, 3.14×10^{-5}, 2.61×10^{-5}, 2.80×10^{-5} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.80×10^{-5} (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
$\ln x = -7.4275 - 6004.5/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.88×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)
1.034×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
1.08×10^{-5}, 1.53×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -5226/(T/K) + 13.57$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
27.66 (calculated-P/C, Burkhard et al. 1985b)
8.845 (calculated-QSPR, Dunnivant et al. 1992)
0.474 (calculated-QSPR, Achman et al. 1993)

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15.1 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

9.14 (RP-TLC-k′ correlation, Bruggeman et al. 1982)
7.94, 7.91, 7.98, 7.94 (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.07 (generator column-GC, Larsen et al. 1992)
7.51 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

13.09, 11.79 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.81 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.71; 7.24 (zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
2.60–4.85 (various marine species, mean dry weight BCF, Hope et al. 1998)
4.37–5.67 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, log K_{OC}:

7.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.15, 5.92, 5.83, 5.69 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg L^{-1} DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
6.152; 6.133 (marine humic substances of 5 mg L^{-1} DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 4940$ d^{-1}; $k_2 = 0.00958$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.016$ d^{-1} with $t_{½} = 45$ d and $k_2 = 0.013$ d^{-1} with $t_{½} = 53$ d for food concn of 20 ng/g and 141 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.005$ d^{-1} with $t_{½} = 140$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½} = 148$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½} > 1000$ d in rainbow trout, and $t_{½} = 84$ d in its muscle (Niimi & Oliver 1983)

Depuration $t_{½}$.= 45–53 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{½} = 140$ d for high-dose treatment, $t_{½} = 148$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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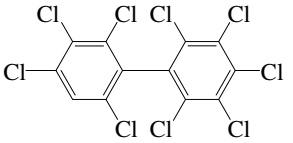
7.1.1.207 2,2′,3,3′,4,4′,5,6,6′-Nonachlorobiphenyl (PCB-207)



Common Name: 2,2′,3,3′,4,4′,5,6,6′-Nonachlorobiphenyl
Synonym: PCB-207, 2,2′,3,3′,4,4′,5,6,6′-nonochloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,4′,5,6,6′-nonachlorobiphenyl
CAS Registry No: 52663-79-3
Molecular Formula: $C_{12}HCl_9$
Molecular Weight: 464.213
Melting Point (°C):
161 (calculated, Abramowitz & Yalkowsky 1990)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
372.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.00167 (supercooled liquid S_L, calculated-TSA, Burkhard et al. 1985b)
4.64×10^{-5}, 3.29×10^{-5}, 4.04×10^{-5}, 3.77×10^{-5} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
0.000058 (calculated-TSA, Abramowitz & Yalkowsky 1990)
2.10×10^{-5} (calculated-MCI χ, Patil 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.47×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985a)
1.30×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.17×10^{-5}, 4.99×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
$\log (P_L/Pa) = -5127/(T/K) + 12.70$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
35.97 (calculated-P/C, Burkhard et al. 1985b)
17.13 (calculated-QSPR, Dunnivant et al. 1992)
0.717 (calculated-QSPR, Achman et al. 1993)
97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.94 (calculated-TSA, Burkhard 1984)
7.84, 7.97, 7.85, 7.86 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
7.52 (generator column-GC, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.74 (calculated-TSA, Hawker & Connell 1988a)
7.80 (calculated-MCI χ, Patil 1991)
7.88 (recommended, Sangster 1993)
7.6190 (calculated-molecular properties MNDO-AM1, Makino 1998)
7.77 (calculated-QSPR, Yeh & Hong 2002)

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Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.60, 11.26 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.94 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

2.65–4.54 (various marine species, mean dry wt. BCF, Hope et al. 1998)
4.02–6.29 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, log K_{OC}:

7.74 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.98, 5.77, 5.67, 5.44 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg L^{-1} DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
5.98, 5.97 (marine humic substances of 5 mg L^{-1} DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)
6.39, 6.17, 6.19 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 162$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.004\ d^{-1}$ with $t_{½} = 155$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 162 d for high-dose treatment, $t_{½}$ = 155 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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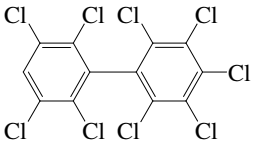
7.1.1.208 2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl (PCB-208)



Common Name: 2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl
Synonym: PCB-208, 2,2′,3,3′,4,5,5′,6,6′-nonochloro-1,1′-biphenyl
Chemical Name: 2,2′,3,3′,4,5,5′,6,6′-nonachlorobiphenyl
CAS Registry No: 52663-77-1
Molecular Formula: $C_{12}HCl_9$
Molecular Weight: 464.213
Melting Point (°C):
180.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
Molar Volume (cm^3/mol):
372.7 (calculated-Le Bas method at normal boiling point)
276.1 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.60 (Ruelle et al. 1993; Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.45 (Shiu & Mackay 1986)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0298 (mp at 180.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1.80×10^{-5} (generator column-GC/ECD, Miller et al. 1984,1985)
6.87×10^{-5}; 4.64×10^{-5}, 6.87×10^{-5}, 3.95×10^{-5}, 4.97×10^{-5} (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
1.74×10^{-7} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
3.78×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)
1.22×10^{-4} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
3.08×10^{-5}, 6.62×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
2.19×10^{-5} (supercooled liquid P_L: GC-RI correlation, Fischer et al. 1992)
$\log (P_L/Pa) = -5127/(T/K) + 12.68$ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
32.53 (calculated-P/C, Burkhard et al. 1985b)
16.93 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:
7.92 (calculated-TSA, Burkhard 1984)
8.16 (generator column-GC/ECD, Miller et al. 1984,1985)
9.05 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
7.72, 7.87, 7,69, 7,78 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
8.18 (calculated-TSA, Hawker & Connell 1988a)

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7.77 (recommended, Sangster 1993)
8.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

12.57, 11.26 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
11.71 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

7.72 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
5.974 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h, calculated-molecular connectivity indices χ, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.005\ d^{-1}$ with $t_{½} = 139$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005\ d^{-1}$ with $t_{½} = 152$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: depuration $t_{½}$ = 139 d for high-dose treatment, $t_{½}$ = 152 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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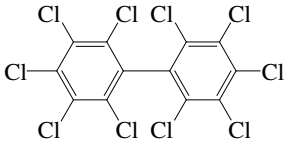
7.1.1.209 2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl (PCB-209)



Common Name: 2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl
Synonym: PCB-209
Chemical Name: 2,2′,3,3′,4,4′,5,5′,6,6′-decachlorobiphenyl
CAS Registry No: 2051-24-3
Molecular Formula: $C_{12}Cl_{10}$
Molecular Weight: 498.658
Melting Point (°C):
309 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.507
Molar Volume (cm^3/mol):
393.6 (calculated-Le Bas method at normal boiling point)
289.0 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.79 (differential scanning calorimetry, Miller et al. 1984; Ruelle & Kesselring 1997)
39.434 (Ruelle et al. 1993)
38.16 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.37 (Miller et al. 1984; Shiu & Mackay 1986; Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00164 (mp at 309°C)
0.0017 (Mackay et al. 1980; Shiu & Mackay 1986; Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.015 (shake flask-GC/ECD, Wallnöfer et al. 1973; Tulp & Hutzinger 1978)
1.6×10^{-5} (generator column-GC/ECD, Weil et al. 1974)
7.43×10^{-6} (generator column-GC/ECD, Miller et al. 1984,1985)
2.12×10^{-8} (calculated-UNIFAC activity coeff., converted from log γ, Arbuckle 1986)
4.1×10^{-4}, 4.6×10^{-4} (exptl., calculated-UNIFAC, converted from log γ, Burkhard et al. 1986)
6.48×10^{-7}* (generator column-GC/ECD, measured range 50–80°C, Dickhut et al. 1986)
6.48×10^{-7}, 8.38×10^{-6}, 1.76×10^{-5}, 4.95×10^{-5} (25, 60, 70, 80°C, generator column-GC/ECD, Dickhut et al. 1986)
$\ln x = -8010.6/(T/K) - 4.608$, temp range 50–80°C, ΔH_{ss} = 66.6 kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)
$\log x = -3478/(T/K) - 2.001$, ΔH_{ss} = 66.6 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or
$S/(mol/L) = 1.80 \times 10^{-13} \exp(0.077 \cdot t/°C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)
7.37×10^{-6}, 8.67×10^{-6}, 7.04×10^{-6}, 9.07×10^{-6} (RP- HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
2.1×10^{-5} (22°C, generator column-GC/ECD, Opperhuizen et al. 1988)
$(7.9 \pm 0.38) \times 10^{-6}$ (generator column-SPME/GC, Paschke et al. 1998)
$\ln x = -4.632 - 8001/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.4×10^{-5} (calculated-volatilization rate, Dobbs & Cull 1982)
4.0×10^{-5} (supercooled liquid P_L, Mackay et al. 1983)

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5.30×10^{-8}* (extrapolated, gas saturation-GC, measured range 50.7–89.8°C, Burkhard et al. 1984)
log (P/Pa) = 14.049 – 6358/(T/K); temp range 50.7–89.8°C (gas saturation, Burkhard et al. 1984)
1.39×10^{-6} (supercooled liquid P_L, GC-RT correlation, Bidleman 1984)
5.36×10^{-8} (GC-RI correlation, Burkhard et al. 1985a)
2.75×10^{-5} (supercooled liquid P_L, GC-RI correlation, Burkhard et al. 1985b)
5.58×10^{-6}, 1.32×10^{-5} (supercooled liquid P_L, GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
5.00×10^{-8}; 3.0×10^{-5} (selected, solid P_S; supercooled liquid P_L, Shiu & Mackay 1986)
9.44×10^{-6} (GC-RT correlation, Watanabe & Tatsukawa 1989)
5.14×10^{-6}, 1.44×10^{-5} (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
1.303×10^{-5} (P_{GC} by GC-RT correlation with *p,p′*-DDT as reference standard, Hinckley et al. 1990)
log (P_L/Pa) = 13.27 – 5402/(T/K) (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
log (P_L/Pa) = –5402/(T/K) + 13.27 (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)
$2.89 \times 10^{-9} – 1.40 \times 10^{-5}$; $(5.58–27.5) \times 10^{-6}$ (literature P_S range; P_L range, Delle Site 1997)
2.6×10^{-5}* (65°C, Knudsen effusion, measured range 65–85°C, Goodman 1997)

Henry's Law Constant (Pa m^3/mol at 25°C):

100 (estimated, Mackay et al. 1983)
12.46 (calculated-P/C, Burkhard et al. 1985b)
20.84 (calculated-P/C, Shiu & Mackay 1986; Shiu et al. 1987)
40.0 (calculated-QSPR, Dunnivant et al. 1992)
97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
ln $K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

11.19 (Hansch & Leo 1979)
9.60 (TLC-RT correlation, Bruggeman et al. 1982; 1984)
8.26 (generator column-GC/ECD, Miller et al. 1984,1985)
8.20 (generator column-HPLC, Woodburn et al. 1984)
8.20 (shake flask/slow stirring-GC, Brooke et al. 1986)
8.20 (generator column-GC/ECD, Doucette & Andren 1987,1988)
8.38, 8.37, 8.41, 8.28 (RP-HPLC-k′ correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
9.45, 11.2 (calculated-UNIFAC activity coeff., π const. or f const., Banerjee & Howard 1988)
8.274 ± 0.001(shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
> 9.0 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
8.24 (HPLC-retention indices correlation, Noegrohati & Hammers 1992)
8.27 (recommended, Hansch et al. 1995)
7.95 ± 0.68 (flask/slow stirring-SPME/GC, Paschke et al. 1998)
7.59 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

13.36, 1.96 (0, 20°C, multi-column GC-k′ correlation, Zhang et al. 1999)
12.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

5.48 (guppy, 3.5% extractable lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)
7.0 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
1.48, 1.41 (human fat of lipid basis, calculated-K_{OW}, Geyer et al. 1987)
1.38, 1.32 (human fat of wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
4.02 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)
4.02 (guppy, calculated-C_B/C_W or k_1/k_2, Connell & Hawker 1988; Hawker 1990)

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5.07 (guppy, estimated, Banerjee & Baughman 1991)
5.44; 6.97 (22°C, zebrafish: log BCF_W wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
2.65–4.54 (various marine species, mean dry wt. BCF, Hope et al. 1998)
> 5.44, > 6.97 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
> 5.53, > 6.99 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
6.95, 8.26 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 3.97 (human, steady-state not reached during whole life: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:

13 (trout in Lake Ontario, Niimi 1996)
0.047, 0.42, 0.10 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:

8.09 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
6.19, 5.99, 5.83, 5.61 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
6.19, 6.17 (marine humic substances of 5 mg L^{-1} DOC, quoted; calculated-MCI χ, reported as log K_h, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: 8.5×10^{-7} g m^{-1} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007$ d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
$k_1 = 40$ d^{-1}; $k_2 = 0.004$ d^{-1} (guppy, Bruggeman et al. 1984)
$k_1 = 600$ d^{-1} (guppy, Opperhuizen 1986)
log $k_1 = 1.60$ d^{-1}; log $1/k_2 = 2.39$ d (fish, quoted, Connell & Hawker 1988)
$k_1 = 3640$ d^{-1}; $k_2 = 0.0132$ d^{-1} (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
$k_2 = 0.013$ d^{-1} with $t_{½} = 52$ d and $k_2 = 0.013$ d^{-1} with $t_{½} = 52$ d for food concn of 62 ng/g and 688 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.005$ d^{-1} with $t_{½} = 127$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
$k_2 = 0.005$ d^{-1} with $t_{½} = 149$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil:
Biota: $t_{½}$ > 1000 d in rainbow trout, and $t_{½} = 122$ d its muscle (Niimi & Oliver 1983);

$t_{½} = 175$ d in guppy (Bruggeman et al. 1984).
Depuration $t_{½} = 52$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
depuration $t_{½} = 127$ d for high-dose treatment, $t_{½} = 149$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

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TABLE 7.1.1.209.1
Reported aqueous solubilities and vapor pressures of decachlorobiphenyl at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure			
Dickhut et al. 1986		Burkhard et al. 1984		Goodman 1997	
generator column-GC/ECD		gas saturation-GC/ECD		Knudsen effusion	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
25	6.48×10^{-7}	50.7	2.69×10^{-6}	65	2.6×10^{-5}
60	8.38×10^{-6}	64.9	1.68×10^{-5}	70	5.1×10^{-5}
70	1.76×10^{-5}	72.3	4.00×10^{-5}	75	8.1×10^{-5}
80	4.95×10^{-5}	80.5	1.43×10^{-4}	80	1.10×10^{-4}
		85.2	1.88×10^{-4}	85	1.80×10^{-4}
ln x = A – B/(T/K)		89.8	3.36×10^{-4}		
A	–4.608	25.0	5.30×10^{-8}		
B	8010.6			log (P/Pa) = A – B/(T/K)	
		log (P/Pa) = A – B/(T/K)			
enthalpy of solution:			P/Pa	A	9.91
ΔH_{sol}/(kJ mol^{-1}) = 66.6 ± 4.9		A	14.049	B	4886
for 40–80°C		B	6358.0		
		temp range 50.7–89.8°C			
		ΔH_{subl}/(kJ mol^{-1}) = 101.7			

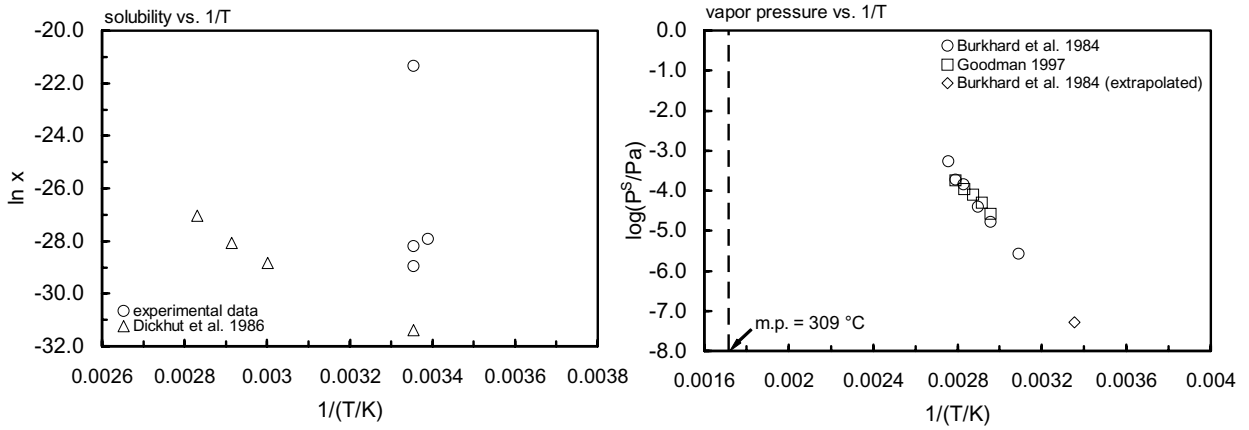

FIGURE 7.1.1.209.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2′,3,3′,4,4′,5,5′,6,6′-decachlorobiphenyl (PCB-209).

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7.1.2 Isomer groups

7.1.2.1 Monochlorobiphenyl

Common Name: Monochlorobiphenyl
Synonym: Dowtherm G
Chemical Name: monochlorobiphenyl
CAS Registry No: 27323-18-8
Molecular Formula: $C_{12}H_9Cl$
No. of Isomers: 3
Molecular Weight: 188.652
Melting Point (°C):
25–77.9 (Shiu et al. 1987)
Boiling Point (°C): 285
Chlorine Content: 18.79% (Hutzinger et al. 1974)
Density (g/cm^3): 1.1
Molar Volume (cm^3/mol):
205.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.30–1.0 (Mackay et al. 1983)
0.301–1.0 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.06–1.5 (selected, Mackay et al. 1983)
7.20 (selected, supercooled liq., Mackay et al. 1983a)
0.795–6.17, 4.08(exptl. range, calculated-UNIFAC, converted from log γ, Burkhard et al. 1986)
1.2–5.5 (selected, Shiu et al. 1987)
2.5–6.73 (selected, supercooled liquid, Shiu et al. 1987)
1.2–9.5 (selected, Formica et al. 1988)
4.0 (selected, Metcalfe et al. 1988)
1.2–5.5 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
1.1–5.6 (selected, Mackay et al. 1983a)
2.30 (supercooled liquid P_L, Mackay et al. 1983a)
1.32 (selected, supercooled liq., Bopp 1983)
1.10 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
0.271–2.04 (selected, solid, Shiu et al. 1987)
0.9–2.5 (selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
79.3 (calculated-P/C, Bopp 1983)
58–74 (calculated, Mackay et al. 1983a)
60.0 (selected, Mackay et al. 1983a,b)
42.56–75.55 (calculated, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
4.66 (selected, Mackay et al. 1983b)
4.70 (selected, Mackay 1986; Metcalfe et al. 1988)
4.3–4.6 (selected, Shiu et al. 1987)
4.73 (calculated-no. Cl atoms, Formica et al. 1988)
4.50 (quoted, Luthy et al. 1997)

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Bioconcentration Factor, log BCF:

3.40 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Half-Lives in the Environment:

Air: atmospheric photodegradation, 0.62–1.4 d (Dilling et al. 1983); calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for monochlorobiphenyls (Kwok et al. 1995).

Surface water: 1.4–4.9 d in Lake Michigan (Neely 1983); 2–3 d for river water (Bailey et al. 1983).

Groundwater:

Sediment:

Soil:

Biota:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: k = 0.25 g/m^2 h (Mackay 1986; Metcalfe et al. 1988).

Photolysis: $t_{½}$ = 0.62–1.4 d for photodegradation in the atmosphere (Dilling et al. 1983).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, k_{OH}(calc) = $(3.1 – 4.7) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp., and the tropospheric lifetime was calculated to be 5–11 d for monochlorobiphenyls (Atkinson 1987)

k_{OH} (exptl) = $(2.8 – 5.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, and k_{OH}(calc) = $(3.2 – 4.6) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp. for reaction with monochlorobiphenyls, the tropospheric lifetime was calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, 7×10^{-8} nmol cell^{-1}·h^{-1} (Furukawa et al. 1978; selected, NAS 1979); time for 50% biodegradation of an initial concentration of 1–100 µg/L by river dieaway test is about 2–5 d (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

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7.1.2.2 Dichlorobiphenyl

Common Name: Dichlorobiphenyl
Synonym:
Chemical Name: dichlorobiphenyl
CAS Registry No: 25512-42-9
Molecular Formula: $C_{12}H_8Cl_2$
No. of Isomers: 12
Molecular Weight: 223.098
Melting Point (°C):
24.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; quoted, Metcalfe et al. 1988)
Boiling Point (°C):
312 (Shiu & Mackay 1986)
Chlorine Content: 31.77%
Density (g/cm^3 at 20°C): 1.30
Molar Volume (cm^3/mol):
226.4 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.06–1.5 (Mackay et al. 1983)
0.059–1.0 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.22 (quoted, Bopp 1983)
0.06–1.5, 2.20 (solid, supercooled liquid, Mackay et al. 1983a)
0.898–1.96, 1.60(exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
1.6 (Mackay 1986; quoted, Metcalfe et al. 1988)
0.06–2.0, 1.02–2.26(selected, solid, supercooled liquid, Shiu et al. 1987)
0.06–2.0 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
0.223 (quoted, supercooled liquid, Bopp 1983)
0.60 (quoted, supercooled liquid, Mackay et al. 1983a)
0.03–0.36 (Mackay et al. 1983)
0.24 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
0.0018–0.279, 0.008–0.60 (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
153.6 (calculated-P/C, Bopp 1983)
60.0 (Mackay et al. 1983a,b)
97.0 (calculated-P/C, Mackay et al. 1983a)
17–92.2 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
5.19 (Mackay et al. 1983a,b)
5.10 (Mackay 1986; Metcalfe et al. 1988)
4.9–5.3 (selected, Shiu et al. 1987)
5.13 (calculated-chlorine atoms, Formica et al. 1988)
5.10 (quoted mean value for isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
3.89 (biota, Mackay et al. 1983b)
3.80 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
4.10 (calculated-MCI χ, Koch 1983)

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Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half Lives, $t_{½}$:

Volatilization/Evaporation: k = 0.065 g m^{-2} h^{-1} (selected, Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(1.4 – 2.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 8–17 d at room temp. (Atkinson 1987)

k_{OH}(exptl) = $(2.0 – 4.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, the tropospheric lifetime is calculated to be 3.4–7.2 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, 6×10^{-8} nmol $cell^{-1} \cdot h^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979);

$t_{½}$ ~ 2–3 d for degradation, using river water dieaway test (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the calculated rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{½}$ = 2–3 d (Bailey et al. 1983).

Groundwater:

Sediment:

Soil:

Biota:

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7.1.2.3 Trichlorobiphenyl

Common Name: Trichlorobiphenyl
Synonym:
Chemical Name: trichlorobiphenyl
CAS Registry No: 25323-68-6
Molecular Formula: $C_{12}H_7Cl_3$
No. of Isomers: 24
Molecular Weight: 257.543
Melting Point (°C):
28–87 (Shiu & Mackay 1986; Metcalfe et al. 1988)
Boiling Point (°C):
337 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 41.4%
Density (g/cm^3):
Molar Volume (cm^3/mol):
247.3 (calculated-Le Bas method at normal boiling point Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.24–0.65 (Mackay et al. 1983)
0.244–0.651 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.05 (Neely 1980)
0.15–0.64, 0.67(solid, supercooled liquid, Mackay et al. 1983)
0.0654–1.09 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.65 (quoted, Mackay 1986; Metcalfe et al. 1988)
0.015–0.40 (selected, Shiu et al. 1987)
0.015–0.40 (quoted, Formica et al. 1988)
0.015–0.40 (quoted range for individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
0.200 (Neely 1980)
0.0375 (supercooled liquid, Bopp 1983)
0.01–0.27, 0.20(solid, supercooled liquid, quoted, Mackay et al. 1983)
0.054 (average, liquid, Mackay 1986; Metcalfe et al. 1988)
0.0136–0.143, 0.003–0.022 (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
81.76 (calculated-P/C, Bopp 1983)
82–102 (calculated-P/C, Mackay et al. 1983)
77 (selected, Mackay et al. 1983)
24.3–92.2 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
5.76 (Mackay et al. 1983)
5.50 (Mackay 1986; Metcalfe et al. 1988)
5.5–5.9 (selected, Shiu et al. 1987)
5.53 (calculated-chlorine atoms, Formica et al. 1988)
5.80 (quoted mean value of isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
4.20 (fish, Mackay 1986; Metcalfe et al. 1988)
4.70 (calculated-MCI χ, Koch 1983)

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Sorption Partition Coefficient, log K_{OC}:

Sorption Partition Coefficient, log K_P:

3.34 (lake sediment, calculated, Formica et al. 1988)
3.50 (calculated-MCI χ, Koch 1983)

Environmental Fate Rate Constants, k, or Half Lives, $t_{½}$:

Volatilization/Evaporation: k = 0.017 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7 – 1.6) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 14–30 d at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0 – 2.1) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radicals for trichlorobiphenyls, the tropospheric lifetime is calculated to be 6.9–15 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of Alcaligenes and Acinetobacter, 5 × 10^{-8} nmol $cell^{-1}·h^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: estimated $t_{½}$ = 134 h from fish in simulated ecosystem (Neely 1980).

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7.1.2.4 Tetrachlorobiphenyl

Common Name: Tetrachlorobiphenyl
Synonym:
Chemical Name: tetrachlorobiphenyl
CAS Registry No: 26914-33-0
Molecular Formula: $C_{12}H_6Cl_4$
No. of Isomers: 42
Molecular Weight: 291.988
Melting Point (°C):
47–180 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
360 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 48.6%
Density (g/cm^3 at 20°C): 1.5
Molar Volume (cm^3/mol):
268.2 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.1–0.68 (Mackay et al. 1983)
0.029–0.606 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.05 (Neely 1980)
0.0008–0.17 (Mackay et al. 1983)
0.017 (McCall et al. 1983)
0.02–0.0955, 0.224 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.26 (quoted, Mackay 1986; Metcalfe et al. 1988)
0.0043–0.10 (selected, Shiu et al. 1987)
0.039–0.38 (selected, supercooled liquid, Shiu et al. 1987)
0.001–0.10 (Formica et al. 1988)
0.001–0.10 (quoted range for individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
0.0653 (Neely 1980)
0.0064 (supercooled liquid, Bopp 1983)
0.003–0.104 (Mackay et al. 1983)
0.06 (supercooled liquid, Mackay et al. 1983)
0.0653 (McCall et al. 1983)
0.012 (Mackay 1986; Metcalfe et al. 1988)
$5.9 \times 10^{-5} - 5.4 \times 10^{-3}$ (selected, Shiu et al. 1987)
0.002 (selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
34.69 (calculated-P/C, Bopp 1983)
75–94 (calculated-P/C, Mackay et al. 1983)
76.0 (Mackay et al. 1983)
1.72–47.59 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
6.35 (suggested, Mackay et al. 1983)
5.90 (Mackay 1986, Metcalfe et al. 1988)
5.6–6.5 (selected, Shiu et al. 1987)

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5.93 (calculated-chlorine atoms, Formica et al. 1988)
6.00 (quoted mean value for isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

3.98 (pinfish, Branson et al. 1975; quoted, Waid 1986)
3.95 (trout, Branson et al. 1975; quoted, NAS 1979)
4.79 (McCall et al. 1983)
4.60 (fish, Mackay 1986; Metcalfe et al. 1988)
5.30 (calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K_{OC}:

4.51 (correlated, McCall et al. 1983)
3.43–5.11 (correlated of literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: $k = 4.2 \times 10^{-3}$ g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.4 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime of 25–60 d at room temp. (Atkinson 1987)
k_{OH}(calc) = $(0.36 – 1.7) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radicals for tetrachlorobiphenyls, the tropospheric lifetime is calculated to be 8.5–40 d (Kwok et al. 1995).
Hydrolysis:
Biodegradation: rate of degradation for both rings substituted with chlorine using species of Alcaligenes and Acinetobacter, 2.5×10^{-8} nmol $cell^{-1}$ h^{-1} (Furukawa et al. 1978; selected, NAS 1979);
no degradation by river dieaway test after 98 d of incubation (Bailey et al. 1983).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil: volatilization $t_{½}$ ~ 10 d from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).
Biota: estimated $t_{½}$ = 139 h from fish in simulated ecosystem (Neely 1980).

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7.1.2.5 Pentachlorobiphenyl

Common Name: Pentachlorobiphenyl
Synonym:
Chemical Name: pentachlorobiphenyl
CAS Registry No: 25429-29-2
Molecular Formula: $C_{12}H_5Cl_5$
No. of Isomers: 46
Molecular Weight: 326.433
Melting Point (°C):
–23.5–124 (Shiu et al. 1987)
76.5–124 (Shiu & Mackay 1986; Metcalfe et al. 1988)
Boiling Point (°C):
381 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 54.4%
Density (g/cm^3 at 20°C): 1.50
Molar Volume (cm^3/mol):
289.1 (Le Bas method at normal boiling point, Shiu & Mackay 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.1–0.31 (Mackay et al. 1983)
0.105–0.311 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.01 (Neely 1980)
0.004–0.03 (Mackay et al. 1983)
0.072 (supercooled liquid, Mackay et al. 1983)
0.0338–0.0525, 0.0829 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.099 (Mackay 1986; Metcalfe et al. 1988)
0.004–0.02 (selected, Shiu et al. 1987)
0.03–0.11 (selected, supercooled liquid, Shiu et al. 1987)
0.004–0.02 (Formica et al. 1988)
0.024 (selected average value of isomers, Mackay 1989)
0.004–0.02 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
0.01026 (Neely 1980)
0.00111 (supercooled liquid, Bopp 1983)
0.015 (supercooled liquid, Mackay et al. 1983)
0.004–0.03 (Mackay et al. 1983)
0.0026 (Mackay 1986; Metcalfe et al. 1988)
0.000304–0.0093(selected, Shiu et al. 1987)
0.0023–0.051(selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
68.0 (suggested, Mackay et al. 1983)
17.34 (calculated-P/C, Bopp 1983)
24.8–151.4 (selected, Shiu et al. 1987)
12.2 (calculated, Mackay 1989)

Octanol/Water Partition Coefficient, log K_{OW}:
6.85 (suggested, Mackay et al. 1983)
6.33 (calculated-chlorine atoms, Formica et al. 1988)

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6.30 (Mackay 1986; Metcalfe et al. 1988)
6.2–6.5 (selected, Shiu et al. 1987)
6.60 (selected, Mackay 1989)
6.40 (quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

5.0 (fish, Mackay 1986; Metcalfe et al. 1988)
5.30 (Mackay 1989)
5.90 (calculated-MCI χ, Koch 1983)

Sorption Partition Coefficient, log K_{OC}:

6.21 (calculated, $0.41K_{OW}$, Mackay 1989)

Sorption Partition Coefficient, log K_P:

4.15 (lake sediment, calculated-K_{OW}, f_{OC}, Formica et al. 1988)
4.51 (calculated-MCI χ, Koch 1983)

Environmental Fate Rate Constants, k, and Half Lives, $t_{½}$:

Volatilization /Evaporation: $k = 1.0 \times 10^{-3}$ g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}(calc) = $(0.2 – 0.4) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp., with a calculated tropospheric lifetime of 60–120 d (Atkinson 1987);
k_{OH}(calc) = $(0.3 – 0.9) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radicals for pentachlorobiphenyls, the tropospheric lifetime is calculated to be 16–48 d (Kwok et al. 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 0.62–1.4 d for atmospheric photodegradation (Dilling et al. 1983);
calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radicals for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radicals for pentachlorobiphenyls (Kwok et al. 1995).
Surface water:
Groundwater:
Sediment:
Soil: volatilization $t_{½}$ = 25 d from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).
Biota: estimated $t_{½}$ = 226 d from fish in simulated ecosystem (Neely 1980).

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7.1.2.6 Hexachlorobiphenyl

Common Name: Hexachlorobiphenyl
Synonym:
Chemical Name: hexachlorobiphenyl
CAS Registry No: 26601-64-9
Molecular Formula: $C_{12}H_4Cl_6$
No. of Isomers: 42
Molecular Weight: 360.878
Melting Point (°C):
85–160 (Shiu et al. 1987)
77–150 (Shiu & Mackay 1986; Metcalfe et al. 1988)
Boiling Point (°C):
400 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 62.77% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.60
Molar Volume (cm^3/mol):
310.0 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.06–0.25 (Mackay et al. 1983)
0.0582–0.256(Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0004–0.01, 0.021 (solid, supercooled liquid, Mackay et al. 1983)
0.00303–0.0504, 0.00297 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.038 (Mackay 1986; Metcalfe et al. 1988)
0.0004–0.001, 0.0022–0.01 (solid, supercooled liquid, Shiu et al. 1987)
0.0004–0.005 (Formica et al. 1988)
0.0035 (Mackay & Paterson 1991)
0.0004–0.001 (quoted range, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C):
0.000182 (supercooled liquid, Bopp 1983)
0.0016, 0.005 (solid, supercooled liquid, Mackay et al. 1983)
5.8×10^{-4} (Mackay 1986; Metcalfe et al. 1988)
$2.0 \times 10^{-5} - 1.59 \times 10^{-3}$, $7.0 \times 10^{-4} - 0.012$ (solid, supercooled liquid, Shiu et al. 1987)
0.0005 (selected, Mackay & Paterson 1991)

Henry's Law Constant (Pa m^3/mol at 25°C):
86.0 (Mackay et al. 1983)
6.70 (calculated-P/C, Bopp 1983)
11.9–81.8 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
6.70–7.30 (selected, Shiu et al. 1987)
6.70 (selected, Mackay 1986; Metcalfe et al. 1988)
6.80 (selected, Mackay & Paterson 1991)
7.00 (quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, log BCF:
6.50 (calculated-MCI χ, Koch 1983)
5.39 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
4.57 (green alga, Mailhot 1987)

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Sorption Partition Coefficient, log K_{OC}:

4.785–6.869 (correlated literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: 2.5×10^{-4} g m^{-2} h^{-1} (Mackay 1986; Metcalf et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = $(0.16 – 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at room temp., the tropospheric lifetime is calculated to be 29–60 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: degradation rate constants estimated to be 1.5×10^{-5} h^{-1} in water, soil and sediment (Mackay & Patterson 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: volatilization $t_{½}$ = 40 d from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).

Biota:

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7.1.2.7 Heptachlorobiphenyl

Common Name: Heptachlorobiphenyl
Synonym:
Chemical Name: heptachlorobiphenyl
CAS Registry No: 28655-71-2
Molecular Formula: $C_{12}H_3Cl_7$
No. of Isomers: 24
Molecular Weight: 395.323
Melting Point (°C):
122.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
417 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 62.77% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.70
Molar Volume (cm^3/mol):
330.9 (Le Bas method at normal boiling point, Shiu & Mackay 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0596–0.109(Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0005, 0.006 (solid, supercooled liquid, Mackay et al. 1983)
0.00816–0.0205, 0.011 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.014 (Mackay 1986; Metcalfe et al. 1988)
0.00045–0.002, 0.0076–0.018 (solid, supercooled liquid, selected, Shiu et al. 1987)
0.00046–0.002(Formica et al. 1988)

Vapor Pressure (Pa at 25°C):
0.0015 (supercooled liquid, Mackay et al. 1983)
1.3×10^{-4} (Mackay 1986; Metcalfe et al. 1988)
2.73×10^{-5}, 2.5×10^{-4} (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol):
100.0 (Mackay et al. 1983)
5.4 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
7.1 (Mackay 1986; Metcalfe et al. 1988)
6.7–7.0 (selected, Shiu et al. 1987)

Bioconcentration Factor, log BCF:
7.10 (calculated-MCI χ, Koch 1983)
5.80 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization/Evaporation: $k = 6.2 \times 10^{-5}$ g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis:

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Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

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7.1.2.8 Octachlorobiphenyl

Common Name: Octachlorobiphenyl
Synonym:
Chemical Name: octachlorobiphenyl
CAS Registry No: 31472-83-0
Molecular Formula: $C_{12}H_2Cl_8$
No. of Isomers: 12
Molecular Weight: 429.768
Melting Point (°C):
159–162 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
432 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 65.98% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.7
Molar Volume (cm^3/mol):
351.8 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.0443–0.0474(Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at 25°C):
0.0002–0.007, 0.020 (solid, supercooled liquid, estimated, Mackay et al. 1983)
0.00345–0.006, 0.00378 (experimental range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.0055 (Mackay 1986; Metcalfe et al. 1988)
0.0002–0.0003, 0.004–0.0068 (solid, supercooled liquid, Shiu et al. 1987)

Vapor Pressure (Pa at 25°C):
2.8×10^{-5} (Mackay 1986; Metcalfe et al. 1988)
2.66×10^{-5}, 6.0×10^{-3} (solid, supercooled liquid, selected, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
100.0 (suggested, Mackay et al. 1983)
38.08 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{OW}:
8.55 (Mackay et al. 1983)
7.50 (Mackay 1986; Metcalfe et al. 1988)
7.1 (selected, Shiu et al. 1987)

Bioconcentration Factor, log BCF:
6.20 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:
Volatilization/Evaporation: $k = 1.5 \times 10^{-5}$ g m^{-2}·h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Half-Lives in the Environment:

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7.1.2.9 Nonachlorobiphenyl

Common Name: Nonachlorobiphenyl
Synonym:
Chemical Name: nonachlorobiphenyl
CAS Registry No: 53742-07-7
Molecular Formula: $C_{12}HCl_9$
No. of Isomers: 3
Molecular Weight: 464.213
Melting Point (°C):
182.8–206 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)
Boiling Point (°C):
445 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)
Chlorine Content: 68.73% (Hutzinger et al. 1974)
Density (g/cm^3 at 20°C): 1.80
Molar Volume (cm^3/mol):
372.7 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.016 (Mackay et al. 1983)
0.0163–0.0276(Shiu et al. 1987)

Solubility (g/m^3 or mg/L at 25°C):
0.0001, 0.0007 (solid, supercooled liquid, Mackay et al. 1983)
0.000678–0.00148, 0.00145 (exptl. range, calculated-UNIFAC, converted from log γ, Burkhard & Kuehl 1986)
0.002 (Mackay 1986; Metcalfe et al. 1988)
0.000018–0.00011, 0.00065–0.0068 (solid, supercooled liquid, selected, Shiu et al. 1987)

Vapor Pressure (Pa at 25°C):
0.00015 (supercooled liquid, Mackay et al. 1983)
6.3×10^{-6} (Mackay 1986; Metcalfe et al. 1988)

Henry's Law Constant (Pa m^3/mol at 25°C):
100.0 (estimated, Mackay et al. 1983)

Octanol/Water Partition Coefficient, log K_{OW}:
9.14 (Mackay et al. 1983)
7.9 (Mackay 1986; Metcalfe et al. 1988)
7.2–8.16 (selected, Shiu et al. 1987)

Bioconcentration Factor, log BCF:
6.60 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:
Volatilization/Evaporation: $k = 3.5 \times 10^{-6}$ g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Half-Lives in the Environment:

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7.1.3 Aroclor mixtures

7.1.3.1 Aroclor 1016

Common Name: Aroclor 1016
Synonym:
Chemical Name:
CAS Registry No: 12674-11-2
Molecular Formula:
Average Molecular Weight: 257
Physical state: mobile oil
Distillation Range (°C):
323–356 (NAS 1979; Brinkman & De Kock 1980)
Chlorine Content: 41%
Density (g/cm^3):
1.37 (20°C, Brinkman & De Kock 1980)
1.36–1.37 (25°C, NAS 1979)
1.33 (Mills et al. 1982)
1.40 (25°C, Mackay 1986)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
0.22–0.25 (estimated, Tucker et al. 1975)
0.906 (23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Lee et al. 1979)
0.42 (shake flask-GC/ECD, Paris et al. 1978; Callahan et al. 1979; Mackay et al. 1980; Mills et al. 1982)
0.906 (shake flask-GC/ECD, Lee et al. 1979)
0.049, 0.490 (shake flask, nephelometric, Hollifield 1979)
0.085 (Kenaga & Goring 1980)
0.34 (quoted, Pal et al. 1980)
0.906 (23°C, shake flask-GC/ECD, Griffin & Chian 1981; quoted, Sklarew & Girvin 1987)
0.40–0.91 (selected, Mackay et al. 1983)
0.84 (selected, Mackay 1986; Metcalfe et al. 1988)
0.332 (quoted, Chou & Griffin 1986)

Vapor Pressure (Pa at 25°C):
0.0533 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
0.060 (quoted, Mackay et al. 1983)
0.200 (quoted, supercooled liquid, Mackay et al. 1983)
0.10 (selected, Mackay 1986; Metcalfe et al. 1988)
0.12, 0.121 (GC-RT correlation, Foreman & Bidleman 1985)

Henry's Law Constant ($Pa\ m^3/mol$ at 25°C):
1368 (calculated, Paris et al. 1978)
33.4 (calculated-P/C, Mabey et al. 1982)
77.0 (calculated, Mackay et al. 1983)

Octanol/Water Partition Coefficient, log K_{OW}:
> 5.58 (shake flask, Chiou et al. 1977; Callahan et al. 1979; Veith et al. 1979a; Kenaga & Goring 1980; Mabey et al. 1982; Mackay 1982)
4.38 (shake flask-GC, Paris et al. 1978; quoted, Callahan et al. 1979; Ryan et al. 1988)
5.88 (HPLC-RT correlation, Veith et al. 1979b; Garten & Trabalka 1983)
3.48 (Pal et al. 1980; Sklarew & Girvin 1987)

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4.3–5.48 (quoted, Mills et al. 1982)
4.40–5.80 (selected, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988)
5.31 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, log BCF:

3.80, 3.81, 3.74 (bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
4.18 (fish in Hudson River, Skea et al. 1979; quoted, Waid 1986)
4.63 (fathead minnow, 32-d exposure, Veith et al. 1979b; Veith & Kosian 1983)
4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
4.69 (quoted, Bysshe 1982)
4.70 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
4.63; 4.56 (fish, quoted; calculated-K_{OW}, Mackay 1982)
0.15 (rodents, Garten & Trabalka 1983)
4.63 (fish, Garten & Trabalka 1983)
4.63 (fathead minnow, quoted, Zaroogian et al. 1985)
4.24, 4.30 (oyster, quoted, Zaroogian et al. 1985)
3.11–4.5 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC}:

5.19, 5.23, 4.96, 4.73 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
5.26 (calculated-K_{OW}, Mabey et al. 1982)
4.87 (calculated, Sklarew & Girvin 1987)
4.25 (soil, calculated-S, Chou & Griffin 1986)
5.03, 4.97 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: volatilization $t_{½}$ = 9.9 h (Paris et al. 1978, quoted Callahan et al. 1979); rate constant k = 0.031 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis: not environmentally significant (Mabey et al. 1982).
Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1} h^{-1} and k << 1 M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).
Biodegradation: 32.9% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972);
33% degraded by activated sludge for 48-h exposure (Tucker et al. 1975; Versar Inc. 1979; quoted, Pal et al. 1980);
rate constant k = 0.2 d^{-1} by acclimated activated sludge with $t_{½}$ = 3.5 d (Callahan et al. 1979).
96% loss by degradation with Nocardia strain NCIB 10603 and 91% loss with NCIB 10643, both within 52 d; > 98% loss with NCIB 10603 and > 96% loss with NCIB 10643, both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).
Biotransformation: k ~ 3×10^{-9} to 3×10^{-12} mL $cell^{-1}$ h^{-1}, estimated for bacteria transformation in water (Mabey et al. 1982).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: $t_{½}$ = 9.9 h in 1 m^3 water of 1-m deep (Paris et al. 1978; selected, Callahan et al. 1979; Mills et al. 1982)
Groundwater:
Sediment:
Soil: $t_{½}$ > 50 d (Ryan et al. 1988).
Sludge: estimated $t_{½}$ = 15 d for the volatilization from activated sludge under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).
Biota: $t_{½}$ ~ 1.2 yr in fish in Hudson River (Armstrong & Sloan 1985).

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7.1.3.2 Aroclor 1221

Common Name: Aroclor 1221
Synonym:
Chemical Name:
CAS Registry No: 11104-28-2
Molecular Formula:
Average Molecular Weight: 192–200.7
Physical State: mobile oil
Distillation Range (°C):
275–320 (NAS 1979; Brinkman & De Kock 1980)
Chlorine Content: 20.5–21.5%
Density (g/cm^3):
1.182–1.19 (25°C, NAS 1979)
1.18 (20°C, Brinkman & De Kock 1980)
1.15 (Callahan et al. 1979; Mills et al. 1982)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
5.00 (Zitko 1970, 1971)
3.5 (23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Chou & Griffin 1986)
15.0 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Pal et al. 1980; Mills et al. 1982)
3.52 (shake flask-GC/ECD, Lee et al. 1979)
0.59 (shake flask-nephelometric, Hollifield 1979)
40.0 (calculated-K_{OW}, Mabey et al. 1982)
3.50–15.0 (selected, Mackay et al. 1983)

Vapor Pressure (Pa at 25°C):
0.893 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
0.93 (Pal et al. 1980)
0.89 (quoted, Mackay et al. 1983)

Henry's Law Constant ($Pa\ m^3/mol$):
0.750 (Hetling et al. 1978)
17.23 (calculated-P/C, Mabey et al. 1982)
60.0 (suggested value, Mackay et al. 1983)
23.10 (calculated, Burkhard et al. 1985b)

Octanol/Water Partition Coefficient, log K_{OW}:
2.8 (Monsanto Co. 1972; quoted, Callahan et al. 1979)
2.81 (Pal et al. 1980)
4.08 (Callahan et al. 1979; Mabey et al. 1982)
4.10–4.70 (quoted, Mackay et al. 1980)
2.78–4.0 (quoted, Mills et al. 1982)
4.09 (quoted, Chou & Griffin 1986)
4.09 (quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:
3.34 (microorganism, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
3.76 (sediment, calculated-K_{OW}, Mabey et al. 1982)
3.62 (soil, calculated-S, Chou & Griffin 1986)

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Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated k ~ 1.74 mg cm^{-2} h^{-1} from liquid substrate at 100°C (Hutzinger et al. 1974; quoted, Pal et al. 1980).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1} h^{-1} and k << 1 M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: 80.6% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980); 81% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980); k = 0.8 d^{-1} and $t_{½}$ = 0.9 d for biodegradation by acclimated activated sludge (Callahan et al. 1979).

Biotransformation: estimated k ~ 3×10^{-9} to 3×10^{-12} mL $cell^{-1}$ h^{-1} rate of transformation for bacteria in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil: $t_{½}$ > 50 d (Ryan et al. 1988).

Sludge: estimated $t_{½}$ = 12 d of volatilization from activated sludge to be 12 d under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).

Biota:

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7.1.3.3 Aroclor 1232

Common Name: Aroclor 1232
Synonym:
Chemical Name:
CAS Registry No: 11141-16-5
Molecular Formula:
Average Molecular Weight: 221–232.2
Physical State: mobile oil
Distillation Range (°C):
270–325 (NAS 1979; Brinkman & De Kock 1980)
Chlorine Content: 32%
Density (g/cm^3):
1.260 (20°C, Brinkman & De Kock 1980)
1.27–1.28 (25°C, NAS 1979)
1.24 (Callahan et al. 1979; Mills et al. 1982)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
1.45 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Chou & Griffin 1986)
1.45 (quoted, Pal et al. 1980; Mackay et al. 1983)
407 (calculated-K_{OW}, Mabey et al. 1982)

Vapor Pressure (Pa at 25°C):
0.54 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)
0.533 (quoted, Mills et al. 1982)
0.54 (quoted, Mackay et al. 1983)

Henry's Law Constant ($Pa\ m^3/mol$):
60.0 (suggested, Mackay et al. 1980)
1.14 (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
3.2 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)
4.54 (Tulp & Hutzinger 1978; Callahan et al. 1979)
3.23 (quoted, Pal et al. 1980)
3.18–4.48 (quoted, Mills et al. 1982)
4.10–5.20 (quoted, Mackay et al. 1983)
4.62 (calculated-S, Chou & Griffin 1986)
4.54 (quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:
2.54 (microorganism, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
2.89 (sediment, calculated-K_{OW}, Mabey et al. 1982)
3.85 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis: not environmentally significant (Mabey et al. 1982).

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Oxidation: calculated rate constant for singlet oxygen k << 360 M^{-1} h^{-1} and k << 1 $M^{-1}{\cdot}h^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: aerobic biodegradation $t_{½}$ = 61.4 d without the addition of polymer chitin, $t_{½}$ = 33.4 d with chitin and $t_{½}$ = 26.8 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: k ~ 3×10^{-9} to 3×10^{-12} mL·$cell^{-1}{\cdot}h^{-1}$, estimated rate of transformation for bacteria in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: aerobic biodegradation $t_{½}$ = 61.4 d without the addition of polymer chitin, $t_{½}$ = 33.4 d with chitin and $t_{½}$ = 26.8 d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Groundwater:

Sediment:

Soil: $t_{½}$ > 50 d (Ryan et al. 1988).

Biota:

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7.1.3.4 Aroclor 1242

Common Name: Aroclor 1242
Synonym:
Chemical Name:
CAS Registry No: 534-692-19
Molecular Formula:
Average Molecular Weight: 261–266.5
Physical State: mobile oil
Distillation Range (°C):
325–366 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)
Chlorine Content: 42%
Density (g/cm^3):
1.38 (Brinkman & De Kock 1980)
1.30–1.39 (quoted, NAS 1979)
1.35 (Callahan et al. 1979; Mills et al. 1982)
1.40 (quoted, Mackay 1986; Metcalfe et al. 1988)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.20 (Monsanto Co. 1972; quoted, Hutzinger et al. 1974; Tucker et al. 1975 Sawhney 1987)
0.20 (20°C, Nisbet & Sarofim 1972)
0.24 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Brinkman & De Kock 1980; Geyer et al. 1980; Pal et al. 1980; Erickson 1986)
0.045 (shake flask-GC, Lawrence & Tosine 1976)
0.085 (Branson 1977; Kenaga & Goring 1980)
0.703 (23°C, shake flask-GC/ECD, Griffin et al. 1978)
0.34 (shake flask-GC/ECD, Paris et al. 1978)
0.1329 (11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)
0.23 (quoted, Callahan et al. 1979; Mabey et al. 1982)
0.23–0.703 (shake flask-GC, Lee et al. 1979)
0.10 (shake flask-nephelometric, Hollifield 1979)
0.703 (20°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)
0.25 (quoted, Eisenreich et al. 1981)
0.34–0.703 (selected, Westcott et al. 1981)
0.10–0.30 (selected, Mills et al. 1982)
0.75 (selected, Mackay 1986; Metcalfe et al. 1988)
0.277 (20°C, calculated from mole fraction, Murphy et al. 1987)
0.097; 0.085–0.34 (21°C, shake flask-GC/ECD; quoted lit. range, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0133 (20°C, Nisbet & Sarofim 1972)
0.12 (20°C, extrapolated, Monsanto 1972; NAS 1979)
$\log (P_L/mmHg) = 8.80 - 3500/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.055 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983; Bidleman & Christinsen 1979)
0.054 (Callahan et al. 1979; Westcott et al. 1981; Eisenreich et al. 1981; Richardson et al. 1983)
0.054 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
0.040 (38°C, average, Wingender & Williams 1984)
0.076, 0.077 (GC-RT correlation, Foreman & Bidleman 1985)
0.077 (quoted, Mackay et al. 1986)
0.0517 (quoted, Eisenreich 1987)

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0.091 (selected, Mackay 1986; Metcalfe et al. 1988)
0.033 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations):

58.06 (calculated, Mackay & Leinonen 1975)
768 (calculated, Paris et al. 1978)
59.5 (Slinn et al. 1978)
56.74 (calculated-P/C, Eisenreich et al. 1981)
20.32–41.62 (Westcott et al. 1981)
20.27–41.54 (calculated, Westcott et al. 1981)
79.02 (batch stripping, Atlas et al. 1982; quoted, Eisenreich et al. 1983; Atlas & Giam 1986)
34.69 (radiotracer-equilibration, Atlas et al. 1982; Atlas & Giam 1986)
200.6 (calculated-P/C, Mabey et al. 1982)
22.29 (direct concn. ratio-GC/ECD, Murphy et al. 1983)
40.3 (16°C, calculated-P/C, Richardson et al. 1983)
34.75 (calculated, Burkhard et al. 1985b)
50.0 (calculated, Mackay et al. 1986)
34.45 (calculated-P/C, Eisenreich 1987)
23.0 (20°C, quoted, Murphy et al. 1987 from Burkhard et al. 1985b)
28.31 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
28.27 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 12.869 - 4339/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

4.11 (Callahan et al. 1979; Mabey et al. 1982; quoted, Ryan et al. 1988)
5.58 (HPLC-RT correlation, Veith et al. 1979a; quoted, Kenaga & Goring 1980)
0.703 (shake flask-GC/ECD, Lee et al. 1979)
3.54 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
4.0–5.6 (quoted, Mills et al. 1982)
4.50–5.80 (quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
5.90 (Rapaport & Eisenreich 1984)
5.74 (literature mean, Di Toro et al. 1985)
5.29 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, log BCF:

3.92, 3.65, 3.46(bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
0.08, –0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
4.69 (quoted, Bysshe 1982)
3.36 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
0.30, 0.13, –0.11, –0.50, –0.27 (rodent, poultry, sheep, small birds, swine, Garten & Trabalka 1983)
3.20–4.51 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
4.69, 5.99 (fish 5% lipid in flow-through system: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.13, 5.18, 4.89, 4.70 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
3.80 (sediment, calculated-K_{OW}, Mabey et al. 1982)
4.17 (Lake Michigan sediment, 0.7–3.8% OC, Eadie et al. 1983)
3.36 (calculated, Sklarew & Girvin 1987)
4.09 (soil, calculated-S, Chou & Griffin 1986)
4.30, 4.12, 4.64(soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 2.0 to > 10, average, Delle Site 2001)
4.82, 4.74 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

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Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: k = 0.23 μg m^{-2} d^{-1} with $t_{½}$ = 17 d (Baker et al. 1986);
k = 0.029 g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1} h^{-1} and k << 1 M^{-1} h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: 26.3% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980);
26% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980);
degraded by acclimated activated sludge with a first-order rate constant k = 0.15 d^{-1} and $t_{½}$ = 4.5 d (Callahan et al. 1979).
88% loss by degradation with Nocardia strain NCIB 10603, 76% loss with NCIB 10643 both within 52 d; 95% loss with NCIB 10603 and 85% loss with NCIB 10643 both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation: estimated k ~ 3×10^{-9} to 3×10^{-12} mL·cell^{-1}·h^{-1} for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 12 h (Paris et al. 1978); volatilization $t_{½}$ ~12 h at 1 m depth in 1 m^3 of water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

Groundwater:

Sediment:

Soil: $t_{½}$ > 50 d (Ryan et al. 1988).

Biota:

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7.1.3.5 Aroclor 1248

Common Name: Aroclor 1248
Synonym:
Chemical Name:
CAS Registry No: 12672-29-6
Molecular Formula:
Average Molecular Weight: 288–299.5
Physical State: mobile oil
Distillation Range (°C):
340–375 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)
Chlorine Content: 48%
Density (g/cm^3):
1.44 (20°C, Brinkman & De Kock 1980)
1.40–1.41 (NAS 1979)
1.41 (Callahan et al. 1979)
1.40 (Mackay 1986; Mills et al. 1982; Metcalfe et al. 1988)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.10 (20°C, Nisbet & Sarofim 1972)
0.10 (Monsanto Co. 1972; selected, Hutzinger et al. 1974; Sawhney 1987)
0.043 (26°C, Hutzinger et al. 1974)
0.054 (Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983, 1986)
0.054 (NAS 1979; Callahan et al. 1979; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Chou & Griffin 1986)
0.060 (shake flask-nephelometry, Hollifield 1979)
0.052 (quoted, Brinkman & De Kock 1980; Erickson 1986)
0.32 (selected, Mackay 1986; Metcalfe et al. 1988)
0.056 (selected, Eisenreich 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.004 (20°C, Nisbet & Sarofim 1972)
0.066 (selected, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; quoted, Mills et al. 1982)
0.11 (20°C, extrapolated, Monsanto 1972; quoted, NAS 1979)
$\log (P_L/mmHg) = 8.40 - 3400/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.017 (Branson 1977; Kenaga & Goring 1980)
0.066 (Callahan et al. 1979; Mabey et al. 1982; Mackay et al. 1983)
0.025, 0.024 (GC-RT correlation, Foreman & Bidleman 1985)
0.0085 (selected, Eisenreich 1987)
0.023 (selected, Mackay 1986; Metcalfe et al. 1988)

Henry's Law Constant ($Pa\ m^3/mol$):
355.7 (calculated, Mackay & Leinonen 1975)
372 (Slinn et al. 1978)
364 (calculated-P/C, Mabey et al. 1982)
86.0 (calculated-P/C, Mackay et al. 1983)
44.58 (calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)
50.0 (calculated-P/C, Mackay et al. 1986)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
5.75 (Callahan et al. 1979; Kenaga & Goring 1980; Mabey et al. 1982; Chou & Griffin 1986)

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6.11 (shake flask-GC, Chiou et al. 1977; quoted, Callahan et al. 1979)
6.11 (HPLC-RT correlation, Veith et al. 1979a,b; quoted, Mackay 1982; Garten & Trabalka 1983)
6.0 (quoted, Mills et al. 1982)
5.8–6.3 (quoted, Mackay et al. 1983, 1986; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
5.60 (quoted, Ryan et al. 1988)
6.10 (selected, Thomann 1989)

Bioconcentration Factor, log BCF:

4.42 (bluegill sunfish, Stalling & Meyer 1972)
4.75–4.79 (channel catfish, Mayer et al. 1977; quoted, Waid 1986)
5.08 (fathead minnow, DeFoe et al. 1978; quoted, Waid 1986)
4.85 (fathead minnow, 32-d exposure, Veith et al. 1979b)
4.86, 4.07 (fish, flowing water, static water, Kenaga & Goring 1980)
4.86 (quoted, Bysshe 1982)
3.86–4.42, 4.19(mussel, range, average, Geyer et al. 1982)
4.86 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
4.85, 4,79 (fish: quoted, calculated-K_{OW}, Mackay 1982)
4.85, 0.82, 0.72(fish, poultry, rodents, Garten & Trabalka 1983)
4.5–5.0 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
4.80, 6.08 (fathead minnow, male: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.08, 6.08 (fathead minnow, female: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

5.44 (sediment, calculated-K_{OW}, Mabey et al. 1982)
4.74 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: $k = 8.3 \times 10^{-3}$ g $m^{-2} \cdot h^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis: TiO_2 catalyzed photolytic process destroyed 80% of total PCBs in an aqueous solution and clay suspension after 4h of radiation, and 50% destroyed in sediment suspension within 6 h (Zhang et al. 1993).

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, $k << 360\ M^{-1}\ h^{-1}$ and $k << 1\ M^{-1}\ h^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: aerobic biodegradation $t_{½} = 77.6$ d without the addition of polymer chitin, $t_{½} = 38.6$ d with chitin and $t_{½} = 31.9$ d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected form the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to 3×10^{-12} $mL \cdot cell^{-1} \cdot h^{-1}$ for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$\log k_2 = -1.92\ d^{-1}$ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air:

Surface water: volatilization $t_{½} \sim 10$ h at 1 m depth in 1 m^3 water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982);
TiO_2 catalyzed photolytic process destroyed 80% of total PCBs in an aqueous solution and clay suspension after 4 h of radiation, and 50% destroyed in sediment suspension within 6 h (Zhang et al. 1993).

Groundwater:

Sediment:

Soil: $t_{½} > 50$ d (Ryan et al. 1988).

Biota:

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7.1.3.6 Aroclor 1254

Common Name: Aroclor 1254
Synonym:
Chemical Name:
CAS Registry No: 11097-69-1
Molecular Formula:
Average Molecular Weight: 327–328.4
Physical State: viscous liquid
Distillation Range (°C):
365–390 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)
Chlorine Content: 54%
Density (g/cm^3):
1.505 (Monsanto 1972)
1.49–1.50 (65°C, NAS 1979)
1.54 (20°C Brinkman & De Kock 1980)
1.50 (Mills et al. 1982; Mackay 1986; Metcalfe et al. 1988)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.30 (Zitko 1971)
0.043 (26°C, Nelson et al. 1972)
0.050 (20°C, Nisbet & Sarofim 1972)
0.040 (Monsanto 1972; selected, Hutzinger et al. 1974; Sawhney 1987)
0.012–0.07 (Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Geyer et al. 1980; Mackay et al. 1983, 1986)
0.056 (shake flask-GC, Haque et al. 1974; quoted, Haque et al. 1980)
0.0001 (20°C, shake flask-GC/ECD, Schoor 1975)
0.045 (shake flask-GC, Lawrence & Tosine 1976)
0.070 (23°C, shake flask-GC/ECD, Griffin et al. 1978)
0.0242 (11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)
0.012 (Brinkman & De Kock 1980; Giam et al. 1980; Pal et al. 1980; Erickson 1986)
0.010 (Kenaga & Goring 1980)
0.031 (Callahan et al. 1979; Mabey et al. 1982)
0.070 (shake flask-GC/ECD, Lee et al. 1979)
0.057 (shake flask-nephelometry, Hollifield 1979)
0.070 (23°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)
0.0115 (quoted, Eisenreich et al. 1981)
0.045–0.07 (quoted literature range, Westcott et al. 1981)
0.010–0.06 (quoted literature range, Mills et al. 1982)
0.042 (quoted, Chou & Griffin 1986)
0.035 (quoted, Eisenreich 1987)
0.14 (selected, Mackay 1986; Metcalfe et al. 1988)
0.043 (20°C, calculated-mole fraction, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00107 (ebulliometry, Burrows 1946)
0.00048 (20°C, Nisbet & Sarofim 1972)
0.0103 (Monsanto 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)
$\log (P_L/mmHg) = 8.80 - 3700/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.0103 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Bidleman & Christinsen 1979 Giam et al. 1980; Westcott et al. 1980)

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0.024 (20°C, extrapolated, Monsanto 1974; quoted, NAS 1979)
0.0101 (quoted, Eisenreich et al. 1981)
0.004 (38°C, Average, Wingender & Williams 1984)
0.00435, 0.00424 (GC-RT correlation, Foreman & Bidleman 1985)
0.043 (selected, Mackay et al. 1986)
0.00263 (quoted, Eisenreich 1987)
6.7×10^{-3} (selected, Mackay 1986; Metcalfe et al. 1988)
0.00294 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

279.7 (calculated, Mackay & Leinonen 1975)
0.0993 (Murphy & Rzeszutko 1977; quoted, Eisenreich et al. 1983)
273 (Slinn et al. 1978)
274 (calculated-P/C, Eisenreich et al. 1981)
0.007 (Eisenreich et al. 1981a)
0.0142 (Doskey & Andren 1981; quoted, Eisenreich et al. 1983)
47.57–74.08 (calculated-P/C, Westcott et al. 1981)
16.60 (radiotracer-equilibration, Atlas et al. 1982; Atlas & Giam 1986)
21.0 (direct concn. ratio-GC/ECD, Murphy et al. 1983)
28.67 (calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)
50.0 (calculated, Mackay et al. 1986)
18.24 (20°C, selected, Murphy et al. 1987 from Burkhard et al. 1985b)
19.25 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
19.25 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 11.880 - 4099/(T/K)$, (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:—See discussion by Linkov et al. 2005.

6.03 (Hansch et al. 1973; Callahan et al. 1979; Mabey et al. 1982)
6.47 (GC-RT correlation, Veith et al. 1979b; Veith & Kosian 1983; quoted, Mackay 1982; Garten & Trabalka 1983; Zaroogian et al. 1985; Södergren 1987; Travis & Arms 1988)
6.72 (HPLC-RT correlation, Veith et al. 1979a)
4.08 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
6.0 (quoted, Mills et al. 1982)
6.79 (literature mean, Di Toro et al. 1985)
6.1–6.8 (selected, Mackay et al. 1983, 1986; Metcalfe et al. 1988)
7.17 (Rapaport & Eisenreich 1984)
6.11 (quoted, Chou & Griffin 1986)
6.50 (quoted, Thomann 1989)

Bioconcentration Factor, log BCF:

4.57 (spot fish, Hansen et al. 1971; quoted, Waid 1986)
4.85 (bluegill sunfish, Stalling & Mayer 1972)
4.75–4.79 (channel catfish, Mayer et al. 1977; quoted, Waid 1986)
5.08, 5.57, 6.08 (Mysis, sculpins, pelagic fish, Veith et al. 1977)
5.00 (fathead minnow, 32-d exposure, Veith et al. 1979b; Veith & Kosian 1983)
5.0–5.22; 4.41; 4.57 (oyster; shrimp, estuarine fish, Hansen et al. 1976; NAS 1979)
0.79, 0.78 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
4.66, 4.08 (fish, flowing water, static water, Kenaga & Goring 1980)
4.66 (quoted, Bysshe 1982)
5.12 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
5.00, 5.15 (fish: quoted, calculated-K_{OW}, Mackay 1982)
4.57 (fish, estuarine, Hansen et al. 1976; NAS 1979)
0.53, 4.70, 0.77, 0.79. 0.18, 0.98, 0.03 (cow, fish, poultry, rodents, sheep, small birds, swine, Garten & Trabalka 1983)

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5.69, 5.63; 6.11, 5.76 (live bacteria, dead bacteria; live algae, dead algae, Weber, Jr. et al. 1983)
5.0 (fathead minnow, quoted, Zaroogian et al. 1985)
4.80, 4.68 (oyster, quoted, Zaroogian et al. 1985)
4.8–5.51 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
5.52 (oyster, Södergren 1987)
–1.28; –1.95; –1.77(beef; milk; vegetable, reported as biotransfer factor log B_b, log B_m, log B_v, Travis & Arms 1988)
4.95, 6.65 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
> 5.0, > 5.98 (fathead minnow, 32-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)

Bioaccumulation Factor, log BAF:

7.21 (field data, lake trout-L/kg(Ip), Thomann 1989)
6.9, 6.51, 6.67, 6.8 (field data, large-mouth bass, L/kg(Ip), Thomann 1989)

Partition Coefficient, log K_P or log K_d

3.21, 3.22, 4.42, 3.56 (clay: Montmorillonite, Kaolinite, natural Blue clay, stripped Blue clay, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
4.38, 3.06, 4.73, 5.18, 4.55, 5.01, 4.50, 4.89, 4.05 (sediments: Saginaw River 1. natural, Saginaw River 1. stripped, Saginaw R. 2. natural, Saginaw River 2. NaOH ext., Saginaw River 2. benzene/MeOH ext., Saginaw River 2. stripped, Saginaw River 2. 12°C, Saginaw River 2. < 75 -m, Saignaw Bay, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
5.06, 4.95, 5.07(suspended solids: Huron River, Saginaw River1, Saginaw River 2, Weber, Jr. et al. 1983)

Sorption Partition Coefficient, log K_{OC}:

6.0 (sediment/pore water 2.0% OC of pond, Halter & Johnson 1977; selected, Di Toro et al. 1985)
5.72 (sediment, calculated-K_{OW}, Mabey et al. 1982)
5.44 (sediment/pore water 0.7–3.8% OC-Lake Michigan, Eadie et al. 1983; selected, Di Toro et al. 1985)
6.17, 6.16, 5.89 (clay: Montmorillonite 0.11% OC, natural Blue clay 1.82% OC, stripped Blue clay 0.47% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
5.84, 5.04, 6.31, 6.68, 6.29, 6.19, 6.34, 7.20 (sediments: Saginaw River 1. natural 3.45% OC, Saginaw River 1. stripped 1.05% OC, Saginaw R. 2. natural 2.61% OC, Saginaw River 2. NaOH ext. 1.98% OC, Saginaw River 2. benzene/MeOH ext. 1.84% OC, Saginaw River 2. stripped 0.67% OC, Saginaw River 2. < 75 μm 3.51% OC, Saignaw Bay 0.07% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
6.10, 5.97, 6.15 (suspended solids: Huron River 9.25% OC, Saginaw River 1. 9.48% OC, Saginaw River 2. 8.30% OC, batch equilibrium, Weber, Jr. et al. 1983)
6.65 (suspended solids/subsurface water, 56% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.88 (sediment/pore water, 0.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
5.61 (sediment/pore water, 1.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
4.82 (sediment/pore water, 3.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
6.62 (calculated, Sklarew & Girvin 1987)
4.81 (soil, calculated-S, Chou & Griffin 1986)
6.02 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization/Evaporation: volatilization rate k ~ 2×10^{-6} g cm^{-2} d^{-1} at 26°C and k = 8.6×10^{-5} g cm^{-2} d^{-1} at 60°C (Haque et al. 1974);
k = 0.10 μg m^{-2} d^{-1} with $t_{½}$ = 28 d (Baker et al. 1985);
k = 2.7×10^{-3} g m^{-2} h^{-1} (Mackay 1986; Metcalfe et al. 1988).
Photolysis:
Hydrolysis: not environmentally significant.

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Oxidation: calculated rate constant for singlet oxygen, $k << 360\ M^{-1}\ h^{-1}$ and, $k << 1\ M^{-1}\ h^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: no reduction of concentration in the spilled transformer fluid contaminant of Aroclor was detected over a two-year period (Moein et al. 1976; quoted, Pal et al. 1980).

15.2% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972);

19% degraded by activated sludge for 48-h exposure (Callahan et al. 1979);

biodegradation with a first-order $k = 0.1\ d^{-1}$ by acclimated activated sludge and $t_{½} = 7.0$ d (Callahan et al. 1979);

aerobic biodegradation $t_{½} = 81.9$ d without the addition of polymer chitin, $t_{½} = 36.4$ d with chitin and $t_{½} = 35.5$ d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to 3×10^{-12} $mL \cdot cell^{-1} \cdot h^{-1}$ for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.023\ d^{-1}$ (0 to 1 d), $k_2 = 0.086\ d^{-1}$ (1 to 2 d), and $k_2 = 0.0899\ d^{-1}$ (2 to 6 d) with a biological $t_{½} = 5.5$ d (mosquito larvae, Gooch & Hamdy 1982; selected, Waid 1986)

$k_2 = 0.131\ d^{-1}$, $0.137\ d^{-1}$ with biological $t_{½} = 4.7$ d (guppies, Gooch & Hamdy 1982; quoted, Waid 1986)

$k_2 = 0.102\ d^{-1}$ (first day), $k_2 = 0.057\ d^{-1}$ (thereafter) with a biological $t_{½} = 6.1$ d (cichlids, Gooch & Hamdy 1982; quoted, Waid 1986)

Half-Lives in the Environment:

Air:

Surface water: volatilization $t_{½} \sim 10$ h from 1 meter depth in 1 m^3 water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

Groundwater:

Sediment:

Soil: volatilization $t_{½} \sim 15$ d from an Ottawa sand (Haque et al. 1974; quoted, Pal et al. 1980);

$t_{½} > 50$ d in soil (Ryan et al. 1988).

Biota: $t_{½} < 12$ d in plant surface (Pal et al. 1980);

$t_{½} = 3.3$ d in guppies, and $t_{½} = 5.1$ d cichlids (Gooch & Hamdy 1982; quoted, Waid 1986).

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7.1.3.7 Aroclor 1260

Common Name: Aroclor 1260
Synonym:
Chemical Name:
CAS Registry No: 11096-82-5
Molecular Formula:
Average Molecular Weight: 372–375.7
Physical State: sticky resin
Distillation Range (°C):
385–420 (NAS 1979; Brinkman & De Kock 1980)
Chlorine Content: 60%
Density (g/cm^3):
1.62 (20°C, Brinkman & De Kock 1980)
1.55–1.56 (90°C, NAS 1979)
1.58 (Callahan et al. 1979; Mills et al. 1982)
1.60 (Mackay 1986; Metcalfe et al. 1988)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
0.025 (Monsanto 1972)
0.025 (20°C, Nisbet & Sarofim 1972)
0.0027 (Mackay & Wolkoff 1973; quoted, Callahan et al. 1979; Geyer et al. 1980; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Richardson et al. 1983; Chou & Griffin 1986)
0.080 (shake flask-nephelometry, Hollifield 1979)
0.003 (quoted, Brinkman & De Kock 1980; Mackay et al. 1983; Eisenreich 1987)
0.0144 (20°C, calculated-mole fraction, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C or indicated and reported temperature dependence equations):
2.67×10^{-5} (38°C, Nisbet & Sarofim 1972)
0.0054 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983)
0.012 (20°C, extrapolated, Monsanto 1972; NAS 1979)
$\log (P_L/mmHg) = 8.50 - 3700/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)
0.0054 (Callahan et al. 1979; Mabey et al. 1982; Richardson et al. 1983)
0.0053 (Pal et al. 1980; Mills et al. 1982)
0.0004 (38°C, average, Wingender & Williams 1984)
0.00183, 0.00162 (GC-RT, Foreman & Bidleman 1985)
0.003 (quoted, Erickson 1986)
0.00064 (Mackay 1986; Metcalfe et al. 1988)
0.000284 (quoted, Eisenreich 1987)
0.000841 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m^3/mol):
722.4 (calculated, Mackay & Leinonen 1975)
718 (Slinn et al. 1978)
719 (quoted, Mills et al. 1982)
88.0 (suggested, Mackay et al. 1983)
72.24 (16°C, calculated-P/C, Richardson et al. 1983)
34.04 (calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)
21.27 (20°C, quoted, Murphy et al. 1987 from Burkhard et al. 1985b)

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17.23 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
17.23 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 11.848 – 4104/(T/K) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

7.14 (Chiou et al. 1977)
6.11 (Chiou et al. 1977; Callahan et al. 1979; quoted, Ryan et al. 1988)
7.15 (Callahan et al. 1979; Mabey et al. 1982)
6.91 (GC-RT correlation, Veith et al. 1979a; Veith & Kosian 1983; quoted, Mackay 1982; Geyer et al. 1987)
4.34 (Pal et al. 1980)
> 6.0 (quoted, Mills et al. 1982)
6.30–7.50 (quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
6.61 (calculated-S, Chou & Griffin 1986)
6.90 (quoted, Thomann 1989)

Bioconcentration Factor, log BCF:

5.43 (fathead minnows, DeFoe et al. 1978; quoted, Waid 1986)
5.29 (fathead minnow, 32-d exposure, Veith et al. 1979a; Veith & Kosian 1983)
0.672 (adipose tissue of male albino rats, Geyer et al. 1980)
5.29, 5.59 (fish: quoted, calculated-K_{OW}, Mackay 1982)
6.11 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
5.0–6.20 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
2.28–2.50 (human fat of lipid basis, calculated-K_{OW}, Geyer et al. 1987)
2.11–2.36 (human fat of wet wt. basis, calculated-K_{OW}, Geyer et al. 1987)
4.38 (*Rhabdosargus holubi*, De Kock & Lord 1988)
4.80, 6.72 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.22, 6.50 (fathead minnow, male, 250-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)
5.43, 6.53 (fathead minnow, female, 250-d uptake, wet wt basis, lipid wt basis, Geyer et al. 2000)
2.24, 2.40 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

6.83 (sediment, calculated-K_{OW}, Mabey et al. 1982)
5.54 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization/Evaporation: estimated evaporation rate from liquid surfaces at 100°C to be 0.009 mg/cm^2·h (Hutzinger et al. 1974);
$t_{½}$ ~ 7.53 h of evaporation from water depth of 1 m (Mackay & Leinonen 1975)
rate of evaporation k = 2.9×10^{-4} g m^{-2}·h^{-1} (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, k << 360 M^{-1}·h^{-1} and k << 1 M^{-1}·h^{-1} for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: no degradation over a 12-week period in natural water samples (Oloffs et al. 1972; quoted, Pal et al. 1980).

Biotransformation: k ~ 3×10^{-9} to 3×10^{-12} mL·$cell^{-1}$·h^{-1}, transformation for bacteria in water (Mabey et al. 1982)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 332 d^{-1}; k_2 = 0.014 d^{-1} (*Rhabdosargus holubi*, De Kock & Lord 1988)
log k_2 = –2.40 d^{-1} (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

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Air:
Surface water: volatilization $t_{½}$ ~ 10 h at 1 m depth of 1 m^3 of water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).
River water: volatilization $t_{½}$ ~ 52 d (Oloffs et al. 1972; selected, Pal et al. 1980).
Sediment:
Soil:
Biota: $t_{½}$ = 50 d in *Rhabdosargus holubi* (De Kock & Lord 1988).

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TABLE 7.2.1
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
0	Biphenyl	92-52-4	154.207	68.93	256.1	0.371	184.6
1	2-	2051-60-7	188.652	34	274	0.816	205.5
2	3-	2051-61-8	188.652	16	284.5	1	205.5
3	4-	2051-62-9	188.652	78.8	292.9	0.297	205.5
4	2,2′-	13029-08-8	223.098	60.5		0.448	226.4
5	2,3-	16605-91-7	223.098	28		0.934	226.4
6	2,3′	25569–80–6	223.098				226.4
7	2,4-	33284-50-3	223.098	24.4		1	226.4
8	2,4′-	34883-43-7	223.098	43		0.666	226.4
9	2,5-	34883-39-1	223.098	22–23		1	226.4
10	2,6-	33146-45-1	223.098	35.5		0.789	226.4
11	3,3′-	2050-67-1	223.098	29	320	0.914	226.4
12	3,4-	2974-92-7	223.098	49	195–200	0.581	226.4
13	3,4′-	2974–90–5	223.098				226.4
14	3,5-	34883-41-5	223.098	31		0.873	226.4
15	4,4′-	2050-68-2	223.098	149.3	317	0.0603	226.4
16	2,2′,3-	38444-78-9	257.543	28		0.934	247.3
17	2,2′,4-	37680–66–3	257.543				247.3
18	2,2′,5-	37680-65-2	257.543	44		0.651	247.3
19	2,2′,6-	38444–73–4	257.543				247.3
20	2,3,3′-	38444-84-7	257.543				247.3
21	2,3,4-	55702-46-0	257.543	102		0.176	247.3
22	2,3,4′-	38444–85–8	257.543	73		0.338	247.3
23	2,3,5-	55720–44–0	257.543	41		0.697	247.3
24	2,3,6-	55702–45–9	257.543	49		0.581	247.3
25	2,3′,4-	55712–37–3	257.543				247.3
26	2,3′,5-	38444–81–4	257.543	40.5		0.705	247.3
27	2,3′,6-	38444–76–7	257.543				247.3
28	2,4,4′-	7012-37-5	257.543	57		0.485	247.3
29	2,4,5-	15862-07-4	257.543	78.5		0.299	247.3

(Continued)

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TABLE 7.2.1 *(Continued)*
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
30	2,4,6-	35693-92-6	257.543	62.5		0.429	247.3
31	2,4′,5-	16606–02–3	257.543	67		0.387	247.3
32	2,4′,6-	38444–77–8	257.543				247.3
33	2,3′,4′-	38444-86-9	257.543	60		0.454	247.3
34	2,3′,5′-	37680–68–5	257.543	58		0.474	247.3
35	3,3′,4-	37680-69-6	257.543	87		0.246	247.3
36	3,3′,5-	38444–87–0	257.543				247.3
37	3,4,4′-	38444-90-5	257.543	87		0.246	247.3
38	3,4,5-	53555–66–1	257.543				247.3
39	3,4′,5-	38444–88–1	257.543	88		0.241	247.3
40	2,2′,3,3′-	38444-93-8	291.988	121		0.114	268.2
41	2,2′,3,4-	52663–59–9	291.988				268.2
42	2,2′,3,4′-	36559–22–5	291.988	69		0.370	268.2
43	2,2′,3,5-	70362–46–8	291.988				268.2
44	2,2′,3,5′-	41464-39-5	291.988	47		0.608	268.2
45	2,2′,3,6-	70362–45–7	291.988				268.2
46	2,2′,3,6′-	41464–47–5	291.988				268.2
47	2,2′,4,4′-	2437-79-8	291.988	83		0.270	268.2
48	2,2′,4,5-	70362–47–9	291.988	65.9		0.397	268.2
49	2,2′,4, 5′-	41464-40-8	291.988	66.5		0.392	268.2
50	2,2′,4,6-	62796-65-8	291.988				268.2
51	2,2′,4,6′-	68194-04-7	291.988	66		0.396	268.2
52	2,2′,5,5′-	35693-99-3	291.988	87		0.246	268.2
53	2,2′,5,6′-	41464-41-9	291.988	104		0.168	268.2
54	2,2′,6,6′-	15968-05-5	291.988	198		0.0201	268.2
55	2,3,3′,4-	74338–24–2	291.988				268.2
56	2,3,3′,4′-	41464–43–1	291.988				268.2
57	2,3,3′,5-	70424–67–8	291.988				268.2
58	2,3,3′,5′-	41464–49–7	291.988				268.2
59	2,3,3′,6-	74472–33–6	291.988				268.2
60	2,3,4,4′-	33025-41-1	291.988	142		0.0711	268.2
61	2,3,4,5-	33284-53-6	291.988	92.2		0.219	268.2
62	2,3,4,6-	54230–23–7	291.988				268.2

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63	2,3,4′,5-	74472–34–7	291.988			268.2
64	2,3,4′,6-	52663–58–8	291.988			268.2
65	2,3,5,6-	33284-54-7	291.988	79	0.295	268.2
66	2,3′,4,4′-	32598-10-0	291.988	124	0.107	268.2
67	2,3′,4,5-	73575–53–8	291.988			268.2
68	2,3′,4,5′-	73575–52–7	291.988			268.2
69	2,3′,4,6-	60233–24–1	291.988			268.2
70	2,3′,4′,5-	32598-11-1	291.988	104	0.168	268.2
71	2,3′,4′,6-	41464–46–4	291.988			268.2
72	2,4′,5,5′-	41464–42–0	291.988			268.2
73	2,3′,5′,6-	74338–23–1	291.988			268.2
74	2,4,4′,5-	32690–93–0	291.988	125	0.104	268.2
75	2,4,4′,6-	32598-12-2	291.988			268.2
76	2,3′,4′,5′-	70362–48–0	291.988			268.2
77	3,3′,4,4′-	32598-13-3	291.988	180	0.0301	268.2
78	3,3′,4,5-	70362–49–1	291.988			268.2
79	3,3′,4,5′-	41464–48–6	291.988			268.2
80	3,3′,5,5′-	33284-52-5	291.988	164	0.0433	268.2
81	3,4,4′,5-	70362–50–4	291.988			268.2
82	2,2′,3,3′,4-	52663–62–4	326.433			289.1
83	2,2′,3,3′,5-	60145-20-2	326.433	65	0.405	289.1
84	2,2′,3,3′,6-	52663–60–2	326.433			289.1
85	2,2′,3,4,4′-	65510–45–4	326.433			289.1
86	2,2′,3,4,5-	55312-69-1	326.433	100	0.184	289.1
87	2,2′,3,4,5′-	38380-02-8	326.433	114	0.134	289.1
88	2,2′,3,4,6-	55215-17-3	326.433	100	0.184	289.1
89	2,2′,3,4,6′-	73575–57–2	326.433			289.1
90	2,2′,3,4′,5-	68194–07–0	326.433			289.1
91	2,2′,3,4′,6-	58194–05–8	326.433			289.1
92	2,2′,3,5,5′-	52663–61–3	326.433			289.1
93	2,2′,3,5,6-	73575–56–1	326.433			289.1
94	2,2′,3,5,6′-	73575–55–0	326.433			289.1
95	2,2′3,5,6-	38379-99-6	326.433	100	0.184	289.1
96	2,2′,3,6,6′-	73575–54–9	326.433			289.1
97	2,2′,3,4′,5′-	41464–51–1	326.433	82	0.276	289.1
98	2,2′,3,4′,6′-	60233–25–2	326.433			289.1
99	2,2′,4,4′,5-	38380-01-7	326.433			289.1

(Continued)

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TABLE 7.2.1 (*Continued*)
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
100	2,2′4,4′,6-	39485-83-1	326.433				289.1
101	2,2′,4,5,5′-	37680-73-2	326.433	78.5		0.299	289.1
102	2,2′,4,5,6′-	68194–06–9	326.433				289.1
103	2,2′,4,5′,6-	60145–21–3	326.433				289.1
104	2,2′,4,6,6′-	56558-16-8	326.433	85		0.258	289.1
105	2,3,3′,4,4′-	32598-14-4	326.433	105		0.164	289.1
106	2,3,3′,4,5-	70424–69–0	326.433				289.1
107	2,3,3′,4′,5-	70424–68–9	326.433				289.1
108	2,3,3′,4,5′-	70362–41–3	326.433				289.1
109	2,3,3′,4,6-	74472–35–8	326.433				289.1
110	2,3,3′,4′,6-	38380-03-9	326.433				289.1
111	2,3,3′,5,5′-	39635–32–0	326.433				289.1
112	2,3,3′,5,6-	74472–36–9	326.433				289.1
113	2,3,3′,5′,6-	68194–10–5	326.433				289.1
114	2,3,4,4′,5-	74472–37–0	326.433	99		0.188	289.1
115	2,3,4,4′,6-	74472–38–1	326.433				289.1
116	2,3,4,5,6-	18259-05-7	326.433	123.5		0.108	289.1
117	2,3,4′,5,6-	68194–11–6	326.433				289.1
118	2,3′,4,4′,5-	31508-00-6	326.433	107		0.157	289.1
119	2,3′,4,4′,6-	56558–17–9	326.433				289.1
120	2,3′,4,5,5′-	68194–12–7	326.433	77		0.309	289.1
121	2,3′,4,5′,6-	56558–18–0	326.433				289.1
122	2,3,3′,4′,5′-	76842–07–4	326.433				289.1
123	2,3′,4,4′,5′-	65510–44–3	326.433				289.1
124	2,3′,4′,5,5′-	70424-70-3	326.433				289.1
125	2,3′,4′,5′,6-	74472–39–2	326.433				289.1
126	3,3′,4,4′,5-	57465–28–8	326.433	106		0.160	289.1
127	3,3′,4,5,5′-	39635–33–1	326.433				289.1
128	2,2′,3,3′,4,4′-	38380-07-3	360.878	151		0.058	310.0
129	2,2′,3,3′4,5-	55215-18-4	360.878	85		0.258	310.0
130	2,2′,3,3′,4,5′-	52663–66–8	360.878				310.0
131	2,2′,3,3′,4,6-	61798–70–7	360.878				310.0
132	2,2′,3,3′,4,6′-	38380–05–1	360.878				310.0

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133	2,2′,3,3′,5,5′-	35694–04–3	360.878	129	0.0954	310.0
134	2,2′,3,3′,5,6-	52704-70-8	360.878	100	0.184	310.0
135	2,2′,3,3′,5,6′-	52744–13–5	360.878			310.0
136	2,2′,3,3′,6,6′-	38411-22-2	360.878	114.2	0.133	310.0
137	2,2′,3,4,4′,5-	35694–06–5	360.878	78	0.302	310.0
138	2,2′,3,4,4′,5′-	35065-28-2	360.878	80	0.289	310.0
139	2,2′,3,4,4′,6-	56030–56–9	360.878			310.0
140	2,2′,3,4,4′,6′-	59291–64–4	360.878			310.0
141	2,2,3,4,5,5′-	52712–04–6	360.878	85	0.258	310.0
142	2,2′,3,4,5,6-	41411–61–4	360.878	136	0.0815	310.0
143	2,2′,3,4,5,6′-	68194–15–0	360.878			310.0
144	2,2′,3,4,5′,6-	68194–14–9	360.878			310.0
145	2,2′,3,4,6,6′-	74472–40–5	360.878			310.0
146	2,2′,3,4′,5,5′-	51908–16–8	360.878			310.0
147	2,2′,3,4′,5,6-	68194–13–8	360.878			310.0
148	2,2′,3,4′,5,6′-	74472–42–7	360.878			310.0
149	2,2′,3,4′,5′,6-	38380-04-0	360.878	oil	1	310.0
150	2,2′,3,4′,6,6′-	68194–08–1	360.878			310.0
151	2,2′,3,5,5′,6-	52663–63–5	360.878	101	0.180	310.0
152	2,2′,3,5,6,6′-	68194–09–2	360.878			310.0
153	2,2′,4,4′,5,5′-	35065-27-1	360.878	103.5	0.170	310.0
154	2,2′,4,4′,5,6′-	60145–22–4	360.878	oil	1	310.0
155	2,2′,4,4′,6,6′-	33979-03-2	360.878	112.5	0.139	310.0
156	2,3,3′,4,4′,5-	38380-08-4	360.878	127	0.100	310.0
157	2,3,3′,4,4′,5′-	69782–90–7	360.878			310.0
158	2,3,3′,4,4′,6	74472–42–7	360.878	107	0.157	310.0
159	2,3,3′,4,5,5′-	39635–35–3	360.878			310.0
160	2,3,3′,4,5,6-	41411–62–5	360.878	99	0.188	310.0
161	2,3,3′,4,5′,6-	74472–43–8	360.878			310.0
162	2,3,3′,4′,5,5′-	39635–34–2	360.878			310.0
163	2,3,3′,4′,5,6-	74472–44–9	360.878			310.0
164	2,3,3′,4′,5′,6-	74472–45–0	360.878			310.0
165	2,3,3′,5,5′,6-	74472–46–1	360.878			310.0
166	2,3,4,4′,5,6-	41411–63–6	360.878	163	0.0433	310.0
167	2,3′,4,4′,5,5′-	52663–72–6	360.878			310.0
168	2,3′,4,4′,5′,6-	59291–65–5	360.878	110–111	0.145	310.0
169	3,3′4,4′,5,5′-	32774-16-6	360.878	202	0.0183	310.0
170	2,2′,3,3′,4,4′,5-	35065-30-6	395.323	135	0.0833	330.9

(Continued)

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TABLE 7.2.1
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V_M (cm^3/mol)
171	2,2′,3,3′,4,4′,6-	52663-71-5	395.323	117.5		0.124	330.9
172	2,2′,3,3′,4,5,5′-	52663–74–8	395.323				330.9
173	2,2′,3,3′,4,5,6-	68194–16–1	395.323				330.9
174	2,2′,3,3′,4,5,6′-	38411–25–5	395.323	130.6		0.0920	330.9
175	2,2′,3,3′,4,5′,6-	40186–70–7	395.323				330.9
176	2,2′,3,3′,4,5,6′-	52663–65–7	395.323				330.9
177	2,2′,3,3′,4′,5,6-	52663–70–4	395.323				330.9
178	2,2′,3,3′,5,5′,6-	52663–67–9	395.323				330.9
179	2,2′,3,3′,5,6,6′-	52663–64–6	395.323				330.9
180	2,2′,3,4,4′,5,5′-	35065-29-3	395.323	110		0.147	330.9
181	2,2′,3,4,4′,5,6-	74472–47–2	395.323				330.9
182	2,2′,3,4,4′,5,6′-	60145–23–5	395.323	152		0.0567	330.9
183	2,2′,3,4,4′,5′,6-	52663–69–1	395.323	83		0.270	330.9
184	2,2′,3,4,4′,6,6′-	74472–48–3	395.323				330.9
185	2,2′,3,4,5,5′,6-	52712-05-7	395.323	149		0.0607	330.9
186	2,2′,3,4,5,6,6′-	74472–49–4	395.323				330.9
187	2,2′,3,4′,5,5′,6-	52663-68-0	395.323	149		0.0607	330.9
188	2,2′,3,4′,5,6,6′-	74487–85–7	395.323				330.9
189	2,3,3′,4,4′,5,5′-	39635–31–9	395.323	170		0.0378	330.9
190	2,3,3′,4,4′,5,6-	41411–64–7	395.323	117		0.125	330.9
191	2,3,3′,4,4′,5′,6-	74472–50–7	395.323				330.9
192	2,3,3′,4,5,5′,6-	74472–51–8	395.323				330.9
193	2,3,3′,4′,5,5′,6-	69782–91–8	395.323				330.9
194	2,2′,3,3′,4,4′,5,5′-	35694-08-7	429.768	159		0.0484	351.8
195	2,2′,3,3′,4,4′,5,6-	52663–78–2	429.768				351.8
196	2,2′,3,3′,4,4′,5,6′-	42740–50–1	429.768				351.8
197	2,2′,3,3′,4,4′,6,6′-	33091–17–7	429.768	132		0.0892	351.8
198	2,2′,3,3′,4,5,5′,6-	68194–17–2	429.768				351.8
199	2,2′,3,3′,4,5,5′,6′-	52663–75–9	429.768				1.759
200	2,2′,3,3′,4,5,6,6'-	52663–73–7	429.768				351.8
201	2,2′,3,3′,4,5′,6,6′-	40186–71–8	429.768				351.8

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202	2,2′,3,3′,5,5′,6,6′-	2136-99-4	429.768	161	0.0463	351.8
203	2,2′,3,4,4′,5,5′,6-	52663–76–0	429.768			351.8
204	2,2′,3,4,4′,5,6,6′-	74472–52–9	429.768			351.8
205	2,3,3′,4,4′,5,5′,6-	74472–53–0	429.768			351.8
206	2,2′,3,3′,4,4′,5,5′,6-	40186-72-9	464.213	206	0.0168	372.7
207	2,2′,3,3′,4,4′,5,6,6′-	52663-79-3	464.213			372.7
208	2,2′,3,3′,4,5,5′,6,6′-	52663-77-1	464.213	180.5	0.0298	372.7
209	2,2′,3,3′,4,4′,5,5′,6,6′-	2051-24-3	498.658	309	0.00164	393.6

* Assuming ΔS_{fus} = 56 J/mol K.

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TABLE 7.2.2
Summary of selected physical-chemical properties of some PCB congeners at 25 °C

IUPAC no.	Congener	Selected properties: Vapor pressure P^S/Pa	Vapor pressure P_L/Pa	Solubility S/(g/m³)	Solubility C^S/(mmol/m³)	Solubility C_L/(mmol/m³)	log K_{OW}	Henry's law const. H/(Pa·m³/mol) calculated P/C
0	Biphenyl	1.3	3.50	7	45.39	122.4	3.9	28.64
1	2-	2.04	2.5	5.5	29.15	35.73	4.3	69.97
2	3-	1	1	2.5	13.25	13.24	4.6	75.46
3	4-	0.271	0.91	1.2	6.36	21.42	4.5	42.60
4	2,2′-	0.265	0.59	1	4.482	10.00	4.9	59.12
7	2,4-	0.254	0.254	1.25	5.603	5.603	5.0	45.33
8	2,4′-			1	4.482	6.730	5.1	
9	2,5-	0.18	0.18	2	8.960	8.960	5.1	20.08
10	2,6-			1.4	6.275	7.840	5.0	
11	3,3′-	0.027	0.030	0.354	1.587	1.736	5.3	17.02
12	3,4-			0.008	0.0358	0.0617		
14	3,5-	0.105	0.120					
15	4,4′-	0.0048	0.080	0.06	0.269	4.460	5.3	17.84
18	2,2′,5-	0.143	0.220	0.4	1.553	2.386	5.6	92.07
26	2,3′,5-			0.251	0.975	1.382		
28	2,4,4′-			0.16	0.621	1.281	5.8	
29	2,4,5-	0.132	0.441	0.14	0.544	1.818	5.6	242.8
30	2,4,6-	0.0384	0.090	0.2	0.777	1.810	5.5	49.45
33	2,3′,4′-	0.0136	0.003	0.08	0.311	0.684	5.8	43.78
37	3,4,4′-			0.015	0.0582	0.237	5.9	
40	2,2′,3,3v-	0.00225	0.0197	0.03	0.103	0.901	5.6	21.90
44	2,2′,3,5′-			0.1	0.342	0.563	6.0	
47	2,2′,4,4′-	0.0054	0.02	0.09	0.308	1.142	5.9	17.52
49	2,2′,4,5′-			0.016	0.0548	0.149	6.1	
52	2,2′,5,5′-	0.0049	0.02	0.03	0.103	0.418	6.1	47.69
53	2,2′,5,6′-						5.5	
54	2,2′,6,6′-						5.48	
60	2,3,4,4′-						6.31	
61	2,3,4,5-			0.02	0.0685	0.313	5.9	
65	2,3,5,6-						5.94	
66	2,3′,4,4′-			0.04	0.137	1.280	5.8	

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75	2,4,4′,6-			0.091	0.312		6.21	
77	3,3′,4,4′-	5.88×10^{-5}	0.002	0.001	0.00342	0.114	6.5	17.16
80	3,3′,5,5′-			0.0012	0.0041	0.0949		
86	2,2′,3,4,5-	0.00927	0.0504	0.02	0.0613	0.333	6.2	151.3
87	2,2′,3,4,5′-	0.000304	0.00227	0.004	0.0123	0.0914	6.5	24.81
88	2,2′,3,4,6-			0.012	0.0368	0.200	6.5	
101	2,2′,4,5,5′-	0.00109	0.00364	0.01	0.0306	0.102	6.4	35.58
104	2,2′,4,6,6′-		0.00434	0.0156	0.0478	0.185		23.43
105	2,3,3′,4,4′-						6.0	
110	2,3,3′,4′,6-			0.004	0.0123		6.3	
116	2,3,4,5,6-			0.008	0.0245	0.227	6.3	
128	2,2′,3,3′,4,4′-	1.98×10^{-5}	0.00034	0.0006	0.00166	0.0286	7.0	11.91
129	2,2′,3,3′4,5-			0.0006	0.00166	0.0064	7.3	
134	2,2′,3,3′,5,6-			0.0004	0.00111	0.0060	7.3	
136	2,2′,3,3′,6,6′-			0.0008	0.00222	0.0167	6.7	
153	2,2′,4,4′,5,5′-	0.000119	0.0007	0.001	0.00277	0.0163	6.9	42.94
155	2,2′,4,4′,6,6′-	0.00048	0.00345	0.002	0.00554	0.0399	7.0	86.62
171	2,2′,3,3′,4,4′,6-	2.73×10^{-5}	0.00022	0.002	0.00506	0.0408	6.7	5.396
185	2,2′,3,4,5,5′,6-			0.00045	0.00114	0.0188	7.0	
194	2,2′,3,3′,4,4′,5,5′-			0.0002	0.00047	0.00962	7.4	
202	2,2′,3,3′,5,5′,6,6′-	2.66×10^{-5}	0.0006	0.0003	0.0007	0.0158	7.1	38.11
206	2,2′,3,3′,4,4′,5,5′,6-	1.96×10^{-7}	1.17×10^{-5}	0.00011	0.000237	0.0141	7.2	0.8271
207	2,2′,3,3′,4,4′,5,6,6′-						7.52	
208	2,2′,3,3′,4,5,5′,6,6′-			1.8×10^{-5}	3.88×10^{-5}	0.00130	8.16	
209	2,2′,3,3′,4,4′,5,5′,6,6′-	5.02×10^{-8}	3.06×10^{-5}	1.0×10^{-6}	2.00×10^{-6}	0.0122	8.26	25.03

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TABLE 7.2.3
Summary of physical properties of PCB isomer groups and Aroclor mixtures

PCB isomer group	CAS no.	Molecular weight, MW g/mol	Cl no.	m.p. °C	Fugacity ratio, F range at 25°C	Le Bas molar volume, V_M (cm^3/mol)
Biphenyl	92-52-4	154.2	0	71	0.352	184.6
Monochloro-	27323-18-8	188.7	1	25.1–78	0.299–1.0	205.5
Dichloro-	25512-42-9	223.1	2	24.4–149	0.0594–1.0	226.4
Trichloro-	25323-68-6	257.5	3	28.1–102	0.173–0.932	247.3
Tetrachloro-	26914-33-0	292.0	4	47–164	0.042–0.606	268.2
Pentachloro-	25429-29-2	326.4	5	76.5–123	0.107–0.310	289.1
Hexachloro-	26601-64-9	360.9	6	70–201	0.0182–0.359	310
Heptachloro-	28655-71-2	395.3	7	109–162	0.0596–0.148	330.9
Octachloro-	31472-83-0	429.8	8	132–161	0.0452–0.0874474	351.8
Nonachloro-	53742-07-7	464.2	9	205–206	0.0163–0.0276	372.7
Decachloro-	2051-24-3	498.7	10	305	0.00167	393.6

Aroclor mixture	CAS no.	Molecular weight, MW g/mol	% Cl	No. of Cl/molecule	Fugacity ratio, F at 25°C	Density g/cm^3 at 25°C	Distillation range °C
Aroclor 1016	12674-11-2	257	41	3	1.0	1.33	323–356
Aroclor 1221	111-042-82	192	20.5–21.5	1.15	1.0	1.15	275–320
Aroclor 1232	111-411-65	221	31.4–32.5	2.04	1.0	1.24	290–325
Aroclor 1242	534-692-19	261	42	3.1	1.0	1.35	325–366
Aroclor 1248	126-722-96	288	48	3.9	1.0	1.41	340–375
Aroclor 1254	110-976-91	327	54	4.96	1.0	1.5	365–390
Aroclor 1260	110-968-25	372	60	6.3	1.0	1.58	385–420

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TABLE 7.2.4
Summary of selected physical-chemical properties of PCB isomer groups and Aroclor mixtures at 20–25°C

PCB isomer group	Aqueous solubility range			Vapor pressure range		Henry's law const. H/(Pa·m³/mol) calculated P/C	log K_{OW} range
	S/(g/m³)	C_S/(mmol/m³)	C_L/(mmol/m³)	P_S/Pa	P_L/Pa		
Biphenyl	7.0	45.39	129.7	1.30	3.69	28.64	3.90
Monochloro-	1.21–5.50	6.36-29.15	1 13.24-35.66	0.271-2.04	0.9-2.5	42.56-75.55	4.3-4.60
Dichloro-	0.060–2.0	0.269-8.96	4.56-10.14	0.0048-0.279	0.008-0.60	17.0-92.21	4.9-5.30
Trichloro-	0.015–0.40	0.0582-1.55	0.24-2.39	0.0136-0.143	0.003-0.22	24.29-92.21	5.5-5.90
Tetrachloro-	0.0043–0.010	0.0147-0.342	0.133-1.30	0.000059-.0054	0.002	1.72-47.59	5.6-6.50
Pentachloro-	0.004–0.020	0.0123-0.0613	0.093-0.337	0.000304-0.0093	0.0023-0.051	24.8-151.4	6.2-6.50
Hexachloro-	0.0004–0.0007	0.0011-0.002	0.0061-0.0286	0.000020-0.00159	0.0007- 0.012	11.9-818	6.7-7.30
Heptachloro-	0.000045–0.0002	0.00114-0.0051	0.0191-0.046	0.0000273	0.00025	5.40	6.7-7.0
Octachloro-	0.0002–0.0003	0.00047-0.0007	0.0098-0.0158	0.0000266	0.0006	38.08	7.10
Nonachloro-	0.00018–0.0012	0.000038-0.00024	0.00141-0.0146	-	-	-	7.2-8.16
Decachloro-	0.000761	0.0000024	0.0144	0.00000005	0.00003	20.84	8.26

Aroclor mixture	Aqueous solubility range		Vapor pressure range	Henry's law const. H/(Pa·m³/mol) calculated P/C	log K_{OW} range
	S/(g/m³)	C_L/(mmol/m³)	P_L/Pa		
Aroclor 1016	0.22-0.84	0.856-0.216	0.06-0.2	70-900	4.4-5.8
Aroclor 1221	0.59-5.0	0.307-26.0	0.89-2.0	34-450	4.1-4.7
Aroclor 1232	1.45	6.56-2.0	0.54	82-270	4.5-5.2
Aroclor 1242	0.1-0.75	0.383-2.87	0.05-0.13	45-130	4.5-5.8
Aroclor 1248	0.1-0.5	0.347-1.74	0.0085-0.11	5-300	5.8-6.3
Aroclor 1254	0.01-0.30	0.306-0.92	0.008-0.02	20-260	6.1-6.8*
Aroclor 1260	0.003-0.08	0.00806-0.215	0.0002-0.012	20-60	6.3-6.8*

* See discussion by Linkov et al. 2005.

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TABLE 7.2.5
Suggested half-life classes of polychlorinated biphenyls (PCBs) in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Biphenyl	3	4	5	6
Monochloro-	4	7	8	8
Dichloro-	4	7	8	8
Trichloro-	5	8	9	9
Tetrachloro-	6	9	9	9
Pentachloro-	6	9	9	9
Hexachloro-	7	9	9	9
Heptachloro-	7	9	9	9
Octachloro-	8	9	9	9
Nonachloro-	8	9	9	9
Decachloro-	9	9	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

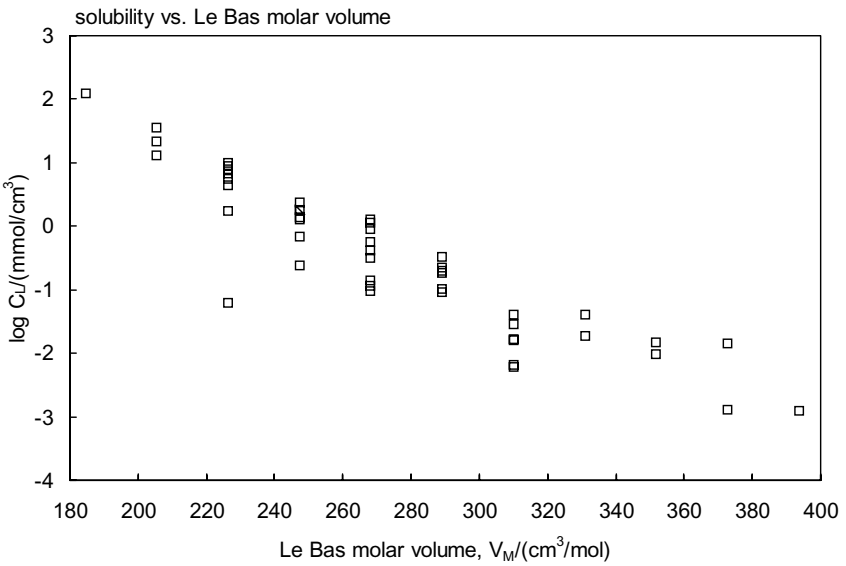

FIGURE 7.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.

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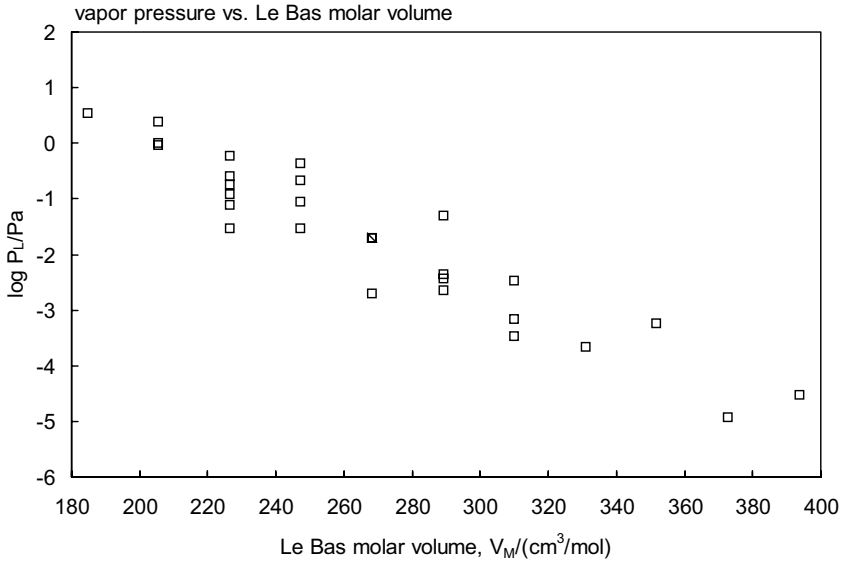

FIGURE 7.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.

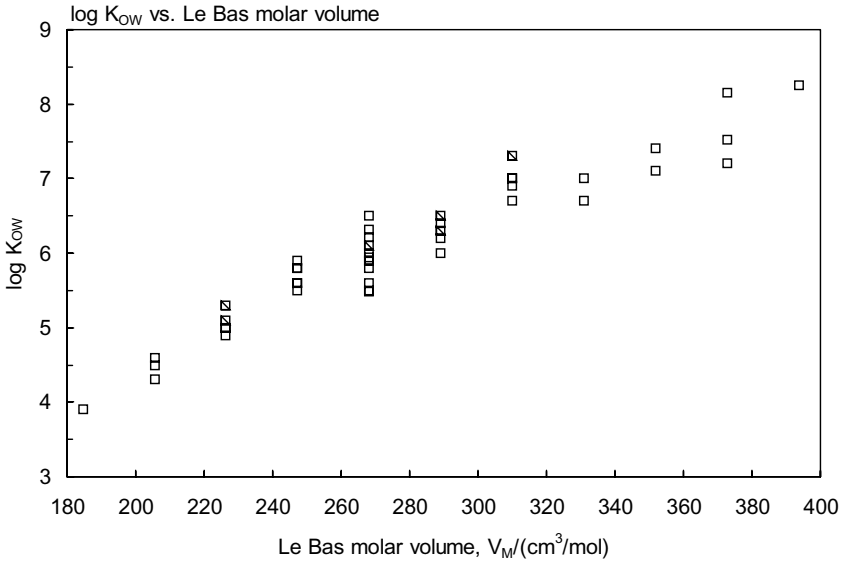

FIGURE 7.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated biphenyls.

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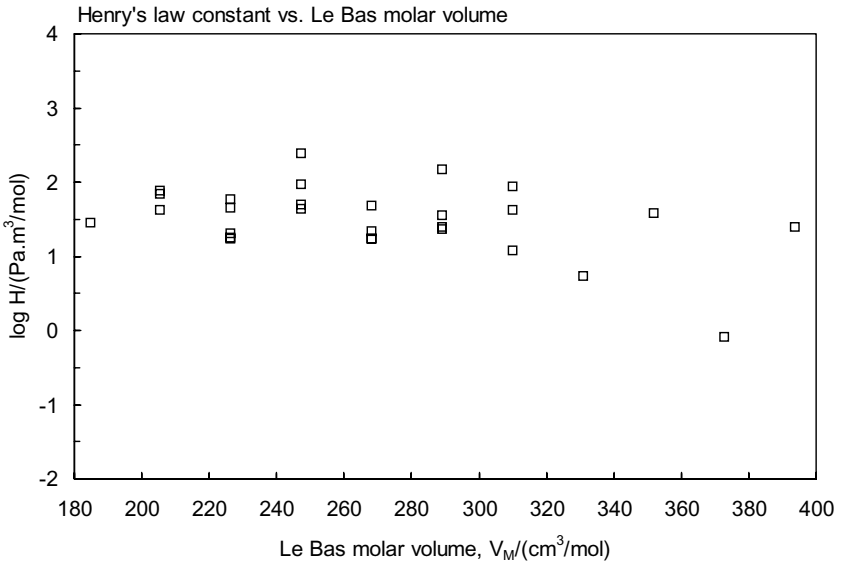

FIGURE 7.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated biphenyls.

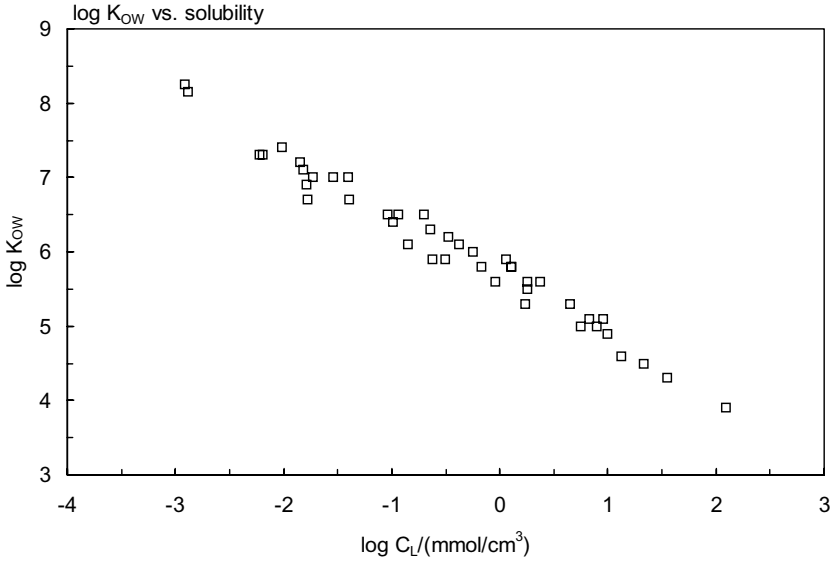

FIGURE 7.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated biphenyls.

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