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# 6 Chlorobenzenes and Other Halogenated Mononuclear Aromatics

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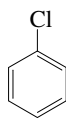
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## 6.1 LIST OF CHEMICALS AND DATA COMPILATIONS

### 6.1.1 CHLOROBENZENES

#### 6.1.1.1 Chlorobenzene



Common Name: Chlorobenzene

Synonym: monochlorobenzene, benzene chloride, phenyl chloride

Chemical Name: chlorobenzene

CAS Registry No: 108-90-7

Molecular Formula:  $C_6H_5Cl$

Molecular Weight: 112.557

Melting Point ( $^{\circ}C$ ):

−45.31 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

131.72 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.1058 (Weast 1972–73; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

101.8 ( $20^{\circ}C$ , calculated-density)

116.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

9.49 (Dean 1985)

11.88 (Riddick et al. 1986)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

488 ( $30^{\circ}C$ , shake flask-interferometer, Gross & Saylor 1931)

551 (Landolt-Börnstein 1951)

488 (Seidell 1941)

< 200 (residue-volume method, Booth & Everson 1948)

500 (shake flask-UV, Andrews & Keefer 1950)

490\* ( $30^{\circ}C$ , shake flask, Kisarov 1962)

546, 523; 534 ( $21^{\circ}C$ , generator column-GC; mean value, Chey & Calder 1972)

463 (shake flask-UV, Vesala 1974)

100 (Stephen & Stephen 1963)

106.8\* (shake flask-GC, measured range  $5-45^{\circ}C$ , Nelson & Smit 1978)

472 (shake flask-GC, Aquan-Yuen et al. 1979)

472 (shake flask-GC, Mackay et al. 1979, 1980, 1982b)

503 (shake flask-UV, Yalkowsky et al. 1979)

420, 450\* ( $20^{\circ}C$ ; elution chromatography, UV adsorption, measured range  $10-30^{\circ}C$ , Schwarz & Miller 1980)

295 (generator column-HPLC/UV, Tewari et al. 1982)

498 (recommended, Horvath 1982)

499 (generator column-HPLC/UV, Wasik et al. 1983)

508 (HPLC- $k'$  correlation, converted from reported  $\gamma_w$ , Hafkenscheid & Tomlinson 1983a)

295 (generator column-GC, Miller et al. 1984, 1985)

495\* (recommended, temp range  $10-70^{\circ}C$ , IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(\text{g/kg}) = 11.3351 - 3.0290 \times 10^{-2} \cdot (T/K) - 1.8716 \times 10^{-4} \cdot (T/K)^2 + 0.559466 \times 10^{-6} \cdot (T/K)^3$ ; temp range 283–363 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

490 (30°C, quoted, Dean 1985)

502 (shake flask-HPLC/UV, Banerjee 1984)

348 (shake flask-radiometric method, Lo et al. 1986)

428 (vapor phase saturation-GC, temp range 15–45°C, Sanemasa et al. 1987)

482\* (20°C vapor-liquid equilibrium-activity coefficient, measured range 20–50°C, Cooling et al. 1992)

477 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

333 (shake flask-GC, Boyd et al. 1998)

496 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)

$\ln x = -41.9062 + 6054.03/(T/K) + 1.3692 \times 10^{-4} \cdot (T/K)^2$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

470\* (shake flask-GC, measured range 5–45°C, Ma et al. 2001)

426, 427, 511 (5, 15, 35°C, estimated-RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

1333\* (22.2°C, summary of literature data, temp range –13.0 to 132.2°C, Stull 1947)

$\log (P/\text{mmHg}) = 7.18473 - 1556.6/(230 + t/^\circ\text{C})$  (Antoine eq., Dreisbach & Martin 1949)

$\log (P/\text{mmHg}) = 6.94504 - 1413.12/(216.0 + t/^\circ\text{C})$ ; temp range 40–200°C (Antoine eq. for liquid state, Dreisbach 1955)

7605\* (56.28°C, ebulliometry, measured range 56.28–131.70°C, Dreisbach & Shrader 1949)

9657\* (62.04°C, ebulliometry, measured range 62.04–131.7°C, Brown 1952)

1580 (interpolated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 10098.0/(T/K)] + 8.5000$ ; temp range –35 to –15°C (Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 9067.3/(T/K)] + 7.717535$ ; temp range –13 to 249.8°C (Antoine eq., Weast 1972–73)

1596, 1610 (extrapolated-Antoine eq., Boublik et al. 1973; 1984)

$\log (P/\text{kPa}) = 6.10416 - 1431.813/(217.655 + t/^\circ\text{C})$ ; temp range 62.04–131.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.07963 - 1419.045/(216.633 + t/^\circ\text{C})$ ; temp range 56.2–131.7°C (Antoine eq. from reported exptl. data of Derisbach & Shrader 1949, Boublik et al. 1984)

1586 (Daubert & Danner 1985)

1596 (extrapolated, Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 6.97808 - 1431.05/(217.65 + t/^\circ\text{C})$ ; temp range 62–131.7°C (Antoine eq., Dean 1985, 1992)

1600 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.11512 - 1438.86/(-54.72 + T/K)$ ; temp range 333–405 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.62988 - 1897.41/(5.21 + T/K)$ ; temp range 405–597 K (Antoine eq.-II, Stephenson & Malanowski 1987)

1410\* (gas saturation-GC, measured range –14.2 to 40°C, Liu & Dickhut 1994)

1828; 1560 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; quoted lit., Spiessma et al. 1994)

$\log (P/\text{mmHg}) = 19.4343 - 2.5801 \times 10^3/(T/K) - 3.9391 \cdot \log (T/K) - 4.4005 \times 10^{-11} \cdot (T/K) + 4.9583 \times 10^{-7} \cdot (T/K)^2$ ; temp range 228–632 K (Yaws 1994)

$\log P/\text{kPa} = 6.11512 - 1438.86/(T/K - 54.72)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m<sup>3</sup>/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):

451 (calculated as  $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

441 (calculated-bond contribution, Hine & Mookerjee 1975)

382 (batch stripping-GC, Mackay et al. 1979)

379 (calculated  $P/C$ , Mackay et al. 1979)

330\* (equilibrium cell-concentration ratio, measured range 1.0–23.0°C, Leighton & Calo 1981)

$\ln (k_H/\text{atm}) = 16.83 - 3466/(T/K)$ ; temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

314 (batch air stripping-GC, Mackay & Shiu 1981)

- 398 (gas stripping-GC, Warner et al. 1987)  
 319 (20°C, EPICS-GC, Yurteri et al. 1987)  
 273 (20°C, calculated-P/C, Yurteri et al. 1987)  
 365\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 3.469 - 2689/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 460 (computer value, Yaws et al. 1991)  
 324\* (extrapolated from equilibrium headspace-GC data, measured range 45–80°C, Ettre et al. 1993)  
 $\log (1/K_{\text{AW}}) = -2.9050240 + 1129.8083/(T/K)$ ; temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)  
 288 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 315 (gas stripping-GC, Shiu & Mackay 1997)  
 293 (headspace equilibrium-GC, de Wolf & Lieder 1998)  
 277.2 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 537 (modified EPICS method-GC, Ryu & Park 1999)  
 297 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 4.225 - 1507/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)  
 384\* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)  
 $\ln K_{\text{AW}} = 10.04 - 3359.7/(T/K)$ ; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient,  $\log K_{\text{OW}}$  at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section:

- 2.84 (Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1985)  
 2.81 (calculated-fragment constant, Rekker 1977)  
 2.18 ( $^{14}\text{C}$ -LSC, Lu & Metcalf 1975)  
 2.84, 2.46, 2.18 (Hansch & Leo 1979)  
 2.79 (HPLC-RT correlation, Veith et al. 1979b)  
 2.84 (HPLC- $k'$  correlation, Könemann et al. 1979)  
 2.80 (HPLC- $k'$  correlation, Hanai et al. 1981)  
 2.81 (HPLC- $k'$  correlation, D'Amboise & Hanai 1982)  
 2.83 (shake flask-HPLC, Hammers et al. 1982)  
 2.18 (HPLC- $k'$  correlation, Miyake & Terada 1982)  
 2.80 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983a)  
 2.98 (generator column-HPLC/UV, Wasik et al. 1983)  
 2.98 (generator column-GC/ECD, Miller et al. 1984; 1985)  
 2.81–2.84 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)  
 2.49 (HPLC- $k'$  correlation, Haky & Young 1984)  
 3.00 (HPLC- $k'$  correlation, De Kock & Lord 1987)  
 2.898 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)  
 $2.784 \pm 0.061$ ,  $2.898 \pm 0.004$  (shake flask methods, interlaboratory studies, Brooks et al. 1990)  
 2.65, 2.73; 2.84 (25°C, 60°C, shake flask-UV/VIS; quoted lit. at 25°C, Kramer & Henze 1990)  
 2.86, 3.02 (centrifugal partition chromatography, Gluck & Martin 1990)  
 2.84 (recommended, Sangster 1993)  
 2.89 (recommended, Hansch et al. 1995)  
 2.98 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)  
 2.96 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)  
 3.05\* (estimated-RP-HPLC- $k'$  correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

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

- 3.45\* (20°C, HPLC- $k'$  correlation, measured range 10–50°C, Su et al. 2002)  
 $\log K_{\text{OA}} = 43910/(2.303\cdot\text{RT}) - 4.107$ ; temp range 10–50°C (HPLC- $k'$  correlation, Su et al. 2002)

Bioconcentration Factor,  $\log \text{BCF}$ :

- 2.65 (fathead minnow, Veith et al. 1979b, 1980)  
 1.30 (Kenaga 1980a)

- 1.08 (fish, flowing water, Kenaga & Goring 1980)
- 2.21 (microorganisms-water, Mabey et al. 1982)
- 1.70 (algae, Freitag et al. 1984, 1985; Halfon & Reggiani 1986)
- 1.88 (fish, Freitag et al. 1984; Halfon & Reggiani 1986)
- 3.23 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
- 1.85 (fish, Freitag et al. 1985)
- 3.23 (activated sludge, Freitag et al. 1985)
- 1.93 (fish, calculated, Figueroa & Simmons 1991)

Sorption Partition Coefficient, log  $K_{OC}$ :

- 2.52 (sediment, Mabey et al. 1982)
- 2.18 (Kenaga 1980a)
- 2.59 (field data, Roberts et al. 1980; Schwarzenbach & Westall 1981; quoted, Voice & Weber 1985)
- 1.84 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 1.73–2.99 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 2.44, 2.50 (calculated from  $K_{OW}$ , Schwarzenbach & Westall 1981)
- 2.73 (soil, calculated- $K_{OW}$ , Calamari et al. 1983)
- 2.10 (calculated-MCI  $\chi$ , Koch 1983)
- 2.92 (calculated- $K_{OW}$ , Yoshida et al. 1983b)
- 2.60 (Offshore Grand Haven sediment, batch equilibrium-sorption isotherm, Voice & Weber, Jr. 1985)
- 2.44 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 1.92–2.59 (soil, Howard 1989)
- 2.50; 2.17 (Captina silt loam, OC 1.49%, pH 4.17; McLaurin sandy loam, OC 0.66%, pH 4.42, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 2.34 (calculated-MCI  $\chi$ , Sabljic et al. 1995)
- 2.19, 2.20 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 1.97, 2.14, 1.77 (soils: organic carbon OC  $\geq 0.1\%$ , OC  $\geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)

Sorption Partition Coefficient, log  $K_{OM}$ :

- 1.68 (Woodburn soil, organic matter 1.9%, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)
- 2.10, 2.32 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

- Volatilization: estimated  $t_{1/2} \sim 1$ –12 h from a flowing stream (Cadena, 1984; selected, Howard 1989);  
 $k = 0.033 \text{ d}^{-1}$  with  $t_{1/2} = 21 \text{ d}$  in spring at 8–16°C,  $k = 0.152 \text{ d}^{-1}$  with  $t_{1/2} = 4.6 \text{ d}$  in summer at 20–22°C,  
 $k = 0.053 \text{ d}^{-1}$  with  $t_{1/2} = 13 \text{ d}$  in winter at 3–7°C for periods when volatilization appears to dominate, and  
 $k = 0.08 \text{ d}^{-1}$  with  $t_{1/2} = 8.9 \text{ d}$  with  $\text{HgCl}_2$  in September 9–15, 1980 in marine mesocosm experiments;  
estimated half-lives from soil:  $t_{1/2} = 0.3 \text{ d}$  of 1-cm depth and  $t_{1/2} = 12.6 \text{ d}$  for 10 cm depth (Wakeham et al. 1983).
- Photolysis: not environmentally significant or relevant (Mabey et al. 1982);  
photolysis  $k = 1.1 \times 10^{-5} \text{ d}^{-1}$  with an estimated  $t_{1/2} \sim 170 \text{ yr}$  by sunlight in surface water at 40°N in the summer (Dulin et al. 1986)  
 $t_{1/2} = 21 \text{ d}$  under sunlight in water (Mansour & Feicht 1994).
- Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with  $\text{NO}_3$  radical and  $k_{O_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures and/or the Arrhenius expression see reference:  
photooxidation  $t_{1/2} = 1553$ –62106 h in water, based on a measured rate for hydroxy radicals in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)  
 $k_{OH} = 9.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 13 d, loss of 7.4% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)  
 $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$  for  $\text{RO}_2$  radical (Mabey et al. 1982)  
 $k = (0.75 \pm 0.2)3 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k = 2.88 \times 10^{-3} \text{ h}^{-1}$  in air (Yoshida et al. 1983b; selected, Mackay et al. 1985)

$k_{\text{OH}} = (8.8 \pm 1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with estimated atmospheric lifetime  $\tau = 13 \text{ d}$  and  $k_{\text{O}_3} < 5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with lifetime  $\tau > 8.8 \text{ yr}$  at room temp. (relative rate method, Atkinson et al. 1985)

$k_{\text{OH}} (\text{obs.}) = 9.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ; and  $k_{\text{OH}} (\text{calc}) = 1.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{\text{OH}} = (5.5 \pm 4.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $23.5^\circ\text{C}$  with an atmospheric lifetime  $\tau = 21 \text{ d}$  (relative rate method, Edney et al. 1986)

$k_{\text{OH}} = 9.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 17 \text{ d}$  for reaction with OH radical, concn of  $5.0 \times 10^5 \text{ molecule/cm}^3$  at room temp. (Atkinson 1987)

$k_{\text{OH}} (\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}} (\text{obs}) = 0.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = (7.41 \pm 0.94) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \text{ K}$ , measured range  $234\text{--}438 \text{ K}$  (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{OH}} = 7.41 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k(\text{soln}) = 9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k = (4.3\text{--}4.6) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{\text{OH}} = 7.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \text{ K}$  (recommended, Atkinson 1989)

$k_{\text{OH}} (\text{calc}) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  with  $t_{1/2} > 900 \text{ yr}$ , based on assumed base mediated 1% disappearance after 16 d at  $85^\circ\text{C}$  and pH 9.7 (Ellington et al. 1988).

$t_{1/2} > 879 \text{ yr}$  based on rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  extrapolated to pH 7 at  $25^\circ\text{C}$  from 1% disappearance after 16 d at  $85^\circ\text{C}$  and pH 9.7 (Ellington et al. 1988)

Biodegradation: significant degradation on anaerobic environment with  $k = 0.5 \text{ d}^{-1}$  (Tabak et al. 1981; Mills et al. 1982)

$k = 1.88 \times 10^{-4} \text{ h}^{-1}$  in air, and  $k = 3.83 \times 10^{-4} \text{ h}^{-1}$  in sediments (Lee & Ryan 1979; selected, Mackay et al. 1985)

$k = 0.24 \text{ L d}^{-1}$  in air, no degradation in water and on the ground (Neely 1982);

$k = 0.07\text{--}0.3 \text{ d}^{-1}$  in river water;  $k = 0.04\text{--}0.2 \text{ d}^{-1}$  in estuary water; and  $k = 0.01 \text{ d}^{-1}$  in marine water (Bartholomew & Pfaender 1983; selected, Battersby 1990)

$k = 0.033 \text{ d}^{-1}$ ,  $t_{1/2} = 21 \text{ d}$  in spring at  $8\text{--}16^\circ\text{C}$ ,  $k = 0.152 \text{ d}^{-1}$ ,  $t_{1/2} = 4.6 \text{ d}$  in summer at  $20\text{--}22^\circ\text{C}$ ,  $k = 0.053 \text{ d}^{-1}$ ,  $t_{1/2} = 13 \text{ d}$  in winter at  $3\text{--}7^\circ\text{C}$ , and  $k = 0.08 \text{ d}^{-1}$ ,  $t_{1/2} = 8.9 \text{ d}$  with  $\text{HgCl}_2$  in September 9–15, 1980 in marine mesocosm system (Wakeham et al. 1983)

$t_{1/2} = 4.6\text{--}21 \text{ d}$  in marine mesocosm (Wakeham et al. 1983);

$t_{1/2} = 7.9 \text{ d}$  in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991);

$k = 0.07 \text{ yr}^{-1}$  with  $t_{1/2} = 37 \text{ d}$  (Olsen & Davis 1990)

$t_{1/2} (\text{aq. aerobic}) = 1632\text{--}3600 \text{ h}$ , based on unacclimated aerobic river dieaway tests;  $t_{1/2} (\text{aq. anaerobic}) = 6528\text{--}14400 \text{ h}$ , based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:  $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$  (estimated, Mabey et al. 1982).

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

#### Half-Lives in the Environment:

Air: photodecomposition  $t_{1/2} = 8.7 \text{ h}$  under simulated atmospheric conditions, with NO (Dilling et al. 1976); residence time of 13 d, loss of 7.4% in one day or 12 sunlit hours at  $300 \text{ K}$  in urban environments (Singh et al. 1981)

estimated atmospheric lifetime  $\tau = 13 \text{ d}$  due to reaction with OH radical and  $\tau > 8.8 \text{ yr}$  due to reaction with  $\text{O}_3$  (Atkinson et al. 1985);

$t_{1/2} = 72.9\text{--}729 \text{ h}$ , based on photooxidation half-life in air (Howard et al. 1991).

Surface Water:  $t_{1/2} = 0.3 \text{ d}$  in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 75 \text{ d}$  for an estuarine river with near natural conditions at  $22^\circ\text{C}$  (Lee & Ryan 1976);

rate constants:  $k = 0.033 \text{ d}^{-1}$ ,  $t_{1/2} = 21 \text{ d}$  in spring at  $8\text{--}16^\circ\text{C}$ ,  $k = 0.152 \text{ d}^{-1}$ ,  $t_{1/2} = 4.6 \text{ d}$  in summer at  $20\text{--}22^\circ\text{C}$ ,  $k = 0.053 \text{ d}^{-1}$ ,  $t_{1/2} = 13 \text{ d}$  in winter at  $3\text{--}7^\circ\text{C}$  for periods when volatilization appears to dominate, and  $k = 0.08 \text{ d}^{-1}$ ,  $t_{1/2} = 8.9 \text{ d}$  with  $\text{HgCl}_2$  in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983)

$t_{1/2} = 1632\text{--}3600$  h, based on unacclimated aerobic river dieaway tests (Howard et al. 1991)

photolysis  $t_{1/2} = 21$  d under sunlight in water (Mansour & Feicht 1994).

Groundwater:  $t_{1/2} = 3264\text{--}7200$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:  $t_{1/2} = 75$  d (Lee & Ryan 1976, 1979; quoted, Anderson et al. 1991).

Soil: disappearance  $t_{1/2} = 2.1$  d from testing soils (Anderson et al. 1991);

$t_{1/2} = 1632\text{--}3600$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

**TABLE 6.1.1.1.1**

**Reported aqueous solubilities of chlorobenzene at various temperatures**

1.

Kisarov 1962		Nelson & Smit 1978		Schwarz & Miller 1980		Horvath & Getzen 1985	
shake flask		vapor equil.-UV spec.		elution chromatography		recommended values	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
30	490	5	40	10	440	10	454
40	705	25	106.8	20	420	15	452
50	960	35	400.5	30	490	20	466
60	1100	45	471.3	shake flask UV		25	495
70	1605			10	460	30	539
80	1805			20	450	35	600
90	2500			30	500	40	677
						45	771
						50	882
						55	1011
						60	1158
						65	1324
						70	1509
						75	1713
						80	1937
						90	2447

2.

Cooling et al. 1992		Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC/MS		shake flask-GC		RP-HPLC- $k'$ correlation	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	482	5	496	5	426
30	608	15	429	15	427
40	840	25	470	35	511
50	1263	35	538		
		45	546		



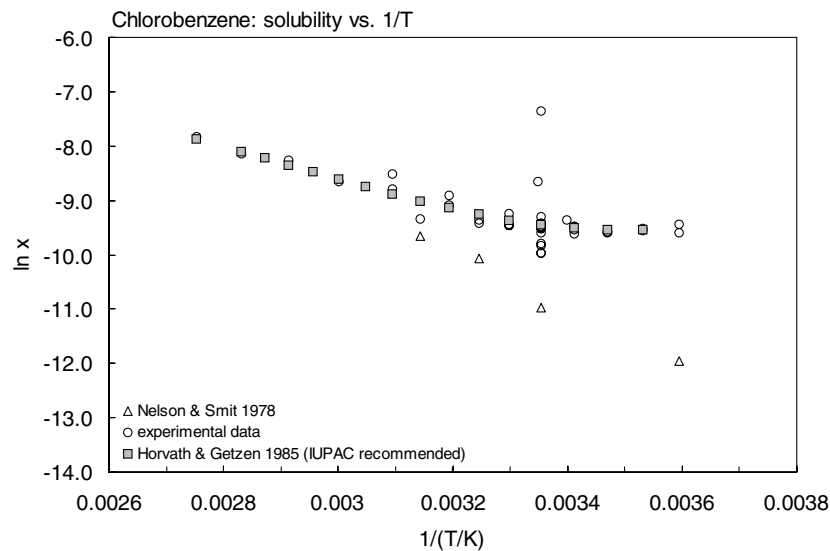


FIGURE 6.1.1.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.2  
Reported vapor pressures of chlorobenzene 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)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Dreisbach & Shrader 1949		Brown 1952		Liu & Dickhut 1994	
summary of lit. data		ebulliometry		ebulliometry		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−13.0	133.3	56.28	7605	62.04	9657	−14.2	66.9
10.6	666.6	63.05	10114	62.06	9663	−5.0	167
22.2	1333	75.22	16500	66.38	11558	10	501
35.3	2666	101.85	42066	74.13	15720	25	1410
49.7	5333	117.30	67661	89.06	27246	40	3270
58.3	7999	131.70	101325	94.04	32276		
70.0	13332			98.79	37961		
89.4	26664			110.35	54794	$\Delta H_v = 35.6 \text{ kJ/mol}$	
110	53329	mp/°C	−45.58	121.1	69774		
132.2	101325	bp/°C	131.67	126.18	87018	$\Delta H_{\text{subl}} = 35.6 \text{ kJ/mol}$	
				130.37	97684		
mp/°C	−45.2	eq. 2	P/mmHg	131.7	101263		
		A	7.18473				
		B	1556.6	eq. 2	P/mmHg		
		C	230	A	6.99893		
				B	1444.75		
				C	219.13		

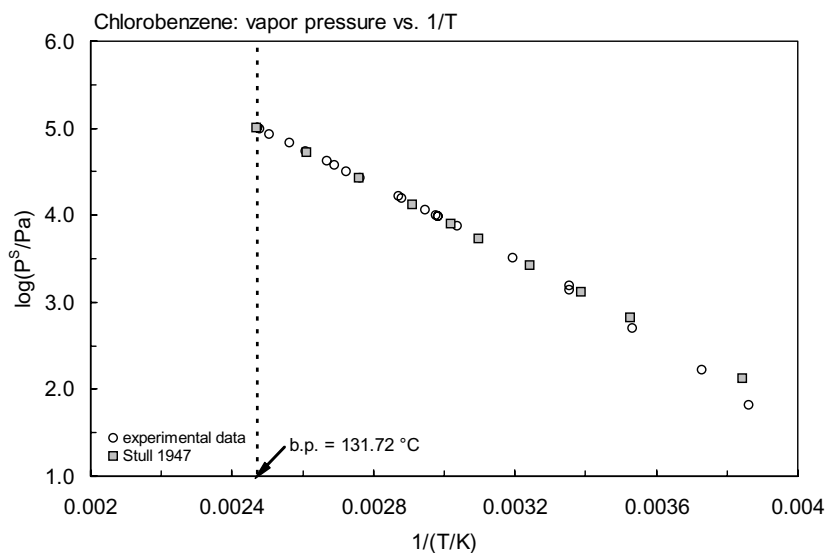


FIGURE 6.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.3

Reported Henry's law constants of chlorobenzene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln k_H = A - B/(T/K)$	(3)	$\log k_H = A - B/(T/K)$	(3a)
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

1.

Leighton & Calo 1981		Ashworth et al. 1988		Ettre et al. 1993		Görgényi et al. 2002	
equilibrium cell-concn ratio		EPICS-GC		equilibrium headspace-GC		EPICS-SPME method	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
1	124	10	247	45	621	2	112
3	125	15	285	60	863	6	155.5
12.4	190	20	346	70	1114	10	183.6
12.5	206	25	365	80	1579	18	283.2
17.9	243	30	479			25	384
19.1	280					30	472.8
22.7	271	eq. 4	H/(atm m <sup>3</sup> /mol)	eq. 2a	1/K <sub>AW</sub>	40	755.8
23	321	A	3.469	A	2.905024	50	1046
		B	2689	B	1129.8083	60	1420
eq. 3	k <sub>H</sub> /atm					70	1804
A	18.46					eq. 1	K <sub>AW</sub>
B	3751					A	10.04
						B	3359.7

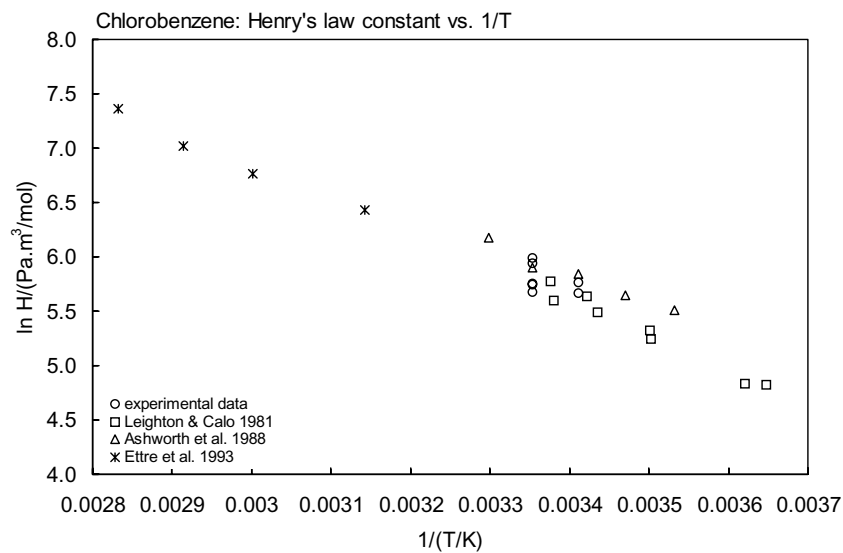


FIGURE 6.1.1.1.3 Logarithm of Henry’s law constant versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.4  
Reported octanol-water and octanol-air partition coefficients of chlorobenzene at various temperatures

log K <sub>OW</sub>		log K <sub>OA</sub>	
Finizio & Di Guardo 2001		Su et al. 2002	
GC-RT correlation		GC-RT correlation	
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
5	3.19	10	3.76
15	3.15	20	3.45
25	3.05	30	3.17
35	3.04	40	2.90
		50	2.65
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 43.91$			
$\log K_{OA} = A + B/T$			
A		− 4.107	
B		43910	

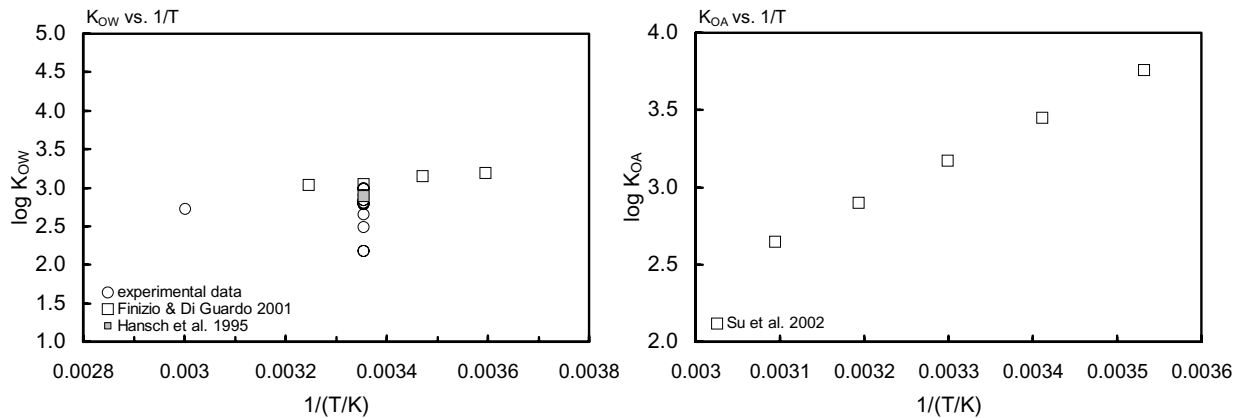
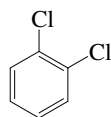


FIGURE 6.1.1.1.4 Logarithm of K<sub>OW</sub> and K<sub>OA</sub> versus reciprocal temperature for chlorobenzene.

## 6.1.1.2 1,2-Dichlorobenzene



Common Name: 1,2-Dichlorobenzene

Synonym: *o*-dichlorobenzene, dowtherm E

Chemical Name: 1,2-dichlorobenzene

CAS Registry No: 95-50-1

Molecular Formula: C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>

Molecular Weight: 147.002

Melting Point (°C):

−17.0 (Pirsch 1956; Dreisbach 1955; Weast 1972–73; 1982–83; Lide 2003)

Boiling Point (°C):

180 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.3048 (Weast 1972–73; Horvath 1982)

1.3059 (Lide 2003)

Molar Volume (cm<sup>3</sup>/mol):

112.6 (20°C, calculated-density)

137.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

12.93 (Weast 1972–73)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

50.46 (Pirsch 1956)

50.63 (Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C, F: 1.0 (Suntio et al. 1988b)

Water Solubility (g/m<sup>3</sup> 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):

145\* (volumetric, measured range 20–60°C, Klemenc & Low 1930; Seidell 1941)

< 260 (residue-volume method, Booth & Everson 1948)

92.7 (Landolt-Börnstein 1951)

79.0 (shake flask-radiolabeled <sup>14</sup>C-LSC, Metcalf et al. 1975)

148\* (20°C, shake flask-GC/ECD, measured 0–34°C, Chiou & Freed 1977)

92.8 (shake flask-UV, Yalkowsky et al. 1979)

154 (shake flask-LSC/<sup>14</sup>C, Veith et al. 1980)

128, 124\* (20°C; elution chromatography, UV, Schwarz & Miller 1980)

155.8 (shake flask-LSC, Banerjee et al. 1980; Banerjee 1985)

99.1 (shake flask-GC, Könemann 1981)

92.6 (recommended, Horvath 1982)

154 (shake flask-GC, Chiou et al. 1982, 1983; Chiou 1981, 1985; Chiou & Schmedding 1981)

125 (quoted average, Yalkowsky et al. 1983)

92.3 (generator column-GC, Miller et al. 1984, 1985)

137 (shake flask-HPLC, Banerjee 1984)

147\* (recommended, temp range 0–60°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)

S/(g/kg) = 19.2314 – 1.81140 × 10<sup>−1</sup> · (T/K) + 5.6509 × 10<sup>−4</sup> · (T/K)<sup>2</sup> – 5.77683 × 10<sup>−7</sup> · (T/K)<sup>3</sup>, temp range 273–333 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

169 (shake flask-radiometry, Lo et al. 1986)

156 (quoted lit. average, Riddick et al. 1986; Howard 1989)

31\* (19.5°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1992)

145 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)

- 159.2 (shake flask-GC/ECD, Tam et al. 1996)  
 144 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 109 (shake flask-GC, Boyd et al., 1998)  
 92, 93, 137; 97 (quoted lit. values; solid-phase micro-extraction SPME-GC, Paschke et al. 1998)  
 $\ln x = -31.5289 + 3834/(T/K) + 8.7172 \times 10^{-5} \cdot (T/K)^2$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)  
 149\*  $\pm 8.2$  (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)  
 140, 124, 158 (5, 15, 25°C, estimated-RP-HPLC-k' correlation, Finizio & Di Guardo 2001)  
 93.7\* (generator column-GC/ECD, measured range 15–55°C, 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):

- 137\* (20°C, summary of literature data, Stull 1947)  
 $\log (P/\text{mmHg}) = 7.32585 - 1824.6/(230 + t/^\circ\text{C})$  (Antoine eq., Dreisbach & Martin 1949)  
 5010\* (56.28°C, ebulliometry, measured range 87.02–180.48°C, Dreisbach & Shrader 1949)  
 171 (calculated by formula., Dreisbach 1955)  
 $\log (P/\text{mmHg}) = 6.92400 - 1538.3/(200.0 + t/^\circ\text{C})$ ; temp range 80–250°C (Antoine eq. for liquid state, Dreisbach 1955)  
 25234\* (130.82°C, ebulliometry, measured range 130.82–181.62°C, McDonald et al. 1959)  
 196 (extrapolated, Antoine eq., Weast 1972–73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 10943.0/(T/K)] + 8.185275$ ; temp range 20–179°C (Antoine eq., Weast 1972–73)  
 174, 197 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)  
 224.87\*; 132, 188 (27.8°C reported; 20°C, 25°C, extrapolated-Antoine eq. from gas saturation-GC measurement, temp range 27.8–70°C, Grayson & Fosbraey 1982)  
 $\log (P/\text{Pa}) = 25.4 - 6013/(T/K)$ , temp range 27.8–70°C (gas saturation-GC, Grayson & Fosbraey 1982)  
 $\log (P/\text{kPa}) = 6.13305 - 1599.034/(206.964 + t/^\circ\text{C})$ ; temp range 87.2–180.5°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.26861 - 1704.435/(219.409 + t/^\circ\text{C})$ ; temp range 130.8–181.62°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1984)  
 197 (extrapolated, Antoine eq., Dean 1985)  
 $\log (P/\text{mmHg}) = 7.14378 - 1704.49/(219.42 + t/^\circ\text{C})$ ; temp range 131–181°C (Antoine eq., Dean 1985, 1992)  
 201.4 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)  
 198 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.26918 - 1705.55/(-52.56 + T/K)$ ; temp range 373–453 K (liquid, Antoine eq., Stephenson & Malanowski 1987)  
 164\* (gas saturation, measured range –15 to 40°C, Liu & Dickhut 1994)  
 137.3\*; 188 (pressure gauge measured at 20.35°C, 25°C, interpolated from reported Antoine eq., Polednicek et al. 1996)  
 $\ln (P/\text{Pa}) = 21.5929 - 4053.86/[(T/K) - 50.2328]$ ; temp range 256–422 K (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)  
 252; 185 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; quoted lit., Spieksma et al. 1994)  
 $\log (P/\text{mmHg}) = 31.3614 - 3.5226 \times 10^3/(T/K) - 7.8886 \cdot \log (T/K) - 2.2250 \times 10^{-10} \cdot (T/K) + 1.1842 \times 10^{-6} \cdot (T/K)^2$ , temp range 256–705 K (Yaws 1994)  
 5729\* (90.193°C, comparative ebulliometry, measured range 90.193–181.633°C, Roháč et al. 1998)  
 133.8\* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)  
 $\ln [(P/\text{Pa})/6.80] = [1 - (T/K)/256.10] \cdot \exp\{3.359374 - 8.5641422 \times 10^{-4} \cdot (T/K) + 6.0235167 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range 256–445 K (Cox eq., recommended, Roháč et al. 1999)  
 $\log (P/\text{kPa}) = 19.40 - 6013/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m<sup>3</sup>/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.):

- 248 (calculated as  $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)  
 375 (calculated-bond contribution, Hine & Mookerjee 1975)  
 193 (batch air stripping-GC, Mackay & Shiu 1981)  
 122 (20°C, gas stripping-GC, Oliver 1985)

- 197 (gas stripping, Warner et al. 1987)  
 159\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = -1.518 - 1422/(T/K)$ ; temp range 10–30°C (EPICS-GC/FID, Ashworth et al. 1988)  
 299 (computer value, Yaws et al. 1991)  
 141 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 195 (gas stripping-GC, Shiu & Mackay 1997)  
 212.7 (modified EPICS method-GC, Ryu & Park 1999)  
 133 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 7.045 - 2636/(T/K)$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 3.55 (Hansch et al. 1968)  
 3.38 (Leo et al. 1971; Hansch & Leo 1979, 1985)  
 3.57 (calculated-fragment constants, Rekker 1977)  
 3.55, 3.39 (shake flask-GC, HPLC- $k'$ , Könemann et al. 1979)  
 3.40; 3.75 (concentration ratio; HPLC-RT correlation, Veith et al. 1980)  
 3.40 (shake flask-LSC, Banerjee et al. 1980)  
 3.71, 3.18–4.36 (shake flask method: mean, range of mean values, OECD 1981)  
 3.34 (shake flask-HPLC, Hammers et al. 1982)  
 3.40 (shake flask-GC, Watarai et al. 1982)  
 3.19, 3.19, 3.31, 3.53, 3.60, 3.84, 4.15, 4.36; 3.61 (shake flask; results of OECD/EEC laboratory comparison tests; mean value, Harnisch et al. 1983)  
 3.34, 3.20; 3.61 (HPLC methods; OECD/EEC shake-flask method; Harnisch et al. 1983)  
 3.61 (OECD/EEC shake-flask method, Harnisch et al. 1983)  
 3.38 (generator column-HPLC/UV, Wasik et al. 1983)  
 3.38 (generator column-GC, Miller et al. 1984, 1985)  
 3.56 (HPLC-RV correlation, Garst 1984)  
 3.433 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)  
 3.49 (shake flask-GC, Pereira et al. 1988)  
 3.38 (recommended, Sangster 1993)  
 3.43 (recommended, Hansch et al. 1995)  
 3.29  $\pm$  0.05 (shake flask-GC/ECD, Bahadur et al. 1997)  
 3.29\* (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)  
 $\log K_{OW} = 0.1831 + 17800/[2.303\cdot R(T/K)]$ ; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)  
 3.447 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)  
 3.70 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

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

- 4.36\*, 4.41 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)  
 $\log K_{OA} = -4.30 + 2574.0/(T/K)$ ;  $\Delta H_{OA} = 49.3$  kJ/mol (generator column-GC, Harner & Mackay 1995)  
 4.68 (solid-phase microextraction SPME-GC, Treves et al. 2001)  
 $\log K_{OA} = -7.90 + 3304/(T/K)$ ,  $\Delta H_{OA} = 63.3$  kJ/mol (SPME-GC, Treves et al. 2001)

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

- 1.95 (bluegill sunfish, Veith et al. 1979b; 1980)  
 2.19–2.48 (fish, calculated, Veith et al. 1980)  
 1.95 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)  
 2.86 (microorganisms-water, Mabey et al. 1982)  
 2.40–2.48 mean 2.43; 2.60–2.85 mean 2.74 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)  
 3.51–3.80 (rainbow trout, lipid-basis, Oliver & Niimi 1983)  
 2.43–2.75 (fish, Oliver 1984)  
 1.95 (correlated-flow through method, bluegill sunfish, Davis & Dobbs 1984)

- 1.60 (fish-normalized, Tadokoro & Tomita 1987)  
 1.89 (fish, calculated-MCI  $\chi$ , Sabljic 1987b)  
 3.94, 4.46, 3.79, 3.82 (field data: Atlantic croaker, blue crabs, spotted sea trout, blue catfish, lipid-based, Pereira et al. 1988)  
 2.4  $\pm$  0.1 (guppies, steady-state conditions, rate const. ratio  $k_1/k_2$ , 96-h exposure, Sijm et al. 1993)  
 3.5  $\pm$  0.1 (guppies, lipid normalized BCF, Sijm et al. 1993)  
 2.70 (fathead minnow, steady-state conditions, rate const. ratio  $k_1/k_2$ , 96-h exposure, Sijm et al. 1993)  
 3.90 (fathead minnow, lipid normalized BCF, Sijm et al. 1993)  
 1.95; 2.43, 2.75 (*Lepomis macrochirus*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)  
 2.40; 2.70 (*Poecilla reticulata*; *Pimephales promelas*, quoted lit., static and semi-static conditions, Devillers et al. 1996)  
 2.43, 3.51; 2.333, 2.549 (quoted: whole fish, lipid content; calculated-MCI  $\chi$ , calculated- $K_{OW}$ , Lu et al. 1999)  
 3.86; 3.84 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

#### Sorption Partition Coefficient, log $K_{OC}$ :

- 2.26 (Willamette silt loam soil, 1.6% organic matter, equilibrium sorption isotherm measurement, Chiou et al. 1979)  
 3.0, 2.96, 2.62 (calculated- $K_{OW}$ , solubility  $C_L$ ,  $C_S$ , Karickhoff 1981)  
 4.60; 4.60; 3.00 (field data of sediment trap material, Niagara River organic matter, calculated from  $K_{OW}$ , Oliver & Charlton 1984)  
 2.34, 2.59 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)  
 2.45 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 3.27, 2.04 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.43 (untreated Marlette soil  $B_t$  horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)  
 3.64, 3.52 (organic cations treated Marlette soil  $B_t$  horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.45–3.51 (aquifer materials, Stauffer et al. 1989)  
 3.10, 2.90; 2.99 (Captina silt loam, OC 1.49% and pH 4.97, McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)  
 2.36–2.61 (16 U.S. soils, 1.03–6.09% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)  
 2.37–2.51 (16 Chinese soils, 0.16–5.61% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)  
 2.48–2.76 (14 U.S. bed sediments, 0.4–2.20% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)  
 2.62–2.78 (21 Chinese bed sediments, 0.11–4.73% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)  
 2.36–2.63 (suspended solids from four U.S. rivers, 1.78–2.87% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)  
 2.48 (suspended solids from Yellow River, China, 0.30% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)  
 2.39, 2.40 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)  
 3.69  $\pm$  0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)  
 2.50, 2.50, 2.47 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, 0.1  $\leq$  OC  $<$  0.5%, average, Delle Site 2001)  
 2.70, 2.69, 2.71 (sediments, organic carbon OC  $\leq$  0.1%, OC  $\leq$  0.5%, 0.1  $\leq$  OC  $<$  0.5%, average, Delle Site 2001)

#### Sorption Coefficient, log $K_{OM}$ :

- 2.25 (Willamette silt loam soil, 1.6% organic matter, equilibrium isotherm, Chiou et al. 1979; quoted, Howard 1989)  
 2.27 (Woodburn silt loam soil, 1.9% organic matter, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)  
 2.50 (soil, Chiou et al. 1983)  
 2.26, 2.54 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)

- 2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.97 (untreated Marlette soil B<sub>t</sub> horizon, OM 0.60%, equilibrium isotherm, Lee et al. 1989)
- 3.97, 3.50, 2.87 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

#### Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$ :

Volatilization/Evaporation: experimental evaporation rate into air,  $1.18 \times 10^{-6} \text{ g cm}^{-2} \text{ s}^{-1}$  (Chiou et al. 1980); estimated  $t_{1/2} = 4.4 \text{ h}$  for a model river of 1-m depth with a flow rate of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant (Mabey et al. 1982); rate constant  $k = 1.22 \times 10^{-4} \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  under photolysis at 25°C in F-113 solution and with  $\text{HO}^-$  in the gas (Dilling et al. 1988).

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{\text{OH}}$  for reaction with OH radical,  $k_{\text{NO}_3}$  with  $\text{NO}_3$  radical, and  $k_{\text{O}_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures see reference:

$k_{\text{OH}} \sim 3.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $\ll 1 \text{ M}^{-1} \text{ h}^{-1}$  for  $\text{RO}_2$  radical (Mabey et al. 1982)

$k_{\text{OH}} = (4.2 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{\text{O}_3} = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K measured range 298–323 K (Atkinson & Carter 1984)

$k_{\text{OH}}$  (obs.) =  $4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ; and  $k_{\text{OH}}$  (calc) =  $4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{\text{OH}}$  (calc) =  $4.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}$  (obs) =  $4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = 4.07 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 22–27°C (Dilling et al. 1988)

$k = (3.7\text{--}4.0) \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$  for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{\text{OH}}$  (calc) =  $4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  in aqueous solutions (Haag & Yao 1992)

$k_{\text{OH}}$  (calc) =  $0.48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982).

base rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  at 25°C with a calculated  $t_{1/2} > 900 \text{ yr}$  at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

Biodegradation:  $t_{1/2}$  (aq. aerobic) = 672–4320 h, based on unacclimated soil grab sample data, and aerobic screening test data (Howard et al. 1991);

$t_{1/2}$  (aq. anaerobic) = 2880–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

significant degradation in an aerobic environment with  $k = 0.05 \text{ d}^{-1}$  (Tabak et al. 1981; Mills et al. 1982); in a continuous flow of activated sludge system; virtually 100% (78% biodegradation and 22% stripping) was observed (Kincannon et al. 1983; selected, Howard 1989).

Biotransformation:  $1 \times 10^{-10} \text{ ml cell}^{-1} \text{ h}^{-1}$  (estimated, Mabey et al. 1982).

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

$k_1 = 870 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 3.90 \text{ d}^{-1}$  (guppy, 96-h exposure., Sijm et al. 1993)

$k_1 = 635 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 1.40 \text{ d}^{-1}$  (fathead minnow, 96-h exposure, Sijm et al. 1993)

#### Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 152.8\text{--}1528 \text{ h}$ , based on the photooxidation half-life in air. (Howard et al. 1991)

Surface water:  $t_{1/2} = 1.2\text{--}37 \text{ d}$  estimated from field data at various locations in the Netherlands,  $t_{1/2} = 0.3\text{--}3 \text{ d}$  for river,  $t_{1/2} = 3\text{--}30 \text{ d}$  for lakes (Zoeteman et al. 1980)

$t_{1/2} = 672\text{--}4320 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater:  $t_{1/2} = 30\text{--}300 \text{ d}$ , estimated from persistence in water (Zoeteman et al. 1980);



$t_{1/2} \sim 1$  yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 1344\text{--}8640$  h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil:  $t_{1/2} = 672\text{--}4320$  h, based on unacclimated aerobic screening test data (Howard et al. 1991)

disappearance  $t_{1/2} = 4.0$  d in testing soils (Anderson et al. 1991).

Biota:  $t_{1/2} < 1$  d in fish (Veith et al. 1980);

$t_{1/2} < 1$  d bluegill sunfish. (Barrows et al. 1980);

$t_{1/2} < 5$  d in worms at  $8^\circ\text{C}$  (Oliver 1987a);

biological half-lives:  $t_{1/2} < 1$  d in trout muscle,  $t_{1/2} < 1$  d in sunfish and  $t_{1/2} < 1$  d in guppy for dichlorobenzenes (Niimi 1987).

**TABLE 6.1.1.2.1**

**Reported aqueous solubilities of 1,2-dichlorobenzene at various temperatures**

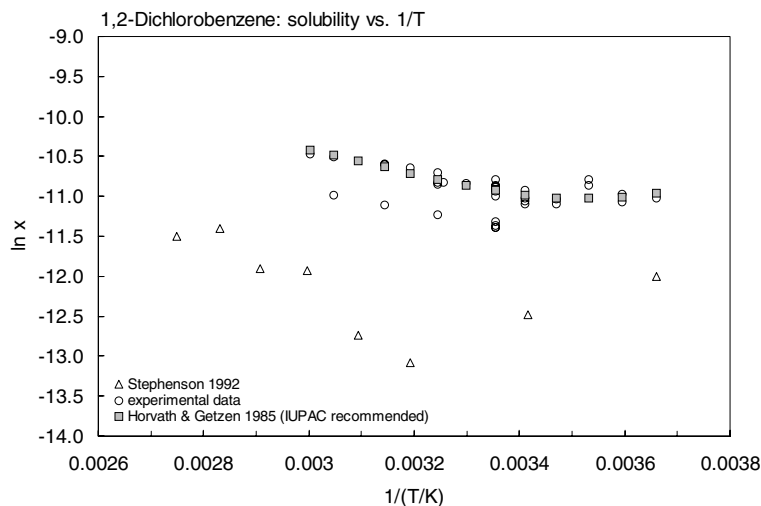
1.

Klemenc & Löw 1930		Chiou & Freed 1977		Schwarz & Miller 1980		Horvath & Getzen 1985	
volumetric method		shake flask-GC		elution chromatography		recommended values	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	134	0	133	10	169	0	142
25	145	20	148	20	128	5	135
30	161	34	162	shake flask-UV		10	133
35	183			10	156	15	134
40	194			20	124	20	139
45	203					25	147
55	223					30	157
60	232					35	169
						40	182
						45	197
						50	212
						55	228
						60	243

2.

Stephenson 1992		Ma et al. 2001		Finizio & Di Guardo 2001		Oleszek-Kudlak et al. 2004	
shake flask-GC		shake flask-GC/FID		RP-HPLC- $k'$ correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
0	50	5	127	5	140	25	93.7
19.5	31	15	132	15	124	25	94.4
40	17	25	149	35	158	35	108.0
50	24	35	162			45	122.7
60.5	54	45	204			55	130.1
70.7	55						
80.0	91						
90.5	83						

$\Delta H_{\text{sol}} = 10.49$  kJ/mol



**FIGURE 6.1.1.2.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,2-dichlorobenzene.

**TABLE 6.1.1.2.2**

**Reported vapor pressures of 1,2-dichlorobenzene 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)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln (P/\text{Pa}) = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_0) = (1 - T/T_0) \cdot \exp[\sum A_i T^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959		Grayson & Fosbraey 1982	
summary of lit. data		ebulliometry		ebulliometry		gas saturation-GC	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
20	133.3	87.02	5010	130.82	25234	20.0	132
46	666.6	97.66	7605	154.83	51778	27.8	224.8
59.1	1333	104.94	10114	178.66	96998	32.0	282.8
73.4	2666	118.32	16500	179.73	99614	41.5	599.3
89.4	5333	147.6	42066	180.54	101655	48.6	780.1
99.5	7999	164.65	67661	181.62	104322	56.3	1253
112.9	13332	180.48	101325			61.1	1645
133.4	26664			mp/ $^{\circ}\text{C}$	-17.0	70.0	2636
155.8	53329						
180	101325	eq. 2	P/mmHg	eq. 2	P/mmHg		
		A	7.32585	A	7.07028	eq. 1	P/Pa
mp/ $^{\circ}\text{C}$	-17.6	B	1824.6	B	1649.55	A	25.4
		C	230	C	213.314	B	6013

TABLE 6.1.1.2.2 (Continued)

2.

Liu & Dickhut 1994		Polednicek et al. 1996		Roháč et al. 1998		Roháč et al. 1999	
gas saturation-GC		pressure gauge		comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
-14.2	7.73	-16.65	7.056	90.193	5729	263.15	12.9
-5.0	14.7	-16.65	7.042	99.529	8333	273.15	30.1
10	56.1	-9.75	13.175	99.53	8335	283.15	65.4
25	164	-9.75	13.195	107.0	11074	283.15	133.8
40	448	0.30	30.815	113.265	13917	303.15	259.1
		10.32	67.088	118.61	16800	313.15	477.9
		20.35	137.3	118.61	16799	232.15	843.3
$\Delta H_v/(\text{kJ mol}^{-1}) = 51.2$		30.28	264.39	124.14	20290	333.15	1430
		40.24	485.45	129.935	24569	343.25	2338
exptl data fitted to the		50.15	848.67	135.547	29394	353.15	3699
modified Watson correlation		60.15	1440.7	141.024	34818	363.15	5681
		60.15	1442.0	146.292	40757	373.15	8491
		70.05	2313.0	146.292	40761	383.15	12380
		70.05	2318.6	151.657	47825	393.15	17640
		80.02	3660.3	160.102	60273	403.15	24630
		80.03	3661.2	168.184	74765	413.15	33720
		88.75	5428.4	176.912	93403	423.15	45370
		88.75	54284	178.845	97970	433.15	60070
		89.94	5606.9	181.633	104893	443.15	78370
		89.94	5601.2			453.15	10080
		98.79	8102.5	bp/°C	180.190	463.15	12810
		98.79	8104.0				
		108.76	11826	eq. 3	P/kPa	Cox eq.	
		118.8	16870	A	6.16161	eq. 5	
		128.19	23583	B	1612.27	A <sub>0</sub>	3.359374
		138.83	32396	C	-64.447	10 <sup>-4</sup> A <sub>1</sub>	-8.5641422
		148.91	43690			10 <sup>-7</sup> A <sub>2</sub>	6.0235167
						T <sub>0</sub> /K	256.10
		eq. 3a	P/Pa			P <sub>0</sub> /Pa	6.80
		A	21.5929			bp/K	453.35
		B	4053.86			temp range	256–445 K
		C	-50.2358				

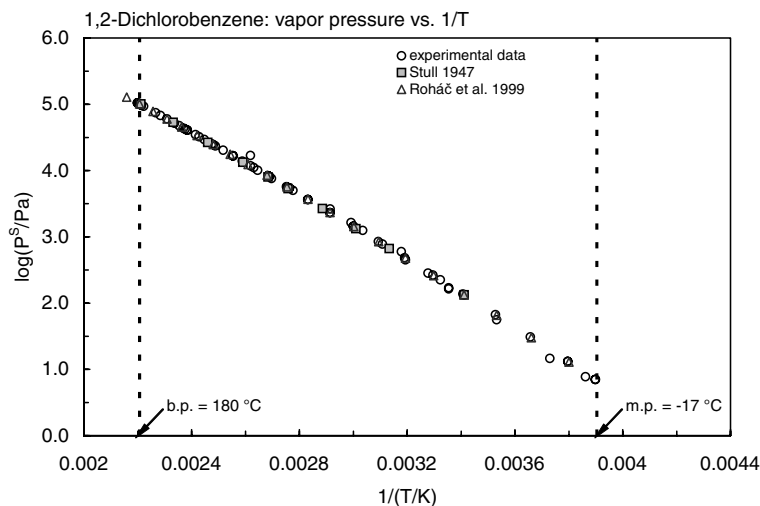
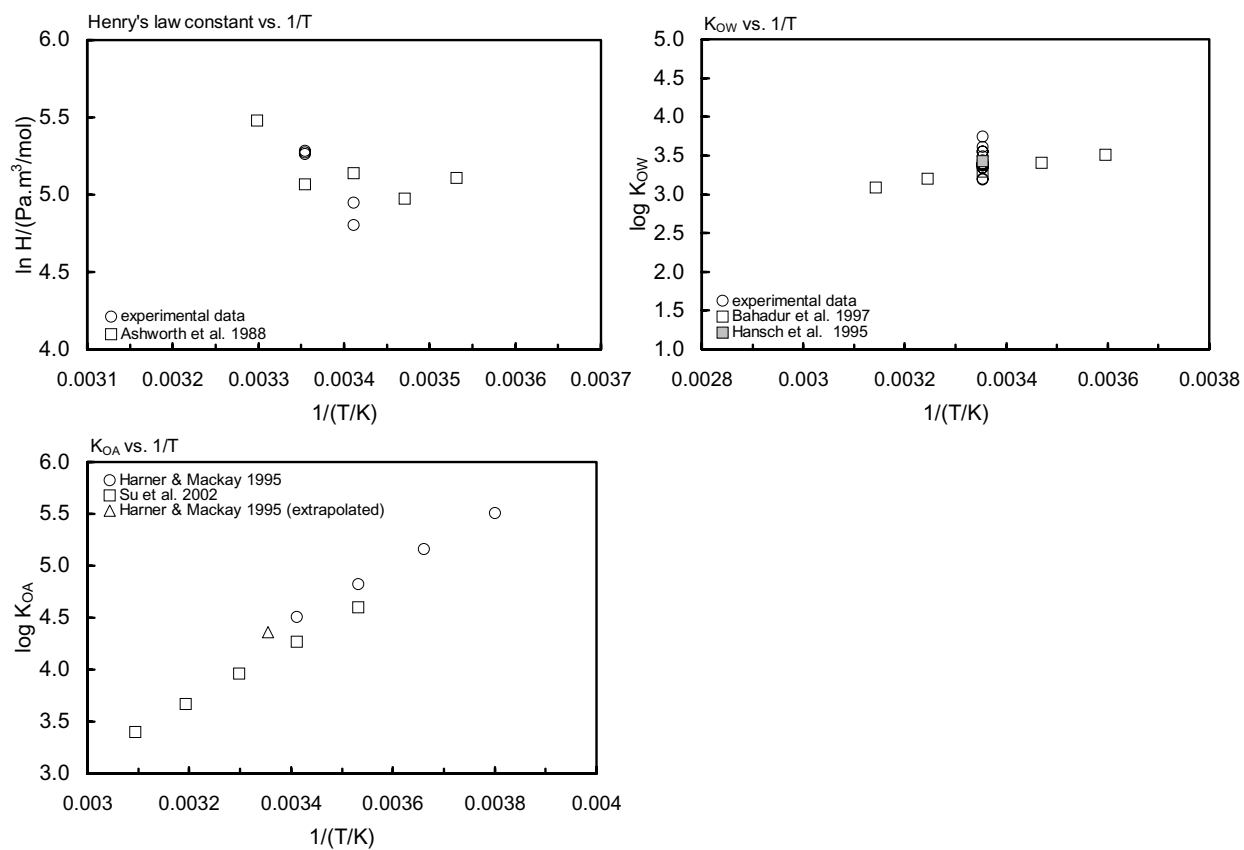


FIGURE 6.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichlorobenzene.

TABLE 6.1.1.2.3

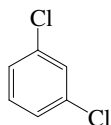
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2-dichlorobenzene at various temperatures and temperature dependence equations

Henry's law constant		log K <sub>OW</sub>		log K <sub>OA</sub>			
Ashworth et al. 1988		Bahadur et al. 1997		Harner & Mackay 1995		Su et al. 2002	
EPICS		shake flask-GC/ECD		generator column-GC		GC-RT correlation	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>	t/°C	log K <sub>OA</sub>
10	165	5	3.51	-10	5.51	10	4.6
15	145	15	3.41	0	5.16	20	4.27
20	170	25	3.29	10	4.82	30	3.96
20	159	35	3.2	20	4.51	40	3.67
30	240	45	3.09			50	3.4
ln H = A - B/(T/K)		enthalpy of transfer ΔH/(kJ mol <sup>-1</sup> ) = -17.8		ΔH <sub>OA</sub> /(kJ mol <sup>-1</sup> ) = 49.3		ΔH <sub>OA</sub> /(kJ mol <sup>-1</sup> ) = 57.02	
H/(atm m <sup>3</sup> /mol)				log K <sub>OA</sub> = A + B/RT		log K <sub>OA</sub> = A + B/2.303RT	
A	-1.518	log K <sub>OW</sub> = A - ΔH/2.303RT		A	-4.3	A	-5.856
B	1422	A		B	2574	B	57020
		ΔH					
		-17800					



**FIGURE 6.1.1.2.3** Logarithm of Henry's law constant,  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for 1,2-dichlorobenzene.

## 6.1.1.3 1,3-Dichlorobenzene



Common Name: 1,3-Dichlorobenzene

Synonym: *m*-dichlorobenzene

Chemical Name: 1,3-dichlorobenzene

CAS Registry No: 541-73-1

Molecular Formula: C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>

Molecular Weight: 147.002

Melting Point (°C):

-24.8 (Lide 2003)

Boiling Point (°C):

173 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.2884 (Dreisbach 1955; Weast 1972–73; Horvath 1982; Lide 2003)

Molar Volume (cm<sup>3</sup>/mol):

114.1 (20°C, calculated-density)

137.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

12.64 (Weast 1972–73)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

50.63 (Pirsch 1956)

51.46 (Yalkowsky 1979)

51.05 (Yalkowsky &amp; Valvani 1980)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> 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):

123\* (volumetric, measured range 20–60°C, Klemenc &amp; Löw 1930)

123.5 (Ginnings et al. 1939)

124 (Landolt-Börnstein 1951)

101.26\* (shake flask-UV, measured range 10–35°C, Vesala 1973)

102.9 (shake flask-UV, Vesala 1974)

119.5 (shake flask-UV, Yalkowsky et al. 1979)

131 (shake flask-LSC-<sup>14</sup>C, Veith et al. 1980)

144\*, 149 (23.5°C, elution chromatography, measured range 10–30°C, Schwarz 1980)

111, 89, 113, 101 (20°C, quoted, UV, elution chromatography, average exptl. value, Schwarz &amp; Miller 1980)

133.5 (shake flask-LSC, Banerjee et al. 1980)

68.6 (shake flask-GC, Könemann 1981)

134 (shake flask-GC/ECD, Chiou &amp; Schmedding 1981; Chiou et al. 1982, 1983; Chiou 1985)

124 (recommended, Horvath 1982)

124.5 (generator column-GC/ECD, Miller et al. 1984, 1985)

143 (shake flask-HPLC, Banerjee 1984)

106\* (recommended, temp range 10–60°C, IUPAC Solubility Data Series, Horvath &amp; Getzen 1985)

S/(g/kg) = 27.6827 – 2.61597 × 10<sup>-1</sup>·(T/K) + 8.19706 × 10<sup>-4</sup>·(T/K)<sup>2</sup> – 8.4698 × 10<sup>-7</sup>·(T/K)<sup>3</sup>, temp range 283–333 K  
(regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

110 (Dean 1985)

111 (20°C, Riddick et al. 1986)

130 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka &amp; Dohnal 1997)

123; 138 (quoted lit.; shake flask-GC, Boyd et al. 1998)

126\*  $\pm$  6.1 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)

71, 104, 132, 166 (5, 15, 25, 35°C, estimated-RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

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\* (12.1°C, summary of literature data, Stull 1947)

$\log(P/\text{mmHg}) = 7.30364 - 1782.4/(C + t/^\circ\text{C})$  (Antoine eq., Dreisbach & Martin 1949)

7605\* (90.72°C, ebulliometry, measured range 90.72–173.0°C, Dreisbach & Shrader 1949)

252 (calculated by formula., Dreisbach 1955)

$\log(P/\text{mmHg}) = 6.88045 - 1496.2/(201.0 + t/^\circ\text{C})$ ; temp range 75–240°C (Antoine eq. for liquid state, Dreisbach 1955)

307 (extrapolated, Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 10446.8/(T/K)] + 8.017555$ ; temp range 12.1–173°C (Antoine eq., Weast 1972–73)

266 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.17083 - 1611.121/(213.817 + t/^\circ\text{C})$ ; temp range 90.7–173°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

179.3 (gas saturation, interpolated from reported graph, Rordorf 1985)

265 (extrapolated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.0401 - 1607.05/(213.38 + t/^\circ\text{C})$ ; temp range 91–173°C (Antoine eq., Dean 1985, 1992)

243 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.00535 - 1496.2/(-72.15 + T/K)$ ; temp range 348–513 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

236 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; Spieksma et al. 1994)

190.4\* (20.39°C, static-pressure gauge, measured range –25 to 159°C, Polednicek et al. 1996)

$\ln(P/\text{Pa}) = 21.6433 - 4031.27/[(T/K) - 47.5846]$ ; temp range 249–432 K (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)

$\log(P/\text{mmHg}) = 3.2904 - 2.5839 \times 10^3/(T/K) + 3.893 \cdot \log(T/K) - 9.5398 \times 10^{-3} \cdot (T/K) + 4.6397 \times 10^{-6} \cdot (T/K)^2$ , temp range 248–684 K, (Yaws 1994)

5731\* (84.353°C, comparative ebulliometry, measured range 84.353–175.207°C, Roháč et al. 1998)

185.0\* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)

$\ln[(P/\text{Pa})/4.85] = [1 - (T/K)/248.39] \cdot \exp\{3.366439 - 8.3811530 \times 10^{-4} \cdot (T/K) + 5.9337577 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range 250–448 K (Cox eq., recommended, Roháč et al. 1999)

$\log(P/\text{Pa}) = 21.6433 - 4031.27/[(T/K) - 47.5846]$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m<sup>3</sup>/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.):

472 (calculated as  $1/K_{AW} \cdot C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975; selected exptl., Nirmalakhandan & Speece 1988a)

375 (calculated-bond contribution, Hine & Mookerjee 1975)

182 (20°C, batch air stripping-GC, Oliver 1985)

267 (gas stripping-GC, Warner et al. 1987)

289\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

$\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 2.882 - 2564/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

328 (computer value, Yaws et al. 1991)

216 (20°C, equilibrium gas stripping-GC, Hovorka & Dohnal 1997)

269 (21°C, headspace equilibrium-GC, de Wolf & Lieder 1998)

288 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 2.436 - 986/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section:

3.55 (Hansch et al. 1968)

3.38 (Leo et al. 1971; Hansch & Leo 1979)

3.57, 3.55 (calculated-fragment constants, Rekker 1977)

- 3.60 (shake flask-GC, Könemann et al. 1979)
- 3.62 (HPLC- $k'$  correlation, Könemann et al. 1979)
- 3.44 (shake flask-LSC, Banerjee et al. 1980)
- 3.44 (shake flask-LSC, Veith et al. 1980; Oliver & Niimi 1983)
- 3.95 (HPLC-RT correlation, Veith et al. 1980)
- 3.53 (shake flask-GC, Watarai et al. 1982)
- 3.46 (shake flask-HPLC, Hammers et al. 1982)
- 3.38–3.62, 3.52 (range, mean, shake flask method, Eadsforth & Moser 1983)
- 3.62–3.95, 3.73 (range, mean, HPLC method, Eadsforth & Moser 1983)
- 3.48 (generator column-HPLC/UV, Wasik et al. 1983)
- 3.48 (generator column-GC/ECD, Miller et al. 1984; 1985)
- 3.57 (HPLC-RV correlation, Garst 1984)
- 3.60 (Hansch & Leo 1985)
- 3.55\* (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)
- 3.50 (shake flask-GC, Pereira et al. 1988)
- 3.525 (slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 3.52 (recommended, Sangster 1993)
- 3.53 (recommended, Hansch et al. 1995)

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:

- 4.36 (calculated- $S_{oct}$  and vapor pressure, Abraham et al. 2001)
- 4.27\* (20°C, HPLC- $k'$  correlation, measured range 10–50°C, Su et al. 2002)
- $\log K_{OA} = 57020/(2.303 \cdot RT) - 5.856$ ; temp range 10–50°C (HPLC- $k'$  correlation, Su et al. 2002)

Bioconcentration Factor,  $\log BCF$ :

- 1.82 (bluegill sunfish, Veith et al. 1979b; 1980)
- 1.82 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 2.86 (microorganisms-water, Mabey et al. 1982)
- 2.57–2.68 mean 2.62; 2.74–2.96 mean 2.87 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
- 3.70–4.02 (rainbow trout, lipid base, Oliver & Niimi 1983)
- 2.62–2.87 (fish, Oliver 1984)
- 1.99 (fathead minnow, flowing water, Carlson & Kosian 1987)
- 3.77, 3.78, 3.83, 3.84 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
- 3.60, 3.86, 3.25, 3.40 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
- 1.82; 2.62, 2.87 (*Lepomis macrochirus*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
- 3.78 (*Poecilla reticulata*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
- 2.62, 3.70; 2.553, 2.305 (quoted: whole fish, lipid content; calculated-QSPR-MCI  $\chi$ ,  $K_{OW}$ , Lu et al. 1999)
- 3.79; 3.75 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient,  $\log K_{OC}$ :

- 4.50; 4.10 (field data of sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)
- 2.14 (soil, Lee et al. 1989)
- 2.48 (soil, calculated-QSAR-MCI  $\chi$ , Sabljic et al. 1995)
- 2.43, 2.58, 2.88 (RP-HPLC- $k'$  correlation on three different stationary phases, Szabo et al. 1995)
- 2.60, 2.60 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 3.47  $\pm$  0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)
- 2.49, 2.53 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, average, Delle Site 2001)



Sorption Partition Coefficient,  $\log K_{OM}$ :

- 2.23 (Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)  
 3.88 (micelle-water, Valsaraj & Thibodeaux 1989)

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Volatilization: estimated  $t_{1/2} = 4.1$  h from a model river of 1 m depth with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982);

$k = 1.9 \times 10^{-4} \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988);  
 pseudo-first-order direct photolysis  $k(\text{exptl}) = (0.008 \pm 0.001) \text{ min}^{-1}$  with  $t_{1/2} = (92.3 \pm 6.4) \text{ min}$  in aqueous solution (Peijnenburg et al. 1992)

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with  $\text{NO}_3$  radical and  $k_{O_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures see reference:

$k_{OH} \sim 3.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$  for  $\text{RO}_2$  radical (Mabey et al. 1982)

$k_{OH} = (7.2 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{OH}(\text{obs.}) = 7.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ; and  $k_{OH}(\text{calc.}) = 11.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{OH}(\text{calc.}) = 1.01 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs.}) = 0.72 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k(\text{aq.}) = (0.57 \pm 0.005) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 22°C, with  $t_{1/2} = 16$  h at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = (5.4\text{--}5.9) \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$  for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{HO\cdot}(\text{aq.}) = (5.0 \pm 1.0) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  in aqueous solutions (Haag & Yao 1992)

$k_{OH} = 0.46 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982)

base rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  at 25°C with a calculated  $t_{1/2} > 900$  yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

first-order  $t_{1/2} > 879$  yr, based on rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation: significant degradation in an aerobic environment with rate constant  $k = 0.05 \text{ d}^{-1}$  (Tabak et al. 1981; Mills et al. 1982);

nearly 100% removed by an apparent combination of biodegradation and stripping in a continuous flow activated sludge system (Kincannon et al. 1983; selected, Howard 1989)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320$  h, estimated from unacclimated soil grab sample data;  $t_{1/2}(\text{aq. anaerobic}) = 2688\text{--}17280$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:  $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$  (estimated, Mabey et al. 1982).

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

## Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 200.6\text{--}2006$  h, based on photooxidation half-life in air (Howard et al. 1991).

Surface Water:  $t_{1/2} = 0.9\text{--}50$  d, various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

$t_{1/2} = 672\text{--}4320$  h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

measured rate constant  $k = (0.57 \pm 0.05) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 22°C, with  $t_{1/2} = 16$  h at pH 7 (Yao & Haag 1991)

direct photolysis  $t_{1/2} = 92.3$  min in aqueous solution (Peijnenburg et al. 1992).

Groundwater:  $t_{1/2} = 1$  yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 1334\text{--}8640$  h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil:  $t_{1/2} = 672\text{--}4320$  h, based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota:  $t_{1/2} < 1$  d in bluegill sunfish (Veith et al. 1980; Barrows et al. 1980)

$t_{1/2} < 5$  d in worm at 8°C (Oliver 1987a);

biological half-lives,  $t_{1/2} < 1$  d in trout muscle,  $t_{1/2} < 1$  d in sunfish, and  $t_{1/2} < 1$  d in guppy for dichlorobenzenes (Niimi 1987).

**TABLE 6.1.1.3.1**

**Reported aqueous solubilities of 1,3-dichlorobenzene at various temperatures**

1.

Klemenc & Löw 1930		Vesala 1973		Schwarz & Miller 1980		Horvath & Getzen 1985	
volumetric method		shake flask-UV spec.		elution chromatography		recommended values	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	111	10	97.63	10	116	10	103
25	123	15.2	97.76	20	89	15	99.9
30	140	19.6	98.32	30	139	20	101
35	150	25.1	101.26	shake flask-UV		25	106
40	167	30.0	112.74	10	120	30	114
45	177	35.0	121.13	20	113	35	125
55	196			30	132	40	137
60	201			average		45	151
				10	118	50	165
				20	101	55	179
				30	135	60	192

2.

Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC		RP-HPLC- $k'$ correlation	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
5	114	5	71
15	108	15	104
25	126	25	132
35	134	35	166
45	141		

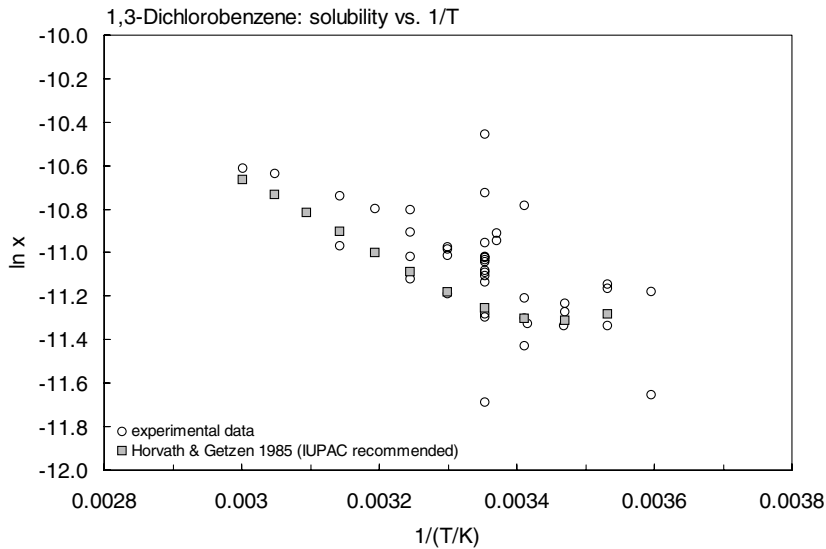


FIGURE 6.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.2  
Reported vapor pressures of 1,3-dichlorobenzene 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)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_o) = (1 - T/T_o) \cdot \exp [\sum A_i T^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		Poledniecek et al. 1996		Roháč et al. 1998	
summary of literature data		ebulliometry		static method-pressure gauge		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.1	133.3	90.72	7605	-23.55	5.459	84.353	5731
39	666.6	98.05	10114	-19.57	7.987	93.65	8343
52.9	1333	111.49	16500	-19.57	7.973	97.99	11076
66.2	2666	140.49	42060	-9.7	19.355	107.17	13922
82	5333	157.37	67660	0.3	44.17	112.433	16799
92.2	7999	173.0	101325	10.34	94.451	117.892	20292
105	13332			10.35	9.459	117.893	20291
125.9	26664	mp/°C	-24.76	20.39	190.4	123.625	24569
149	53329	bp/°C	173.0	30.28	360.02	129.141	29396
173	101325			40.26	652.82	134.535	34819
		eq. 2	P/mmHg	50.15	1122.2	139.715	40761
mp/°C	-24.2	A	7.30364	50.16	1125.0	144.993	47623
		B	1782.4	60.18	1872.9	144.993	47623
		C	230	60.18	1875.7	153.301	60276
				70.03	2980.9	161.253	74765
				70.03	2978.4	169.859	93403
				80.0	4661.7	172.047	98670

(Continued)

TABLE 6.1.1.3.2 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Poledniecek et al. 1996		Roháč et al. 1998	
summary of literature data		ebulliometry		static method-pressure gauge		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				89.94	7042.6	174.92	105933
				89.94	7049.0	175.207	106716
				98.86	10180		
				108.83	14713	bp/°C	173.095
				118.87	20859		
				128.93	28986	eq. 3	P/kPa
				138.94	39411	A	6.16151
				149.05	52842	B	1595.19
				159.06	69604	C	−62.398
				eq. 3a	P/Pa		
				A	21.6433		
				B	4031.27		
				C	−47.5846		

2.

Roháč et al. 1999	
recommended	
T/K	P/Pa
253.15	7.70
263.15	18.9
273.15	43.1
283.15	92.0
283.15	185.0
303.15	352.9
313.15	641.6
232.15	1117
333.15	1871
343.25	3016
353.15	4737
363.15	7205
373.15	10670
383.15	15420
393.15	21810
403.15	30210
413.15	41080
423.15	54920
433.15	72270
443.15	93730
453.15	12000
Cox eq.	
eq. 5	P/Pa
A <sub>0</sub>	3.366439
10 <sup>−4</sup> A <sub>1</sub>	−8.3811530

TABLE 6.1.1.3.2 (Continued)

Roháč et al. 1999	
recommended	
T/K	P/Pa
$10^{-7}A_2$	5.9337577
$T_o/K$	248.39
$P_o/Pa$	4.85
bp/K	446.25
temp range 250–448 K	

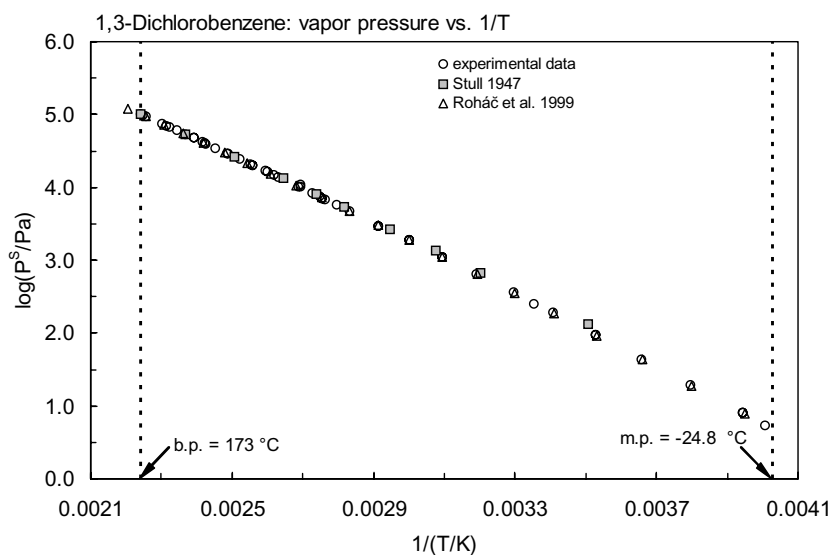
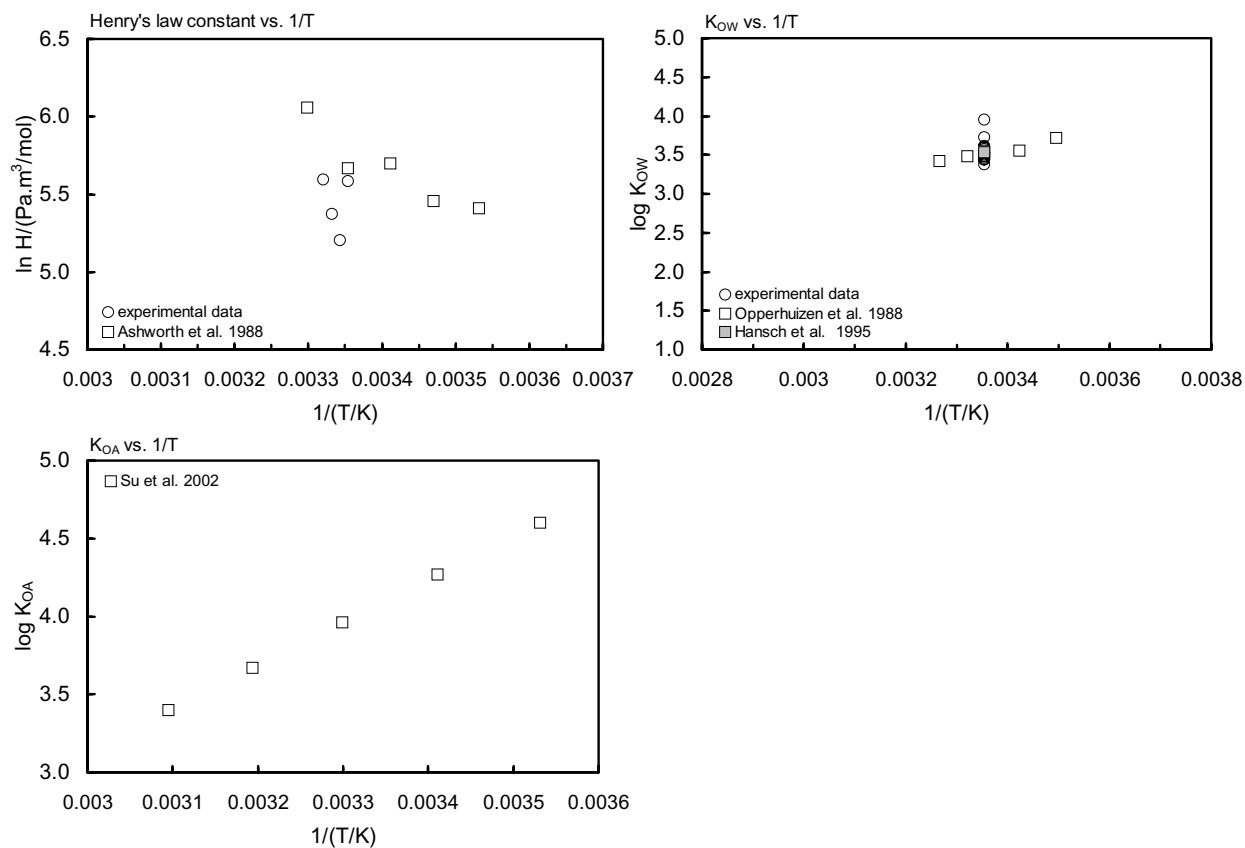


FIGURE 6.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.3

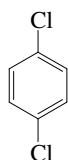
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,3-dichlorobenzene at various temperatures and temperature dependence equations

Henry's law constant		log K <sub>OW</sub>		log K <sub>OA</sub>	
Ashworth et al. 1988		Opperhuizen et al. 1988		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
10	224	13	3.72	10	4.6
15	234	19	3.55	20	4.27
20	298	28	3.48	30	3.96
20	289	33	3.42	40	3.67
30	428			50	3.4
ΔH/(kJ mol <sup>-1</sup> ) = -15.0 .				ΔH <sub>OA</sub> /(kJ mol <sup>-1</sup> ) = 57.02	
ln H = A - B/(T/K)					
	H/(atm m <sup>3</sup> /mol)				
A	-2.882	log K <sub>OA</sub> = A + B/2.303RT			
B	2564	A			
		B			



**FIGURE 6.1.1.3.3** Logarithm of Henry's law constant,  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for 1,3-dichlorobenzene.

## 6.1.1.4 1,4-Dichlorobenzene



Common Name: 1,4-Dichlorobenzene

Synonym: *p*-dichlorobenzene, paradichlorobenzene

Chemical Name: 1,4-dichlorobenzene

CAS Registry No: 106-46-7

Molecular Formula:  $C_6H_4Cl_2$

Molecular Weight: 147.002

Melting Point ( $^{\circ}C$ ):

53.09 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

174 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.2457 (Dreisbach 1955; Weast 1972–73; Horvath 1982)

Molar Volume ( $cm^3/mol$ ):

118.0 ( $20^{\circ}C$ , calculated-density)

137.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

18.72 (Dreisbach 1955)

17.882 (Weast 1972–73)

18.16, 18.70 (Wauchope & Getzen 1972)

18.20 (Tsonopoulos & Prausnitz 1971; Dean 1985)

19.0 (Miller et al. 1984)

17.153 (Ruelle et al. 1993)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

56.484 (Pirsch 1956)

55.65 (Tsonopoulos & Prausnitz 1971)

54.81 (Weast 1976–77; Amidon & Williams 1982; Yalkowsky 1979)

56.07 (Yalkowsky & Valvani 1980)

58.16 (Miller et al. 1984)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ),  $F$ : 0.53 (mp at  $53.09^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

79.1\* (volumetric method, measured range  $20$ – $60^{\circ}C$ , Klemenc & Löw 1930)

77 ( $30^{\circ}C$ , shake flask-interferometer, Gross & Saylor 1930)

< 500 (residue-volume method, Booth & Everson 1948)

76 (shake flask-UV, Andrew & Keefer 1950)

89.8 (Landolt-Börnstein 1951)

83.4\* ( $24.6^{\circ}C$ , shake flask-UV, measured  $22.2$ – $73.4^{\circ}C$ , Wauchope & Getzen 1972)

85.5 (shake flask-UV, Vesala 1974)

56.9 ( $20^{\circ}C$ , shake flask-GC/ECD, Chiou & Freed 1977)

34 (shake flask-GC, Jones et al. 1977/1978)

87.2 (shake flask-GC, Aqun-Yuen et al. 1979)

90.6 (shake flask-UV, Yalkowsky et al. 1979)

73.7 (shake flask-LSC, Veith et al. 1980)

73.8 (shake flask-LSC, Banerjee et al. 1980)

48.7 (shake flask-GC, Könnemann 1981)

73, 137 (shake flask-GC, solid, supercooled liquid, Chiou et al. 1982)

90.0	(recommended, Horvath 1982)
25	(calculated-UNIFAC activity coefficients, Arbuckle 1983)
175	(calculated-HPLC- $k'$ , converted from reported $\gamma_w$ , Hafkenscheid & Tomlinson 1983a)
154	(30°C, shake flask-GC, McNally & Grob 1983)
30.9	(generator column-GC, Miller et al. 1984, 1985)
65.3	(shake flask-HPLC, Banerjee 1984)
158	(30°C, shake flask-GC, McNally & Grob 1984)
82.9*	(recommended, temp range 10–75°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)
$S/(g/kg) = 13.974 - 8.5829 \times 10^{-2} \cdot (T/K) + 1.3365 \times 10^{-4} \cdot (T/K)^2$ ; temp range 328–348 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)	
100	(Dean 1985)
141	(20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
81.4* $\pm$ 1.5	(shake flask-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
42.0	(shake flask-GC, Boyd et al. 1998)
$\ln x = -4.178 - 2186.7/(T/K)$ ; 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):

1333*	(54.8°C, summary of literature data, temp range 54.8–173.9°C, Stull 1947)
$\log (P/\text{mmHg}) = 7.30697 - 1788.7/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)	
7605*	(92.0°C, ebulliometry, measured range 92.0–174.12°C, Dreisbach & Shrader 1949)
235	(calculated by formula., Dreisbach 1955; quoted, Hine & Mookerjee 1975; Riddick et al. 1986; Howard 1989)
$\log (P/\text{mmHg}) = 6.89797 - 1507.3/(201.0 + t/^\circ\text{C})$ ; temp range 75–240°C (Antoine eq. for liquid state, Dreisbach 1955)	
8514*	(94.8°C, ebulliometry, measured range 94.8–174.04°C, McDonald et al. 1959)
93.33*	(20.4°C, $\alpha$ - <i>p</i> -dichlorobenzene, manometry, measured range 20.4–39.6°C, Walsh & Smith 1961)
402.6*	(37.9°C, $\beta$ - <i>p</i> -dichlorobenzene, manometry, measured range 37.9–52.5°C, Walsh & Smith 1961)
90.2	(solid vapor pressure, extrapolated, Antoine eq., Weast 1972–73)
$\log (P/\text{mmHg}) = [-0.2185 \times 17260.5/(T/K)] + 12.4800$ ; temp range 30–50°C, (Antoine eq., Weast 1972–73)	
$\log (P/\text{mmHg}) = [-0.2185 \times 10611.0/(T/K)] + 8.073632$ ; temp range 54.8–173.9°C (Antoine eq., Weast 1972–73)	
137.2*	(diaphragm pressure gauge, measured range: 0–20°C, De Kruif et al. 1981)
128	(extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 5.94201 - 1668.355/(186.212 + t/^\circ\text{C})$ ; temp range 164.7–237.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)	
158*	(gas saturation-GC, measured range 20–100°C, Rordorf 1985)
243	(extrapolated-Antoine eq., Dean 1985)
$\log (P/\text{mmHg}) = 7.0208 - 1590.9/(210.2 + t/^\circ\text{C})$ , temp range 95–174°C (Antoine eq., Dean 1985, 1992)	
86.7	(20°C, gas saturation, Chiou & Shoup 1985)
134	(interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_s/\text{kPa}) = 10.472 - 3382.9/(T/K)$ ; temp range 293–313 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)	
$\log (P_s/\text{kPa}) = 10.181 - 3290.4/(T/K)$ ; temp range 310–336 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)	
$\log (P_L/\text{kPa}) = 6.12695 - 1578.51/(-64.22 + T/K)$ ; temp range 341–448 K (liquid, Antoine eq., Stephenson & Malanowski 1987)	
133*	(gas saturation-GC, measured range –15 to 40°C, Liu & Dickhut 1994)
216; 257	(supercooled liquid $P_L$ , GC-Kovács retention indices correlation; quoted lit., Spieksma et al. 1994)
$\log (P/\text{mmHg}) = 36.2276 - 3.6756 \times 10^3/(T/K) - 9.6308 \cdot \log (T/K) - 1.3372 \times 10^{-9} \cdot (T/K) + 1.9905 \times 10^{-6} \cdot (T/K)^2$ ; temp range 326–685 K (vapor pressure eq., Yaw et al. 1994)	
135*	(25°C; pressure gauge measurement; interpolated from reported Antoine eq., Poledniecek et al. 1996)
$\ln (P_s/\text{Pa}) = 28.4986 - 6272.86/[(T/K) - 32.2741]$ ; temp range 273–323 K (Antoine eq. from exptl data, pressure gauge measurement, solid, Poledniecek et al. 1996)	
$\ln (P_L/\text{Pa}) = 21.0472 - 3665.96/[(T/K) - 62.3849]$ ; temp range 333–442 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Poledniecek et al. 1996)	



- 5729\* (85.139°C, comparative ebulliometry, measured range 85.139–175.626°C, Roháč et al. 1998)  
 87.0\* (20°C, recommended, summary of literature data, temp range 273.15–453.15 K, Roháč et al. 1999)  
 $\ln [(P_s/P_a)/1280] = [1 - (T/K)/326.3] \cdot \exp\{3.251427 - 2.853921 \times 10^{-4} \cdot (T/K)\}$ ; temp range 273–323 K (Cox eq. solid, recommended, Roháč et al. 1999)  
 $\ln [(P_L/P_a)/1280] = [1 - (T/K)/326.3] \cdot \exp\{3.100023 - 1.0557743 \times 10^{-3} \cdot (T/K) + 7.816354 \times 10^{-7} (T/K)^2\}$ ; temp range 328–449 K (Cox eq., liquid, recommended, Roháč et al. 1999)  
 $\log (P/P_a) = 11.63209 - 2829.32/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m<sup>3</sup>/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.):

- 330 (equilibrium cell-GC, concentration ratio, Leighton & Calo 1981)  
 240 (gas stripping-GC, Mackay & Shiu 1981)  
 152 (20°C, gas stripping-GC, Oliver 1985)  
 276 (gas stripping-GC, Warner et al. 1987)  
 321\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 3.373 - 2720/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 438 (computer value, Yaws et al. 1991)  
 244 (gas stripping-GC, Shiu & Mackay 1997)  
 188 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 275 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 2.649 - 1054/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

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

- 3.39 (shake flask, Leo et al. 1971; Hansch & Leo 1979)  
 3.57, 3.55 (calculated-fragment constants, Rekker 1977)  
 3.38 (Hansch & Leo 1979)  
 3.62, 3.39 (shake flask-GC, HPLC-k' correlation, Könnemann et al. 1979)  
 3.37, 3.78 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)  
 3.37 (shake flask-LSC, Banerjee et al. 1980)  
 3.46 (HPLC-k' correlation, Hammers et al. 1982)  
 3.52 (shake flask-GC, Watarai et al. 1982)  
 3.43 (HPLC-k' correlation, Miyake & Terada 1982)  
 3.67, 3.90 (calculated-UNIFAC activity coefficients, Arbuckle 1983)  
 3.37 (generator column-HPLC/UV, Wasik et al. 1983)  
 3.38 (generator column-GC/ECD, Miller et al. 1984; 1985)  
 3.37 (HPLC-RV correlation, Garst 1984; Garst & Wilson 1984)  
 3.52 (Hansch & Leo 1985)  
 3.444 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 3.85–4.30, 4.0 (range, average: round robin work, shake flask or HPLC-k' correlation, Kishi & Hashimoto 1989)  
 3.355 ± 0.053, 3.444 ± 0.001 (shake flask methods, interlaboratory studies, Brooke et al. 1990)  
 3.45 (recommended, Sangster 1993)  
 3.44 (recommended, Hansch et al. 1995)  
 3.23\* ± 0.03 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)  
 $\log K_{OW} = 0.2338 + 17100/[2.303 \cdot R(T/K)]$ ; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)  
 3.65 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

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:

- 4.46 (calculated- $S_{oct}$  and vapor pressure P, Abraham et al. 2001)  
 4.32\* (20°C, HPLC-k' correlation, measured range 10–50°C, Su et al. 2002)  
 $\log K_{OA} = 55590/(2.303 \cdot RT) - 5.556$ ; temp range 10–50°C (HPLC-k' correlation, Su et al. 2002)

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

- 2.33 (rainbow trout, Neely et al. 1974)
- 2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 1.78 (bluegill sunfish, Veith et al. 1979b, 1980)
- 1.78 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 3.26 (guppy, lipid basis, Könnemann & van Leeuwen 1980)
- 2.53–2.59 mean 2.57; 2.79–2.96 mean 2.86 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
- 3.64–3.96 (rainbow trout, lipid basis, Oliver & Niimi 1983)
- 3.40 (15°C, guppy, Banerjee et al. 1984)
- 2.83–2.86 (fish, Oliver 1984)
- 2.00, 1.70, 2.75 (algae, fish, activated sludge, Freitag et al. 1984)
- 2.0, 1.70, 2.75 (algae, fish, activated sludge, Freitag et al. 1985)
- 2.32–2.72 mean 2.71; 2.74–3.15 mean 2.95 (15°C, rainbow trout, wet wt., steady-state BCF on 7- to 96-d laboratory study in two tanks with different water concn, Oliver & Niimi 1985)
- 2.04 (fathead minnow, flowing water, Carlson & Kosian 1987)
- 5.3–5.6, 5.5 (Niagara River plume, range, mean; Oliver 1987b)
- 3.91, 4.53, 4.09, 3.51 (field data-lipid based: Atlantic creakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
- 3.25 (guppy, lipid weighted-based, 12 to 31 d exposure-GC, Gobas et al. 1989)
- 2.47, 3.56 (flagfish: whole fish, lipid, Smith et al. 1990)
- 1.7 ± 0.2 (guppy, steady-state conditions, rate const. ratio  $k_1/k_2$ , 96-h exposure, Sijm et al. 1993)
- 3.5 ± 0.1 (guppy, lipid normalized BCF, Sijm et al. 1993)
- 2.40 (fathead minnow, steady-state conditions, rate const. ratio  $k_1/k_2$ , 96-h exposure, Sijm et al. 1993)
- 3.60 (fathead minnow, lipid normalized BCF, Sijm et al. 1993)
- 1.78; 2.47; 2.57–2.95 (*Lepomis macrochirus*; *Jordanella floridae*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
- 1.70; 2.40 (*Poecilia reticulata*; *Pimephales promelas*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
- 2.57, 3.65; 2.517, 2.242 (quoted: whole fish, lipid content; calculated-MCI  $\chi$ ,  $K_{OW}$ , Lu et al. 1999)
- 3.70; 3.75 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log  $K_{OC}$ :

- 2.59 (Kenaga 1980a)
- 2.78–3.14 (organic carbon, Schwarzenbach & Westall 1981)
- 2.29 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 2.18–3.44 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 4.80; 5.00 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
- 2.82, 2.45 (Aprison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium Southworth & Keller 1986)
- 5.30–5.60; 5.50 (Niagara River plume: range; average value; Oliver 1987b)
- 2.92; 2.91 (Aldrich humic acid, equilibrium dialysis; Aldrich and Fluka humic acid, Flory-Huggins model, Chin & Weber 1989)
- 2.43 (organic polymers in Huron River water, Chin et al. 1990)
- 2.88 (HPLC- $k'$  correlation, Szabo et al. 1995)
- 2.60, 2.61 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 2.66, 2.57, 2.77 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
- 2.99–3.46 (three wetland soils, batch equilibrium-sorption isotherm-LSC, Lee et al. 2003)

Sorption Coefficient, log  $K_{OM}$ :

- 2.20 (Woodburn silt loam soil, organic matter 1.9%, equilibrium sorption isotherm, Chiou et al. 1983)

Environmental Fate Rate Constants,  $k$  or Half-Lives.  $t_{1/2}$ :

Volatilization:  $t_{1/2} = 4.3$  h from a model river of 1 m depth and with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982);

rate constants:  $k = 0.04$  d<sup>-1</sup>,  $t_{1/2} = 18$  d in spring at 8–16°C,  $k = 0.068$  d<sup>-1</sup>,  $t_{1/2} = 10$  d in summer at 20–22°C,  $k = 0.054$  d<sup>-1</sup>,  $t_{1/2} = 13$  d in winter at 3–7°C for the periods when volatilization appears to dominate, and  $k = 0.066$  d<sup>-1</sup>,  $t_{1/2} = 10.6$  d with HgCl<sub>2</sub>, and  $k = 0.063$  d<sup>-1</sup>,  $t_{1/2} = 11$  d without HgCl<sub>2</sub> in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982)

Direct photolysis unimportant (Zepp & Cline 1977; Zepp 1978);

$t_{1/2} = 25$  d under sunlight in water (Mansour & Feicht 1994)

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with NO<sub>3</sub> radical and  $k_{O_3}$  with O<sub>3</sub> or as indicated, \*data at other temperatures see reference:

$k = 9.63 \times 10^{-3}$  h<sup>-1</sup> in air (Ware & West 1977; selected, Mackay et al. 1985)

$k_{OH} \sim 3.0 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360$  M<sup>-1</sup> h<sup>-1</sup> for singlet oxygen and  $k \ll 1$  M<sup>-1</sup> h<sup>-1</sup> for RO<sub>2</sub> radical (Mabey et al. 1982)

$k \ll 3$  M<sup>-1</sup> s<sup>-1</sup> for the reaction with ozone in water using 0.5 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (3.2 \pm 0.2) \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{OH}$  (obs.) =  $3.2 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>; and  $k_{OH}$  (calc) =  $4.9 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (Atkinson 1985)

$k_{OH}$  (calc) =  $0.41 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}$  (obs) =  $0.32 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (0.32 - .52) \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 295–300 K (literature review, Atkinson 1989)

$t_{1/2} = 200.6$ – $2006$  h based on vapor phase reaction with OH radicals (Howard et al. 1991)

$k = (5.0 - 5.3) \times 10^9$  M<sup>-1</sup> s<sup>-1</sup> for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{HO\cdot} = 4.0 \times 10^9$  M<sup>-1</sup> s<sup>-1</sup> in aqueous solutions (Haag & Yao 1992)

$k_{OH}$  (calc) =  $0.44 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> (molecular orbital calculations, Klamt 1993).

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant  $k < 0.9$  M<sup>-1</sup> h<sup>-1</sup> at 25°C with a calculated  $t_{1/2} > 900$  yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

first order  $t_{1/2} > 879$  yr, based on rate constant  $k < 0.9$  M<sup>-1</sup> h<sup>-1</sup> extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation:

$k = 1.09 \times 10^{-2}$  h<sup>-1</sup> degradation in water (Verschuereen 1977)

$t_{1/2}$  (aq. aerobic) = 672–4320 h, based on unacclimated aerobic screening test data (Canton et al. 1985) and aerobic soil grab sample data (Haider et al. 1981; Howard et al. 1991)

$k = 0.05$  d<sup>-1</sup>, significant degradation in aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2}$  (aq. anaerobic) = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:  $1 \times 10^{-10}$  mL cell<sup>-1</sup> h<sup>-1</sup> (estimated, Mabey et al. 1982).

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

$k_1 = 5.67$  h<sup>-1</sup>;  $k_2 = 0.0264$  h<sup>-1</sup> (trout muscle, Neely et al. 1974; Neely 1979)

$k_1 = 7.44$  h<sup>-1</sup> (10°C, yellow perch, Neely et al. 1974; Neely 1979)

$k_1 = 17.0$  h<sup>-1</sup> (25°C, yellow perch, Neely et al. 1974; Neely 1979)

$kk_1 = 1800$  d<sup>-1</sup>;  $k_2 = 1.00$  d<sup>-1</sup> (guppy, Könemann & van Leeuwen 1980)

$k_1 = 4.1$  h<sup>-1</sup>;  $1/k_2 = 24$  h (guppy, quoted from Könemann & van Leeuwen 1980, Hawker & Connell 1985)

$k_1 = 5.7$  h<sup>-1</sup>;  $1/k_2 = 38$  h (rainbow trout, quoted from Neely et al. 1974, Hawker & Connell 1985)

$k_1 = 97$  d<sup>-1</sup> (fish, quoted, Opperhuizen 1986)

$\log k_2 = 0, -0.2$  d<sup>-1</sup> (fish, calculated- $K_{OW}$ , Thomann 1989)

$\log k_1 = 1.99$  d<sup>-1</sup>;  $\log k_2 = 0.0$  (guppy, 12–31 d exposure experiments, Gobas et al. 1989)

$\log k_1 = 1.99$  d<sup>-1</sup> (fish, quoted, Connell & Hawker 1988)

$k_1 = 291$  d<sup>-1</sup>, 4230 d<sup>-1</sup>;  $k_2 = 0.98$  d<sup>-1</sup>, 1.18 d<sup>-1</sup> (American flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 0.98 \text{ d}^{-1}$ ,  $1.46 \text{ d}^{-1}$  (American flagfish: bioconcentration exptl., toxicity data, Smith et al. 1990)

$k_1 = 760 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 4.80 \text{ d}^{-1}$  (guppy, 96-h exposure, Sijm et al. 1993)

$k_1 = 600 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 2.50 \text{ d}^{-1}$  (fathead minnow, 96-h exposure, Sijm et al. 1993)

#### Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 200.6\text{--}2006 \text{ h}$ , based on photooxidation half-life in air (Howard et al. 1991)

#### Surface Water:

$t_{1/2} = 1.1\text{--}26 \text{ d}$ , various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980);

half-lives from marine mesocosm:  $t_{1/2} = 18 \text{ d}$  in the spring at  $8\text{--}16^\circ\text{C}$ ,  $t_{1/2} = 10 \text{ d}$  in the summer at  $20\text{--}22^\circ\text{C}$  and  $t_{1/2} = 31 \text{ d}$  in the winter at  $3\text{--}7^\circ\text{C}$  when volatilization dominates, and  $t_{1/2} = 10.6 \text{ d}$  and  $11 \text{ d}$  for experiments with and without  $\text{HgCl}_2$ , respectively, in September 9–15 (Wakeham et al. 1983);

hydrolysis  $t_{1/2} > 900 \text{ yr}$  at pH 7 and  $25^\circ\text{C}$  (Ellington et al. 1988)

$t_{1/2}(\text{aerobic}) = 672\text{--}4320 \text{ h}$ , based on unacclimated aerobic screening test data and aerobic soil grab sample data;  $t_{1/2}(\text{anaerobic}) = 2688\text{--}17280 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

photolysis  $t_{1/2} = 25 \text{ d}$  under sunlight in water (Mansour & Feicht 1994).

Groundwater:  $t_{1/2} \sim 1 \text{ yr}$  estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 1344\text{--}8640 \text{ h}$ , based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

#### Sediment:

Soil:  $t_{1/2} = 672\text{--}4320 \text{ h}$ , based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota:  $t_{1/2} < 1 \text{ d}$  in fish tissues (Veith et al. 1980);

$t_{1/2} < 1 \text{ d}$  in bluegill sunfish (Barrows et al. 1980);

$t_{1/2} = 16 \text{ h}$ , clearance from fish (Neely 1980);

$t_{1/2} < 5 \text{ d}$  in worms at  $8^\circ\text{C}$  (Oliver 1987a);

biological half-lives,  $t_{1/2} < 1 \text{ d}$  in trout muscle,  $t_{1/2} < 1 \text{ d}$  in sunfish and  $t_{1/2} < 1 \text{ d}$  in guppy for dichlorobenzenes (Niimi 1987);

depuration  $t_{1/2} = 0.70 \text{ d}$  for whole fish,  $t_{1/2} = 0.59 \text{ d}$  for fish lipid (American flagfish, Smith et al. 1990).

TABLE 6.1.1.4.1  
Reported aqueous solubilities of 1,4-dichlorobenzene at various temperatures

Klemenc & Löw 1930		Wauchope & Getzen 1972		Horvath & Getzen 1985		Shiu et al. 1997	
volumetric method		shake flask-UV		recommended values		shake flask-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
		liquid		liquid			
20	68.1	22.2	77.8	10	51.2	5	48.6
20	79.1	24.6	83.4	15	60.5	15	63.0
30	93.3	25.5	86.9	20	71.0	25	81.4
35	104	30.0	92.6	25	82.9	35	104.5
35	83	34.5	102	30	96.3	45	130
40	101	38.4	121	35	111.3		
45	122	47.5	169	40	128		
55	156	50.1	173	45	147		
60	163	solid		30	167		
		59.2	210	55	190		
		60.7	218	solid			
		65.1	230	55	201		
		65.2	237	60	214		
		73.4	281	65	233		
				70	259		
				75	292		

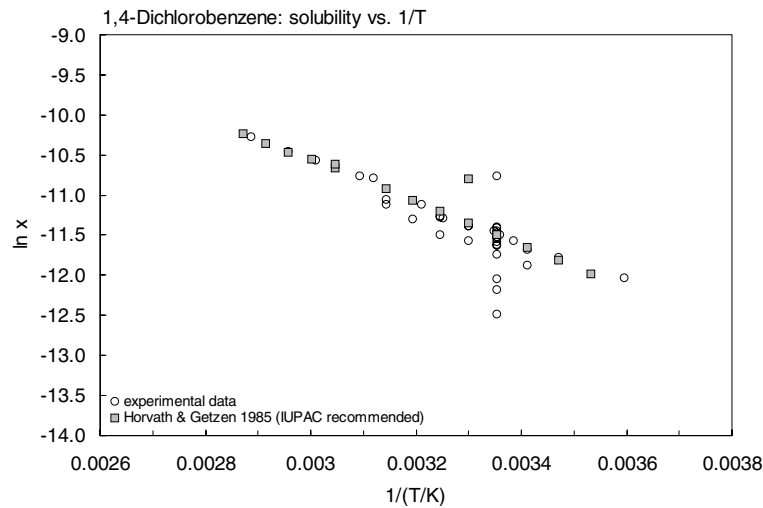


FIGURE 6.1.1.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,4-dichlorobenzene.

TABLE 6.1.1.4.2

Reported vapor pressures of 1,4-dichlorobenzene 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)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_0) = (1 - T/T_0) \cdot \exp[\Sigma A_i T^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959		Walsh & Smith 1961	
summary of lit. data		ebulliometry		ebulliometry		manometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
54.8	1333	92.0	7605	94.8	8514	$\alpha$ -p-dichlorobenzene	
69.2	2666	99.41	10114	98.55	9844	20.4	93.33
84.8	5333	112.66	16500	104.81	12444	23.9	121.32
95.2	7999	141.65	42066	116.28	18808	26.8	156.0
108.4	13332	158.52	67660	143.52	44465	29.8	202.65
128.3	26664	174.12	101325	159.79	70117	33.2	269.3
150.2	53329			171.87	95945	33.7	277.3
173.9	101325			174.04	101325	35.0	312.0
						36.4	317.3
						37.3	350.6
mp/ $^{\circ}\text{C}$	53.0			mp/ $^{\circ}\text{C}$	52.90	37.5	382.6
						39.2	440.0
				eq. 2	P/mmHg	39.6	454.6
				A	6.99800		
				B	1575.11	mp/ $^{\circ}\text{C}$	53.23
				C	208.513		
						eq. 1	P/mmHg
						A	11.347
						B	3382.9
						$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 64.79$	

2.

Walsh & Smith 1961		de Kruif et al. 1981		Rordorf 1985		Liu & Dickhut 1994	
manometry		static manometry		gas saturation		gas saturation-GC	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
$\beta$ -p-dichlorobenzene							
37.9	402.6	1.47	14.14	25	158.1*	-14.5	4.67
39.8	469.3	3.94	18.32	50	1217.6*	-5.0	16.0
40.2	477.3	6.45	23.67	75	6992.7	10	31.7
40.5	490.6	8.43	28.88	100	31774	25	133
40.8	501.3	10.33	34.83	125	119380	40	452
41.1	508.0	12.35	42.44	150	383592		
41.3	522.6	14.3	51.13				
41.7	534.6	16.63	63.79				
42.4	568.0	19.84	85.98		*solid		
42.6	584.0			eq. 1	P/Pa	$\Delta H_v/(\text{kJ mol}^{-1}) = 35.0$	
42.9	593.3			A	13.384		
43.2	597.3	eq. 1	P/Pa	B	3450		

TABLE 6.1.1.4.2 (Continued)

Walsh & Smith 1961		de Kruif et al. 1981		Rordorf 1985		Liu & Dickhut 1994	
manometry		static manometry		gas saturation		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.7	629.3	A	13.6459				
44.1	640.0	B	3431.3		liquid		
45.8	727.9			eq. 1	P/Pa		
46.4	766.6			A	10.472		
48.0	859.3	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 65.7$		B	3382.9		
49.4	955.9	11°C					
51.3	955.9			$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 65.40$			
51.7	1135			30–50°C			
52.5	1192						
eq. 1	P/mmHg						
A	11.056						
B	3290.4						
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 63.01$							
3.							
Polednicek et al. 1996				Roháč et al. 1998		Roháč et al. 1999	
pressure gauge				comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
	solid		liquid				
0.34	12.2	60.12	1838.2	85.139	5729	273.15	12.2
0.35	11.98	60.15	1839.6	94.305	8334	283.15	33.8
10.35	34.25	70.03	2948.1	101.656	11074	283.15	87.0
10.35	34.21	80.03	4629.1	107.836	13921	303.15	209.3
20.35	88.75	80.04	4627.7	113.103	16800	313.15	474.2
20.35	88.61	89.99	7038.6	118.564	20290	232.15	1017
30.31	214.6	90.0	7041.4	118.568	20292	333.15	1817
40.25	485.5	98.72	9904.2	124.29	24570	343.25	2941
50.15	1037	108.68	1434.2	129.822	29388	353.15	4611
25	135.0	118.73	20385	135.223	34809	363.15	7020
	interpolated	128.78	28351	140.416	40752	373.15	10410
		138.8	38541	145.702	47615	383.15	15060
for solid:		148.28	51728	154.032	60269	393.15	21310
eq. 3a	P/Pa	158.9	68186	154.033	60271	403.15	29550
A	28.4986	168.93	88642	162.009	74759	413.15	40220
B	6272.86			170.622	93393	423.15	53800
C	–32.2741			172.86	98793	433.15	70850
		for liquid:		175.626	105783	443.15	91950
		eq. 3a	P/Pa			453.15	11780
		A	21.0472	bp/°C	173.864		
		B	3665.96			Cox eq.	for solid
		C	–62.3849	eq. 3	P/kPa	eq. 5	$P_s/\text{Pa}$
				A	6.13050	$A_0$	3.251427
				B	1575.69	$10^{-4}A_1$	–2.8153921
				C	–65.007	$A_2$	0
						temp range 273–323 K	

(Continued)

TABLE 6.1.1.4.2 (Continued)

Poledniecek et al. 1996				Roháč et al. 1998		Roháč et al. 1999	
pressure gauge				comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						eq. 5	P <sub>L</sub> /Pa
						A <sub>0</sub>	3.100023
						10 <sup>-3</sup> A <sub>1</sub>	-1.0557743
						10 <sup>-7</sup> A <sub>2</sub>	7.8161354
						T <sub>0</sub> /K	326.3
						P <sub>0</sub> /Pa	1280.0
						bp/K	447.01
						temp range 328–449 K	

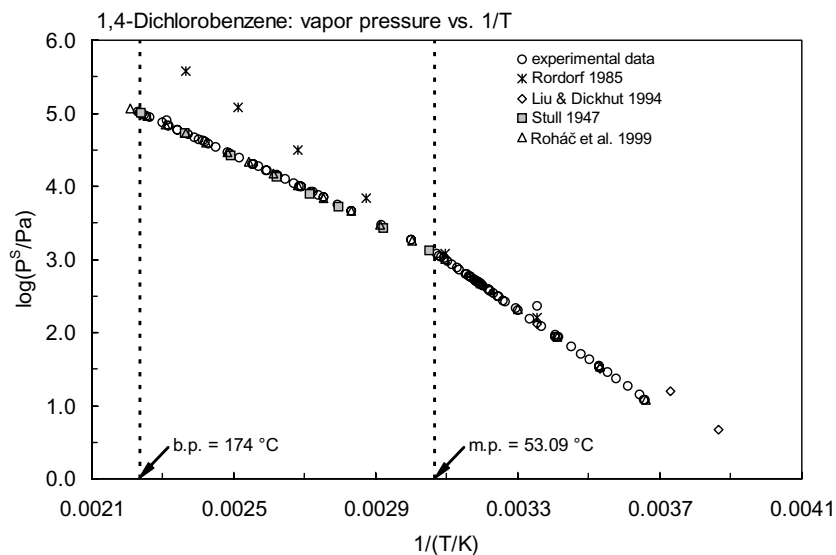


FIGURE 6.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for 1,4-dichlorobenzene.

TABLE 6.1.1.4.3  
Reported Henry’s law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,4-dichlorobenzene at various temperatures

Henry’s law constant		log K <sub>OW</sub>		log K <sub>OA</sub>	
Ashworth et al. 1988		Bahadur et al. 1997		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
10	215	5	3.42	10	4.65
15	220	15	3.35	20	4.32
20	262	25	3.23	30	4.01
20	321	35	3.12	40	3.72
30	394	45	3.03	50	3.45



TABLE 6.1.1.4.3 (Continued)

Henry's law constant		log K <sub>OW</sub>		log K <sub>OA</sub>	
Ashworth et al. 1988		Bahadur et al. 1997		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
ln H = A – B/(T/K)		enthalpy of transfer ΔH/(kJ mol <sup>-1</sup> ) = –17.1		ΔH <sub>OA</sub> /(kJ mol <sup>-1</sup> ) = 55.59	
	H/(atm m <sup>3</sup> /mol)				
A	3.373	log K <sub>OW</sub> = A – ΔH/2.303RT		log K <sub>OA</sub> = A + B/2.303RT	
B	2720	A	0.2338	A	–5.556
		ΔH	–17100	B	55590

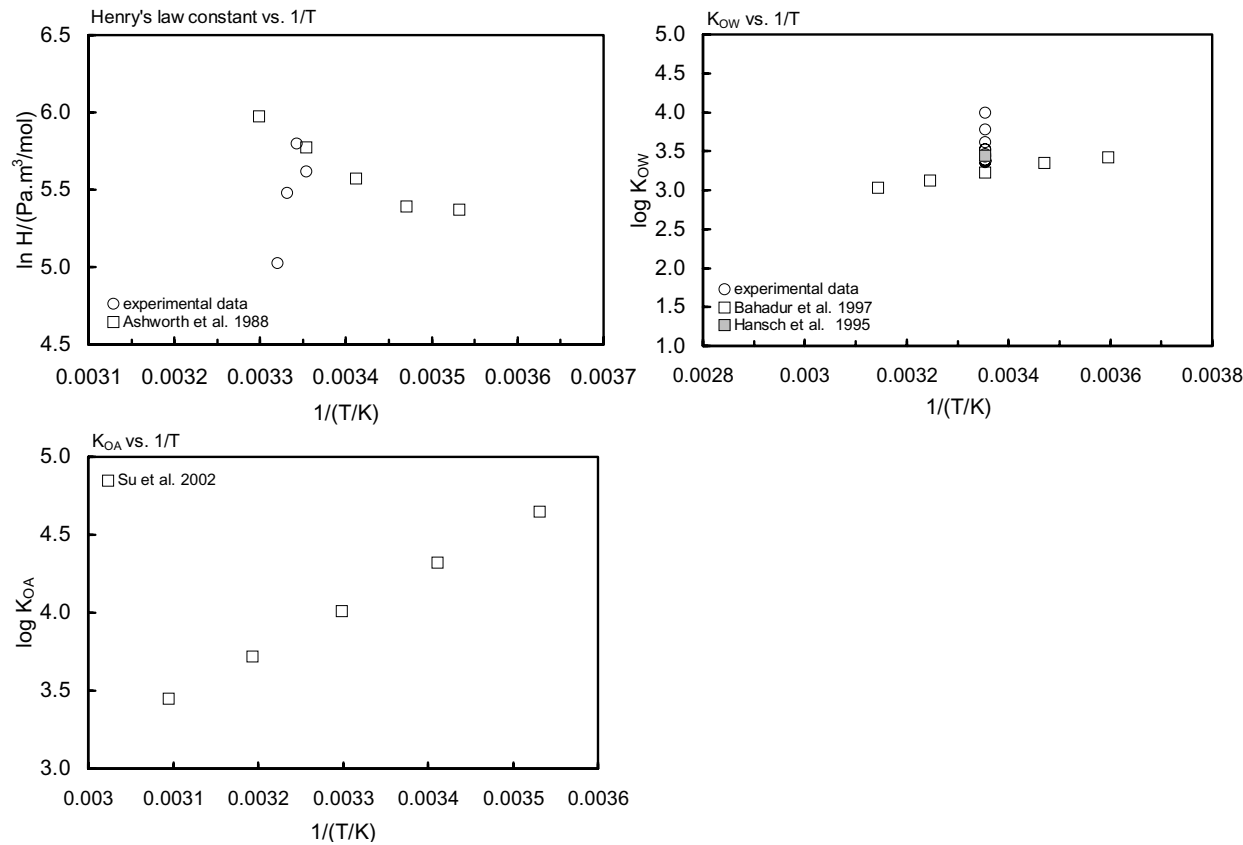
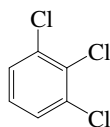


FIGURE 6.1.1.4.3 Logarithm of Henry's law constant,  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for 1,4-dichlorobenzene.

## 6.1.1.5 1,2,3-Trichlorobenzene



Common Name: 1,2,3-Trichlorobenzene

Synonym: vic-trichlorobenzene

Chemical Name: 1,2,3-trichlorobenzene

CAS Registry No: 81-61-6

Molecular Formula:  $C_6H_3Cl_3$

Molecular Weight: 181.447

Melting Point ( $^{\circ}C$ ):

51.3 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

218.5 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.4533 ( $40^{\circ}C$ , Weast 1972–73; Horvath 1982)

1.4533 ( $25^{\circ}C$ , Lide 2003)

1.69 (Dean 1985, 1992)

Molar Volume ( $cm^3/mol$ ):

124.9 ( $25^{\circ}C$ , calculated-density)

158.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

17.364 (Tsonopoulos & Prausnitz 1971)

17.99 (Miller et al. 1984)

17.153 (Ruelle et al. 1993)

20.50 (Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

53.14 (Tsonopoulos & Prausnitz 1971)

56.90 (Miller et al. 1984)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.552 (mp at  $51.3^{\circ}C$ )

0.53 ( $25^{\circ}C$ , mp at  $53^{\circ}C$ , Suntio et al. 1988b)

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

25.1 (Tsonopoulos & Prausnitz 1971)

31.5 (shake flask-UV, Yalkowsky et al. 1979, 1983)

16.6 (shake flask-GC, Mackay & Shiu 1981)

12.0 (shake flask-GC, Könemann 1981)

31.6 (recommended, Horvath 1982)

12.27 (generator column-GC/ECD, Miller et al. 1984, 1985)

18.0 (shake flask-HPLC, Banerjee 1984)

16.3 ( $23^{\circ}C$ , shake flask-GC, Chiou 1985)

18.0 (shake flask-GC, Chiou et al. 1986; Chiou et al. 1991)

$19.3^* \pm 0.24$ ;  $23.7 \pm 1.3$  (generator column-GC/ECD; shake flask-GC/ECD, measured range  $5$ – $45^{\circ}C$ , Shiu et al. 1997)

13.0 (shake flask-GC, Boyd et al. 1998)

$\ln x = -1.773 - 3418.9/(T/K)$ , temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

19.71, 14.8, 21.04, 40.25 (5, 15, 25,  $35^{\circ}C$ , estimated- RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

133.3\* ( $40^{\circ}C$ , summary of literature data, Stull 1947)

- 52.4 (extrapolated-Antoine eq., supercooled liquid  $P_L$ , Weast 1972–73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 11349.5/(T/K)] + 7.91649$ ; temp range 40–218.5°C (Antoine eq., Weast 1972–73)  
 28.0 (selected-converted from reported  $P_L$ , with fugacity ratio, Mackay & Shiu 1981)  
 25.1 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)  
 17.7 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_S/\text{kPa}) = 9.787 - 3440/(T/K)$ ; temp range 289–303 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.23008 - 2624.09/(10.506 + T/K)$ ; temp range 343–492 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)  
 11.20\* (gas saturation-GC, measured range –15 to 40°C, Liu & Dickhut 1994)  
 8.82\* (20.35°C, static method-pressure gauge measurement; Antoine eq., measured range 0.36–169°C, Polednicek et al. 1996)  
 $\ln (P_S/\text{Pa}) = 33.2977 - 9327.37/[(T/K) + 6.13445]$ ; temp range 272–3 (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)  
 $\ln (P_L/\text{Pa}) = 21.1681 - 4077.21/[(T/K) - 71.6539]$ ; temp range 334–2 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)  
 44.1 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; Spijksma et al. 1994)  
 8.50\* (20°C, recommended, summary of literature data, temp range 233.15–503.15 K, Roháč et al. 1999)  
 $\ln [(P_S/\text{Pa})/173.0] = [1 - (T/K)/325.6] \cdot \exp\{3.380608 - 2.5802866 \times 10^{-4} \cdot (T/K)\}$ ; temp range 273–323 K (Cox eq., solid, recommended, Roháč et al. 1999)  
 $\ln [(P_L/\text{Pa})/173.0] = [1 - (T/K)/325.6] \cdot \exp\{3.274398 - 1.0923018 \times 10^{-3} \cdot (T/K) + 7.8603029 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range 333–448 K (Cox eq., liquid, recommended, Roháč et al. 1999)  
 $\log (P/\text{kPa}) = 9.787 - 3440/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

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

- 127 (gas stripping-GC, Mackay & Shiu 1981)  
 90.0 (gas stripping-GC, Oliver 1985)  
 72.0 (20°C, gas stripping-GC, ten Hulscher et al. 1992)  
 147 (equilibrium air stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section:

- 4.27 (Leo et al. 1971; Hansch & Leo 1979)  
 4.11, 3.99 (shake flask-GC, HPLC- $k'$  correlation, Könemann et al. 1979)  
 4.02 (HPLC- $k'$  correlation, McDuffie 1981)  
 3.97 (shake flask-GC, Watarai et al. 1982)  
 3.96 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 4.04 (generator column-GC, Miller et al. 1984, 1985)  
 4.14 (shake flask-GC, Chiou 1985)  
 4.14 (shake flask-GC, Pereira et al. 1988)  
 4.139 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 4.05 (recommended, Sangster 1993)  
 4.14 (recommended, Hansch et al. 1995)  
 3.81\* (estimated- RP-HPLC- $k'$  correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

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:

- 5.19\*, 5.11 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)  
 6.491, 6.073, 5.699, 5.385 (–10, 0, 9.88, 19.85°C, generator column-GC, Harner & Mackay 1995)  
 $\log K_{OA} = -4.6 + 20 - 8.7/(T/K)$ ;  $\Delta H_{OA} = 55.7 \text{ kJ/mol}$  (Harner & Mackay 1995)  
 5.19 (calculated- $S_{oct}$  and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor,  $\log \text{BCF}$ :

- 4.11 (guppy, lipid basis, Könemann & van Leeuwen 1980)  
 3.00–3.20 mean 3.08; 3.34–3.52 mean 3.41 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

- 4.15–4.47 (rainbow trout, lipid basis, Oliver & Niimi 1983)  
 3.08–3.42 (fish, Oliver 1984)  
 4.35 (rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Geyer et al. 1985)  
 4.11 (guppy, 5.4% lipid, wet wt basis, Geyer et al. 1985)  
 4.11 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1987, 1989)  
 2.85 (fish, calculated-concentration ratio  $C_B/C_W$  or rate constant ratio  $k_1/k_2$ , Connell & Hawker 1988)  
 3.28 (guppy, Van Hoogan & Opperhuizen 1988)  
 4.76, 4.90, 3.54, 4.68 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)  
 3.30 (guppy, steady-state conditions, rate const. ratio  $k_1/k_2$ , 96-h exposure, Sijm et al. 1993)  
 4.50 (guppy, lipid normalized BCF, Sijm et al. 1993)  
 2.99 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption, Koelmans et al. 1993)  
 2.90, 3.28; 3.08, 3.41 (*Poecilla reticulata*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)  
 2.94–3.23 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)  
 3.08, 4.16; 2.812, 3.055 (quoted: whole fish, lipid content; calculated- MCI  $\chi$ ,  $K_{OW}$ , Lu et al. 1999)  
 3.68; 3.72 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

#### Sorption Partition Coefficient, log $K_{OC}$ :

- 2.85 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)  
 2.73–4.00 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)  
 4.70; 4.10 (field data of Lake Ontario sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)  
 3.0, 2.0 (Sanhedron soil humic acid, Suwannee River humic acid, batch equilibrium-sorption isotherm, GC/ECD, Chiou et al. 1986)  
 2.3, 2.0 (Sanhedron soil fulvic acid, Suwannee River fulvic acid, batch equilibrium-sorption isotherm, GC/ECD, Chiou et al. 1986)  
 3.21, 3, 14 (Riddles soil: top layer 1.84% OC; below top layer, batch equilibrium-sorption isotherm, Boyd et al. 1990)  
 3.18, 3.38, 3.43, 3.26, 3.23 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)  
 3.91 (Isora soil 1.87% OC, batch equilibrium, GC, Paya-Perez et al. 1991)  
 3.81 (lake sediment 2.5% OC, batch equilibrium, Schrap et al. 1994)  
 3.61  $\pm$  0.39 (suspended particulates in coastal waters, Masunaga et al. 1996)  
 3.16 (HPLC-screening method; Müller & Kördel 1996)  
 3.48, 3.37 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, average, Delle Site 2001)

#### Environment Fate Rate Constants, k, or Half-Lives, $t_{1/2}$ :

Volatilization:

Photolysis:

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

$k_{OH} \sim 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

$k(aq.) \leq 0.06 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 3 and 21°C, with  $t_{1/2} > 6 \text{ d}$  at pH 7 (Yao & Haag 1991).

$k_{HO}(\text{calc}) = 4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  in aqueous solutions (Haag & Yao 1992)

Hydrolysis: base rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  at 25°C with a calculated  $t_{1/2} > 900 \text{ yr}$  at pH 7 (Ellington et al. 1988)

Biodegradation: dechlorination pseudo-first order rate constant  $k = 0.387 \text{ d}^{-1}$  with  $t_{1/2} = 1.8 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

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

$k_1 = 8300 \text{ d}^{-1}$ ;  $k_2 = 0.45 \text{ d}^{-1}$  (guppy, exptl., Könemann & van Leeuwen 1980)

$k_2 = 0.45 \text{ d}^{-1}$  (guppy, exptl., Könemann & van Leeuwen 1980)

$k_1 = 18.7 \text{ h}^{-1}$ ;  $1/k_2 = 53 \text{ h}$  (guppy, quoted, Hawker & Connell 1985)  
 $\log k_1 = 2.50 \text{ d}^{-1}$ ;  $\log k_2 = -0.35 \text{ d}^{-1}$  (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)  
 $k_1 = 780 \text{ mL g}^{-1} \cdot \text{d}^{-1}$ ;  $k_2 = 0.42 \text{ d}^{-1}$  (guppy, Van Hoogan & Opperhuizen 1988)  
 $k_1 = 780 \pm 220 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 0.42 \pm 0.06 \text{ d}^{-1}$  (guppy, 96-h exposure studies, Sijm et al. 1993)  
 $k_1 = (23\text{--}29) \text{ mL g}^{-1} \text{ d}^{-1}$ ,  $k_2 = (5\text{--}3) \text{ d}^{-1}$  (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

#### Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

Surface Water:  $t_{1/2} = 1.9\text{--}30 \text{ d}$ , surface waters in various locations in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

hydrolysis  $t_{1/2} > 900 \text{ yr}$  at pH 7 and 25°C (Ellington et al. 1988)

$k(\text{exptl}) \leq 0.006 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 21°C, with  $t_{1/2} > 6 \text{ d}$  at pH 7 (Yao & Haag 1991)

Groundwater:

Sediment: dechlorination  $t_{1/2} = 1.8 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

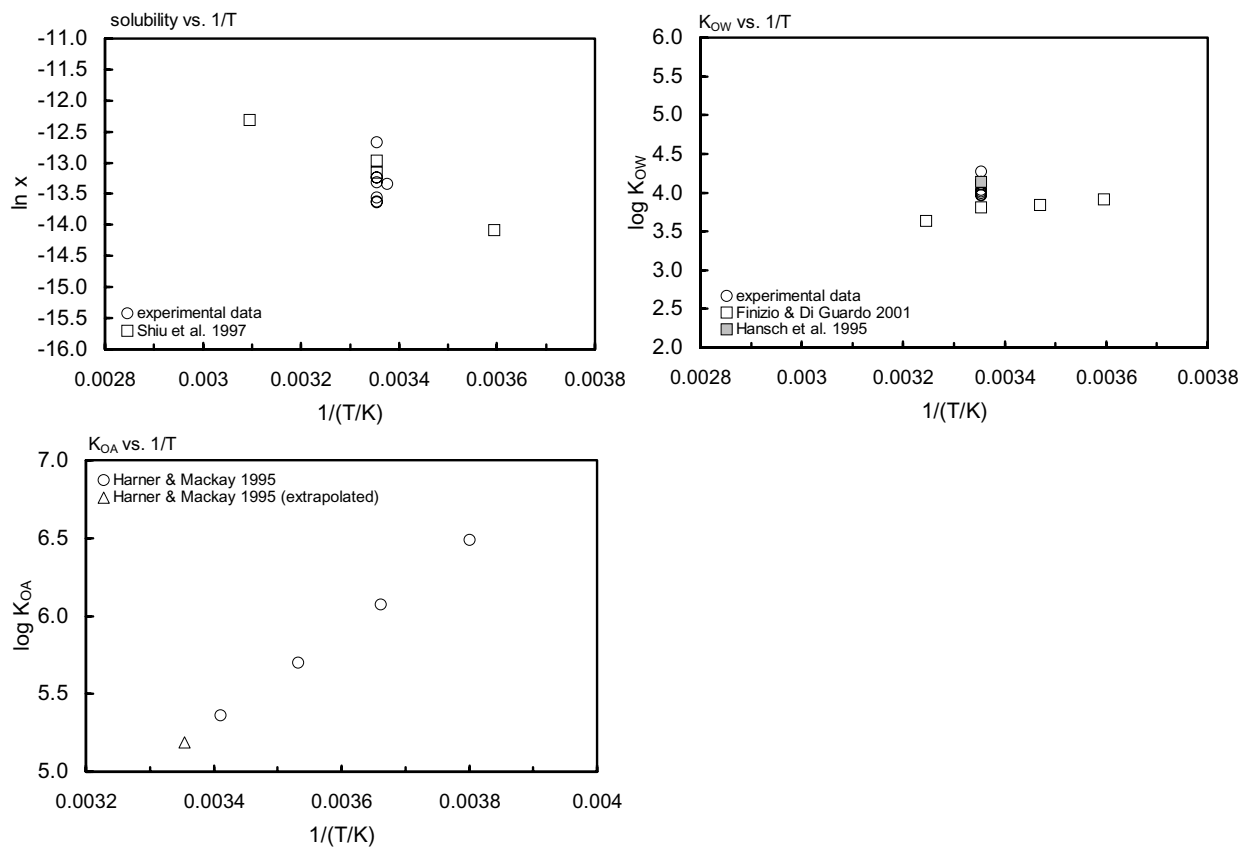
Soil:

Biota: biological  $t_{1/2} < 1 \text{ d}$  in trout,  $t_{1/2} = 2 \text{ d}$  in sunfish and  $t_{1/2} = 2 \text{ d}$  in guppy for trichlorobenzenes (Niimi 1987)  
 $t_{1/2} < 5 \text{ d}$  in worm at 8°C (Oliver 1987a).

**TABLE 6.1.1.5.1**

**Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3-trichlorobenzene at various temperatures**

Aqueous solubility		log $K_{OW}$		log $K_{OA}$	
Shiu et al. 1997		Finizio & Di Guardo 2001		Harner & Mackay 1995	
shake flask-GC		GC-RT correlation		generator column-GC/ECD	
$t/^{\circ}\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$	$t/^{\circ}\text{C}$	log $K_{OW}$	$t/^{\circ}\text{C}$	log $K_{OA}$
5	7.66	5	3.91	25	5.19
25	19.31	15	3.84	-10	6.491
50	45.61	25	3.81	0	6.073
		35	2.64	9.88	5.699
				19.85	5.829
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 55.7$					
$\log K_{OA} = A + B/T$					
A					-4.6
B					2909



**FIGURE 6.1.1.5.1** Logarithm of mole fraction solubility,  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for 1,2,3-trichlorobenzene.

TABLE 6.1.1.5.2

Reported vapor pressures of 1,2,3-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/(C + T/K) & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \\ \ln (P/P_o) = (1 - T/T_o) \cdot \exp[\Sigma A_i T^i] & (5) - \text{Cox eq.} & & \end{array}$$

1.

Stull 1947		Liu & Dickhut 1994		Poledniecek et al. 1996			
summary of lit. data		gas saturation-GC		static method-pressure gauge			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
40	133.3	−15	0.124	0.36	0.94	60.11	268.14
70	666.6	5.0	0.445	0.38	0.955	70.04	472.25
85.5	1333	10	2.80	10.35	2.971	80.01	789.67
101.8	2666	25	11.2	10.36	2.965	80.01	799.36
119.8	5333	40	50.5	20.35	8.820	88.72	1241.7
131.5	7999			20.37	8.834	88.73	1238.8
146.0	13332	$\Delta H_v/(\text{kJ mol}^{-1}) = 54.5$		30.28	23.62	92.95	1305.6
168.2	26664	(−15 to 40°C)		30.28	23.66	98.72	1995.1
193.5	53329			50.12	146.0	108.67	3055.0
218.5	101325	for solid		50.12	145.5	118.69	4618.2
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 72.7$		25	14.07	128.73	6805.3
mp/°C	52.5				interpolated	138.77	9800.6
						138.78	9788.7
					solid	148.88	13815
				eq. 3a	P/Pa	158.88	19090
				A	33.2977	168.95	25970
				B	9327.37		
				C	6.13455		
							liquid
						eq. 3a	P/Pa
						A	21.1681
						B	4077.21
						C	−71.5639

Sears & Hopke 1949	
Rodebush gauge	
t/°C	P/Pa
measure range: 16–30°C	
mp/°C	52.55 to 52.70
eq. 1	P/micron
A	13.662
B	3440.2

2.

Roháč et al. 1999			
recommended			
T/K	P/Pa	T/K	P/Pa
	solid		liquid
233.15	0.003	333.15	272.4
243.15	0.015	343.25	479.4
253.15	0.065	353.15	812.0

(Continued)

TABLE 6.1.1.5.2 (Continued)

Roháč et al. 1999			
recommended			
T/K	P/Pa	T/K	P/Pa
263.15	0.26	363.15	1329
273.15	0.90	373.15	2106
283.15	2.90	383.15	3245
283.15	8.50	393.15	4868
303.15	23.1	403.15	7130
313.15	58.9	413.15	10220
323.15	140.9	423.15	14340
		433.15	19760
Data fitted to Cox eq.		443.15	26760
For solid		453.15	35700
eq. 5	P/Pa	463.15	46860
$A_0$	3.380608	473.15	6730
$10^{-4}A_1$	-2.5802866	483.15	77730
$A_2$	0	493.15	98350
$T_0/K$	325.6	503.15	123100
$P_0/Pa$	173.0		
bp/K	494.45	Cox eq.	
temp range 273–323 K		eq. 5	P/Pa
		$A_0$	3.274398
		$10^{-3}A_1$	-1.0923018
		$10^{-7}A_2$	7.8603029
		$T_0/K$	325.6
		$P_0/Pa$	173.0
		bp/K	494.45
		temp range 333–448 K	

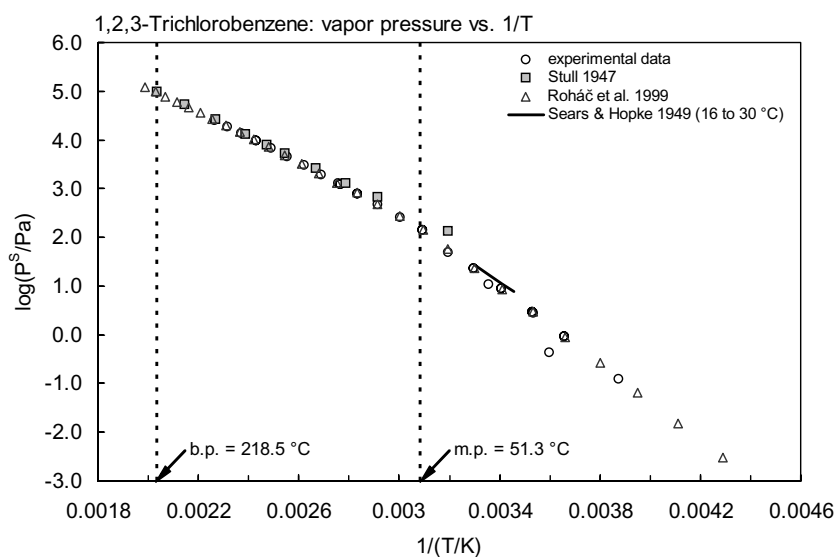
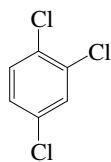


FIGURE 6.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3-trichlorobenzene.



## 6.1.1.6 1,2,4-Trichlorobenzene



Common Name: 1,2,4-Trichlorobenzene

Synonym: unsym-trichlorobenzene

Chemical Name: 1,2,4-trichlorobenzene

CAS Registry No: 120-82-1

Molecular Formula:  $C_6H_3Cl_3$ 

Molecular Weight: 181.447

Melting Point ( $^{\circ}C$ ):

16.92 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

213.5 (Weast 1972–73; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.4542 (Weast 1972–73)

1.446 (Dean 1985, 1992)

1.459 (Lide 2003)

Molar Volume ( $cm^3/mol$ ):124.8 ( $20^{\circ}C$ , calculated-density)

158.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

15.48 (Tsonopoulos &amp; Prausnitz 1971)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

53.56 (Tsonopoulos &amp; Prausnitz 1971)

Fugacity Ratio, at  $25^{\circ}C$ , F: 1.0 (Suntio et al. 1988b)

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

25.03 (Irmann 1965)

34.7 (shake flask-UV, Yalkowsky et al. 1979)

30.0 (Callahan et al. 1979)

19.4 (shake flask-GC, Könemann 1981)

30.0 (recommended, Hovarth 1982)

48.8 ( $20^{\circ}C$ , shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; 1983)

46.1 (generator column-GC/ECD, Miller et al. 1984; 1985)

31.3 (shake flask-HPLC/UV, Banerjee 1984)

30.9 (recommended, IUPAC Solubility Data Series, Horvath &amp; Getzen 1985)

34.6 (shake flask-GC, Chiou 1985)

52.0 (shake flask-GC, Boyd et al. 1998)

36.5\*  $\pm$  0.36 (shake flask-GC/FID, measured range  $5$ – $45^{\circ}C$ , Ma et al. 2001)7.71, 10.39, 13.58, 19.82 (5, 15, 25,  $35^{\circ}C$ , estimated- RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

133.3\* ( $38.4^{\circ}C$ , summary of literature data, temp range  $38.4$ – $213^{\circ}C$ , Stull 1947)

38.6 (calculated by formula, Dreisbach 1955)

 $\log(P/mmHg) = 7.19608 - 1827.0/(210.0 + t/^{\circ}C)$ ; temp range  $110$ – $280^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

60.6 (extrapolated-Antoine eq., supercooled liquid, Weast 1972–73)

 $\log(P/mmHg) = [-0.2185 \times 11425.1/(T/K)] + 8.030523$ ; temp range  $38.4$ – $213^{\circ}C$  (Antoine eq., Weast 1972–73)

- 26.4 (gas saturation, Politzki et al. 1982)  
 28.5 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)  
 38.7 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log (P_g/\text{kPa}) = 9.570 - 3254/(T/K)$ ; temp range 279–290 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.31998 - 1827/(-63.15 + T/K)$ ; temp range 383–553 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.6802 - 2064.4/(-43.05 + T/K)$ ; temp range 293–383 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)  
 53.4 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; Spieksma et al. 1994)  
 $\log (P/\text{mmHg}) = 15.5947 - 2.8920 \times 10^3/(T/K) - 2.5549 \cdot \log (T/K) + 2.0384 \times 10^{-4} \cdot (T/K) - 7.0601 \times 10^{-14} \cdot (T/K)^2$ , temp range 290–725 K, (Yaws 1994)  
 5728\* (118.671°C, comparative ebulliometry, measured range 118.671–215.887°C, Roháč et al. 1998)  
 24.2\* (20°C, recommended, summary of literature data, temp range 293.15–493.15 K, Roháč et al. 1999)  
 $\ln [(P/\text{Pa})/19.0] = [1 - (T/K)/290.07] \cdot \exp\{3.352607 - 9.0343639 \times 10^{-4} \cdot (T/K) + 6.0501757 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range 294–489 K (Cox eq., recommended, Roháč et al. 1999)  
 $\log (P/\text{kPa}) = 9.570 - 3254/(T/K)$ ; temp range 6–17°C (solid, regression eq. from literature data, Shiu & Ma 2000)  
 $\log (P/\text{kPa}) = 6.682 - 2064.4/[(T/K) - 43.5]$ ; temp range 20–110°C (liquid, regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  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.):

- 122 (gas stripping-GC, Oliver 1985)  
 144 (gas stripping-GC, Warner et al. 1987)  
 195\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = -16.34 + 3307/(T/K)$ ; temp range 10–30°C (EPICS-GC/FID, Ashworth et al. 1988)  
 101 (gas stripping-GC, ten Hulscher et al. 1992)  
 375.2 (modified EPICS method-GC, Ryu & Park 1999)  
 172 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 4.381 - 1622/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section:

- 4.05 (Leo et al. 1971)  
 4.26 (Callahan et al. 1979)  
 4.02 (Hansch & Leo 1979; Hansch & Leo 1985)  
 3.93 (shake flask-GC, HPLC-k' correlation, Könemann et al. 1979)  
 4.02 (20°C, shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; Chiou 1985)  
 3.97 (shake flask-GC, Watarai et al. 1982)  
 3.96 (HPLC-k' correlation, Hammers et al. 1982)  
 3.93–4.18, 4.09 (range, mean, shake flask method, Eadsforth & Moser 1983)  
 4.12–4.32, 4.21 (range, mean, HPLC method, Eadsforth & Moser 1983)  
 3.98 (generator column-GC/ECD, Miller et al. 1984; 1985)  
 4.22 (HPLC-k' correlation, De Kock & Lord 1987)  
 4.02 (shake flask-GC, Pereira et al. 1988)  
 4.05 (slow stirring-GC, De Bruijn et al. 1989)  
 4.02 (recommended, Sangster 1993)  
 4.02 (recommended, Hansch et al. 1995)  
 3.92\* (estimated- RP-HPLC-k' correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

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.

- 5.10\* (20°C, HPLC-k' correlation, measured range 10–50°C, Su et al. 2002)  
 $\log K_{OA} = 62080/(2.303 \cdot RT) - 6.031$ ; temp range 10–50°C (HPLC-k' correlation, Su et al. 2002)

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

- 3.32 (fathead minnow, 32-d exposure, Veith et al. 1979b)
- 3.45; 3.37; 2.95 (fathead minnow; green sunfish; rainbow trout, Veith et al. 1979b)
- 2.69 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980a)
- 2.26 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 3.52 (microorganism-water, Mabey et al. 1982)
- 3.04–3.11 mean 3.11; 3.43–3.60 mean 3.51 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
- 4.19–4.56 (rainbow trout, lipid base, Oliver & Niimi 1983)
- 3.26–3.61 (fish, Oliver 1984, 1985)
- 2.40 (algae, Geyer et al. 1984)
- 3.15 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
- 2.40, 2.69, 3.15 (algae, fish, sludge, Klein et al. 1984)
- 3.15–3.72 mean 3.36; 3.30–3.75 mean 3.57 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)
- 3.11; 3.08 (rainbow trout, wet wt. basis, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)
- 4.19–4.56 (rainbow trout, lipid base, Oliver & Niimi 1985)
- 2.09; 3.84 (quoted, rainbow trout, 1.8% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.28, 2.40, 2.34, 2.66 (quoted, carp, 2.2% lipid, wet wt basis, Geyer et al. 1985)
- 3.94, 3.96, 4.0, 4.32 (quoted, carp, 2.2% lipid, lipid basis, Geyer et al. 1985)
- 2.54; 4.04 (quoted, rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.66, 2.73; 4.02, 4.09 (quoted, carp, 4.4% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.96; 4.26 (quoted, golden ide, 5.0% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.86, 2.94; 4.15, 4.19 (quoted, zebra fish, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 2.83, 3.12; 4.12, 4.22 (quoted, tilapia, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 2.98, 3.12; 4.23, 4.36 (quoted, bluegill sunfish, 5.7% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.13, 3.14; 4.37, 4.38 (quoted, guppy, 5.8% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.11, 3.20; 4.23, 4.38 (quoted, rainbow trout, 7.7%, wet wt basis; lipid basis, Geyer et al. 1985)
- 2.96, 3.03; 4.05, 4.23 (quoted, guppy, 8.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.11; 4.19 (quoted, rainbow trout, 8.3% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.32; 4.30 (quoted, fathead minnow, 10.5% lipid, wet wt basis, lipid basis Geyer et al. 1985)
- 2.69; 2.40; 3.15 (fish; algae; activated sludge, Freitag et al. 1985)
- 2.61 (fathead minnow, Carlson & Kosian 1987)
- 4.76, 4.90, 3.54, 4.68 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
- 3.31, 4.25 (American flagfish, whole fish, fish lipid, Smith et al. 1990)
- 2.95–3.57; 3.31; 3.32; 3.36 (*Oncorhynchus mykiss*; *Jordanella floridae*; *Pimephales promelas*; *Lepomis cyanellus*, quoted lit., flow through conditions, Devillers et al. 1996)
- 3.0, 3.06, 3.06 (guppy:  $k_1/k_2$ -best fit exptl. data,  $k_1/k_2$ -slope method,  $C_f/C_w$ -steady state, van Eck et al. 1997)
- 3.81; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log  $K_{oc}$ :

- 2.80 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 2.68–3.94 (5 soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 4.70; 4.40 (field data of sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
- 4.3–5.1, 5.10; 5.10 (suspended sediment, average; algae > 50  $\mu$ m, Oliver 1987c)
- 4.8–5.3, 5.0 (Niagara River plume, range, mean, Oliver 1987b)
- 3.91 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.66, 3.40 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.27 (untreated Marlette soil B<sub>1</sub> horizon, 0.30% OC, equilibrium isotherm, Lee et al. 1989)

- 3.91, 3.64, 3.04 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.32 (calculated- $K_{OW}$ , Aldrich or Fluka humic acid polymers, Chin & Weber 1989)
- 3.32; 2.62 (Aldrich humic acid, organic polymers, Chin et al. 1990)
- 4.02 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
- 2.71, 2.71 (RP-HPLC- $k'$  correlation including: MCI-related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 3.86  $\pm$  0.40 (suspended particulates in coastal waters, Masunaga et al. 1996)
- 3.15, 3.19, 3.10 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, 0.1  $\leq$  OC < 0.5%, average, Delle Site 2001)
- 4.38–3.24 (NIST SRM diesel particulate matter, sorption isotherm, Ngyuen et al. 2004)

#### Sorption Partition Coefficient, log $K_{OM}$ :

- 2.70 (Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)
- 2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.97 (untreated Marlette soil B<sub>t</sub> horizon, 0.30% OC, equilibrium sorption isotherm, Lee et al. 1989)
- 3.97, 3.50, 2.87 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

#### Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$ :

Volatilization: rate constants:  $k = 0.032 \text{ d}^{-1}$  with  $t_{1/2} = 22 \text{ d}$  in spring at 8–16°C,  $k = 0.066 \text{ d}^{-1}$  with  $t_{1/2} = 11 \text{ d}$  in summer at 20–22°C,  $k = 0.058 \text{ d}^{-1}$  with  $t_{1/2} = 12 \text{ d}$  in winter at 3–7°C for the periods when volatilization appears to dominate, and  $k = 0.073 \text{ d}^{-1}$  with  $t_{1/2} = 9.5 \text{ d}$  with  $\text{HgCl}_2$ , and  $k = 0.066 \text{ d}^{-1}$  with  $t_{1/2} = 10.6 \text{ d}$  without  $\text{HgCl}_2$  in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Photolysis: not environmentally relevant (Mabey et al. 1982)

$t_{1/2} = 450 \text{ yr}$  for surface water photolysis at 40°N latitude in the summer (Dulin et al. 1986)

$k = 1.16 \times 10^{-3} \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  at 25°C in F-113 solution and with HO $\cdot$  in the gas (Dilling et al. 1988)

$k = 0.03 \text{ h}^{-1}$ , the maximum summer photolysis rate calculated at midday clear sky, the minimum photolytic  $t_{1/2} \sim 4 \text{ months}$ , but a realistic value is likely to be at least 1 yr (Bunce et al. 1989)

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with  $\text{NO}_3$  radical and  $k_{O_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures see reference:

$k = 7.22 \times 10^{-3} \text{ h}^{-1}$  (Simmons et al. 1976; selected, Mackay et al. 1985)

$k_{OH} \sim 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

$k(\text{singlet oxygen}) \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ ;  $k(\text{RO}_2 \text{ radical}) \ll 1 \text{ M}^{-1} \text{ h}^{-1}$  (Mabey et al. 1982)

$k \ll 1.6 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 10 mM *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 5.32 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 273–368 K (flash photolysis-resonance fluorescence, Rinke & Zetzsch 1984)

$k_{OH}(\text{obs.}) = 5.32 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ; and  $k_{OH}(\text{calc}) = 3.47 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{OH}(\text{calc}) = 0.29 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs}) = 0.532 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(\text{aq.}) = 4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  in aqueous solutions (Haag & Yao 1992)

$k_{OH}(\text{calc}) = 0.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  at 25°C with a calculated  $t_{1/2} > 900 \text{ yr}$  at pH 7 (Ellington et al. 1988)

first-order rate constant  $k = 2.3 \times 10^{-5} \text{ h}^{-1}$  with  $t_{1/2} = 3.4 \text{ yr}$  at pH 7 and 25°C (Howard et al. 1991).

Biodegradation:  $k = 1.92 \times 10^{-2} \text{ h}^{-1}$ , degradation in water (Simmons et al. 1976)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320 \text{ h}$  estimated from unacclimated soil grab sample data (Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 2688\text{--}17280 \text{ h}$  based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$k = 0.05 \text{ d}^{-1}$ , significant degradation in an aerobic environment (Tabak et al. 1981; Mills 1982)

$k = 0.029 \text{ d}^{-1}$  in river water,  $k = 0.026 \text{ d}^{-1}$  in estuarine water, and  $k = 0.012 \text{ d}^{-1}$  in marine water (Bartholomew & Pfaender 1983; Battersby 1990)

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 110 \text{ d}$  in natural waters (Capel & Larson 1995)

$k = 0.035 \text{ d}^{-1}$ , the dechlorination pseudo-first order rate constant, with  $t_{1/2} = 19.8 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000)

Biotransformation:  $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$  (estimated, Mabey et al. 1982).

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

$k_1 = 8300 \text{ d}^{-1}$ ;  $k_2 = 0.45 \text{ d}^{-1}$  (guppy, exptl., Könemann & Van Leeuwen 1980)

$k_1 = 18.7 \text{ h}^{-1}$ ;  $1/k_2 = 53.0 \text{ h}$  (guppy, selected, Hawker & Connell 1985)

$\log k_1 = 2.65 \text{ d}^{-1}$ ;  $\log 1/k_2 = 0.34 \text{ d}$  (guppy, selected, Connell & Hawker 1988)

$\log k_2 = -1.85 \text{ d}^{-1}$ ;  $\log k_2 = 0.23 \text{ d}^{-1}$  (fish, calculated- $K_{ow}$ , fast-biphasic, Thomann 1989)

$k_1 = 1158 \text{ d}^{-1}$ ,  $10140 \text{ d}^{-1}$ ;  $k_2 = 0.57 \text{ d}^{-1}$ ,  $0.57 \text{ d}^{-1}$  (American flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 0.57 \text{ d}^{-1}$ ,  $0.46 \text{ d}^{-1}$  (American flagfish: bioconcentration data, toxicity data, Smith et al. 1990)

$k_1 = 492 \pm 234 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 0.49 \pm 0.22 \text{ d}^{-1}$  (guppy, exptl., van Eck et al. 1997)

#### Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

calculated minimum photolytic  $t_{1/2} \sim 4$  months, but realistically at least 1 yr (Bunce et al. 1989);

tropospheric lifetime of 25 d based on reaction principally with OH radical and other photochemical reactions (Bunce 1991);

$t_{1/2} = 128.4\text{--}1284 \text{ h}$ , based on the photooxidation with OH radical (Howard et al. 1991).

Surface Water:  $t_{1/2} = 2.1\text{--}28 \text{ d}$  estimated for various locations in the Netherlands,  $t_{1/2} = 0.3\text{--}3 \text{ d}$  for river water,  $t_{1/2} = 3\text{--}30 \text{ d}$  for lakes estimated from persistence (Zoeteman et al. 1980);

half-lives from marine mesocosm:  $t_{1/2} = 22 \text{ d}$  in the spring at  $8\text{--}16^\circ\text{C}$ ,  $t_{1/2} = 11 \text{ d}$  in the summer at  $20\text{--}22^\circ\text{C}$  and  $t_{1/2} = 12 \text{ d}$  in the winter at  $3\text{--}7^\circ\text{C}$  when volatilization dominates, and  $t_{1/2} = 9.5 \text{ d}$  and  $10.6 \text{ d}$  for experiments with and without  $\text{HgCl}_2$  respectively in September 9–15 (Wakeham et al. 1983)

hydrolysis  $t_{1/2} > 900 \text{ yr}$  at pH 7 and  $25^\circ\text{C}$  (Ellington et al. 1988)

$t_{1/2}(\text{aerobic}) = 672\text{--}4320 \text{ h}$ , based on unacclimated aerobic soil grab sample data;  $t_{1/2}(\text{anaerobic}) = 2688\text{--}17280 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life; and first order hydrolysis  $t_{1/2} = 3.4 \text{ yr}$  (Howard et al. 1991);

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 110 \text{ d}$  in natural waters (Capel & Larson 1995)

Groundwater:  $t_{1/2} = 1344\text{--}8640 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 30\text{--}300 \text{ d}$  estimated from persistence (Zoeteman et al. 1980).

Soil:  $t_{1/2} < 10 \text{ d}$  (Ryan et al. 1988)

$t_{1/2} = 672\text{--}4320 \text{ h}$ , based on unacclimated aerobic soil grab sample data (Howard et al. 1991).

Sediment: dechlorination  $t_{1/2} = 19.8 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biota:  $1 < t_{1/2} < 3 \text{ d}$  in blue bluegill sunfish (Barrows et al. 1980);

biological half-lives,  $t_{1/2} < 1 \text{ d}$  in trout,  $t_{1/2} = 2 \text{ d}$  in sunfish, and  $t_{1/2} = 2 \text{ d}$  in guppy for trichlorobenzenes (Niimi 1987);

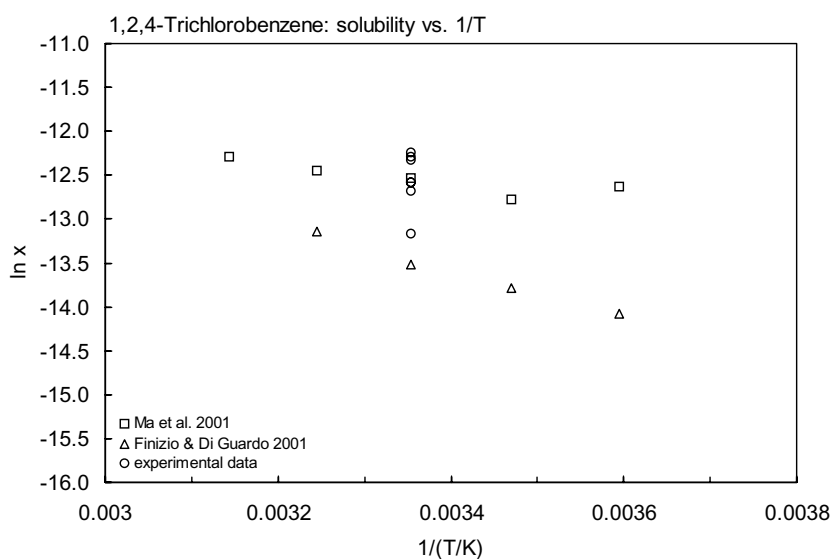
$t_{1/2} < 5 \text{ d}$  in worms at  $8^\circ\text{C}$  (Oliver 1987a);

depuration  $t_{1/2} = 1.21 \text{ d}$  from whole fish,  $t_{1/2} = 1.20 \text{ d}$  from fish lipid (American flagfish, Smith et al. 1990).

TABLE 6.1.1.6.1

Reported aqueous solubilities of 1,2,4-trichlorobenzene at various temperatures

Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC		RP-HPLC-k' correlation	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
5	32.9	5	7.71
15	28.5	15	10.39
25	36.5	25	13.58
35	39.8	35	19.82
45	46.5		



**FIGURE 6.1.1.6.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,2,4-trichlorobenzene.

TABLE 6.1.1.6.2

Reported vapor pressures of 1,2,4-trichlorobenzene 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)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)	$\ln P = A - B/(C + T/K)$		(3a)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
$\ln (P/P_o) = (1 - T/T_o) \cdot \exp[\Sigma A_i T^i]$		(5) - Cox eq.					
Stull 1947		Sears & Hopke 1949		Roháč et al. 1998		Roháč et al. 1999	
summary of literature data		Rodebush gauge		comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
38.4	133.3	measured range: 6–25°C		118.671	5728	293.15	24.2
67.3	666.6			128.383	8331	303.15	51.2
81.7	1333	mp/°C	17.05–17.40	136.228	11070	313.15	102.4
97.2	2666			142.813	13911	232.15	194.7
114.8	5333	for solid:-		142.819	13914	333.15	354.0
125.7	7999	eq. 1	P/micron	148.44	16794	343.25	617.7
140	13332	A	13.445	154.289	20281	353.15	1038
162	26664	B	3254.0	154.308	20290	363.15	1687
187.7	53329			160.441	24566	373.15	2658
213	101325	for liquid:-		166.386	29387	383.15	4071
mp/°C	17.0	eq. 1	P/micron	172.180	34807	393.15	6075
		A	10.682	177.755	40745	403.15	8854
		B	2452.3	183.424	47613	413.15	12630
				192.328	60271	423.15	17650
				192.331	60264	433.15	224210
				200.386	74748	443.15	32650
				209.989	93380	453.15	43360
				212.397	98847	463.15	56740
				215.887	107216	473.15	73260
						483.15	93420
		bp/°C	213.492	493.15	117800		
		eq. 3	P/kPa	eq. 5	P/Pa		
		A	6.11973	A <sub>0</sub>	3.352607		
		B	1677.35	10 <sup>-3</sup> A <sub>1</sub>	–9.0343639		
		C	–78.926	10 <sup>-7</sup> A <sub>2</sub>	6.0501757		
				T <sub>o</sub> /K	290.07		
				P <sub>o</sub> /Pa	19.0		
				bp/K	486.60		
				temp range 294–489 K			

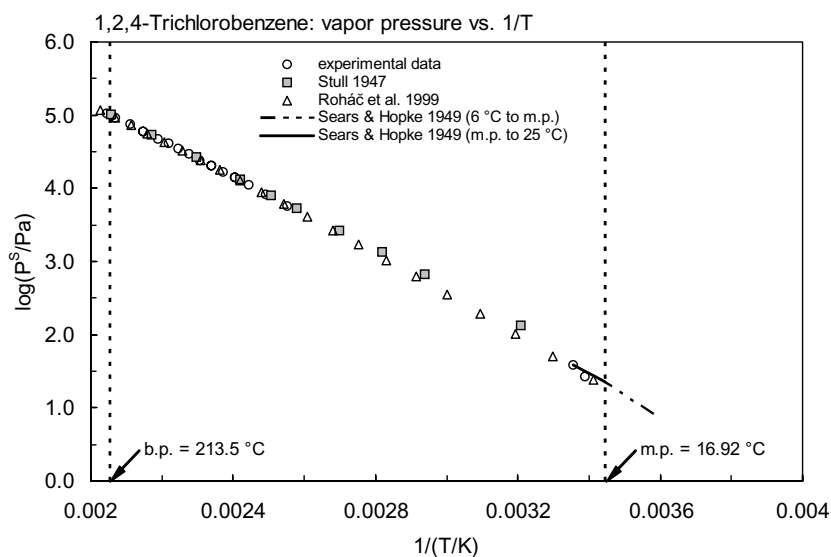


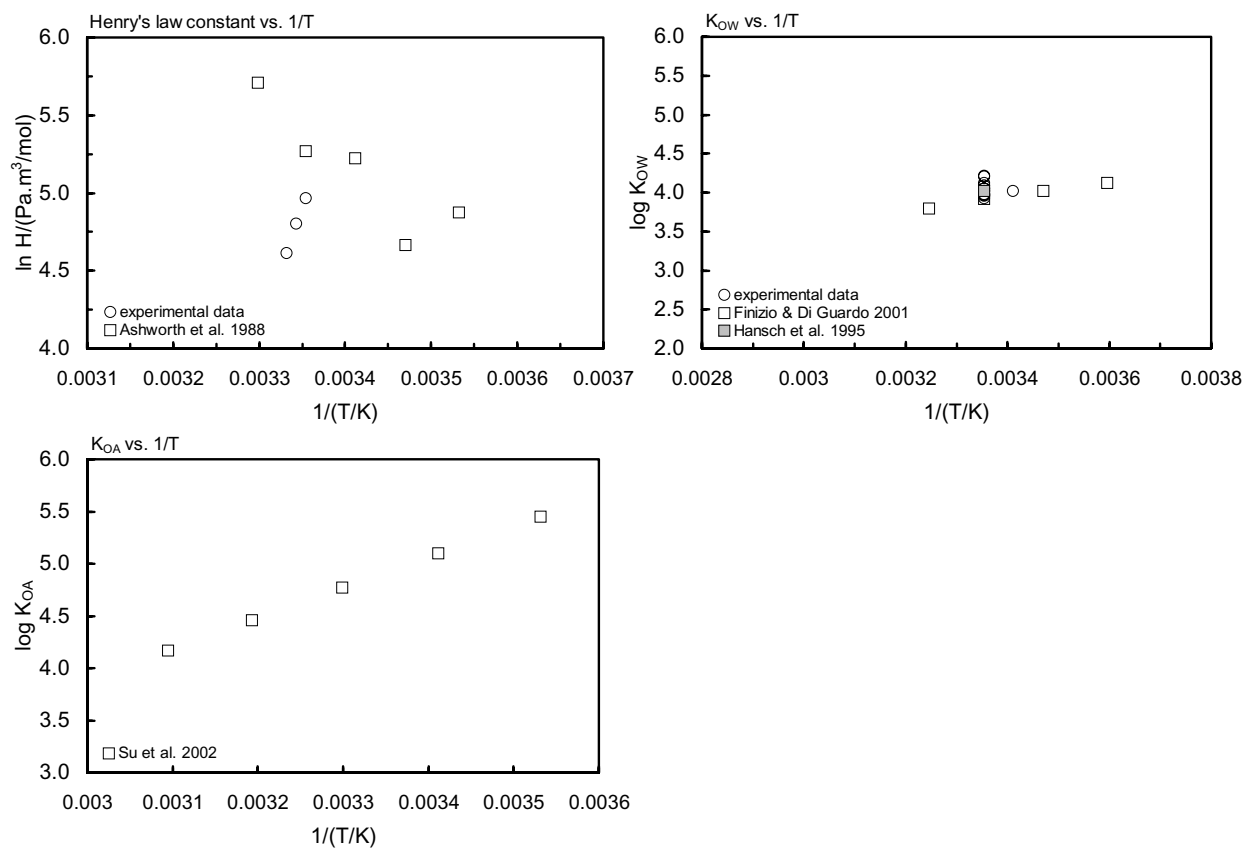
FIGURE 6.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4-trichlorobenzene.

TABLE 6.1.1.6.3

Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4-trichlorobenzene at various temperatures

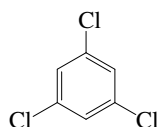
Henry's law constant		log K <sub>OW</sub>		log K <sub>OA</sub>	
Ashworth et al. 1988		Finizio & Di Guardo 2001		Su et al. 2002	
EPICS-GC		HPLC-RT correlation		GC-RT correlation	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
10	131	5	4.12	10	5.45
15	106	15	4.02	20	5.1
20	185	25	3.92	30	4.77
20	195	35	3.8	40	4.46
30	301			50	4.17
ln (H/(atm m <sup>3</sup> /mol)) = A - B/(T/K)				ΔH <sub>OA</sub> /(kJ mol <sup>-1</sup> ) = 62.08	
A	7.261			log K <sub>OA</sub> = A + B/2.303RT	
B	4028			A	-6.031
				B	62080





**FIGURE 6.1.1.6.3** Logarithm of Henry's law constant,  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for 1,2,4-trichlorobenzene.

## 6.1.1.7 1,3,5-Trichlorobenzene



Common Name: 1,3,5-Trichlorobenzene

Synonym: sym-trichlorobenzene

Chemical Name: 1,3,5-trichlorobenzene

CAS Registry No: 108-70-3

Molecular Formula:  $C_6H_3Cl_3$ 

Molecular Weight: 181.447

Melting Point ( $^{\circ}C$ ):

62.8 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

208.0 (Weast 1972–72, 1982–83; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):1.3865 ( $64^{\circ}C$ , Weast 1972–73; Horvath 1982)Molar Volume ( $cm^3/mol$ ):130.9 ( $64^{\circ}C$ , calculated-density)

125 (calculated-density, liquid molar volume, Chiou 1985)

158.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

19.622 (Tsonopoulos &amp; Prausnitz 1971)

18.786 (Miller et al. 1984)

18.198 (Ruelle et al. 1993; Ruelle &amp; Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

58.16 (Tsonopoulos &amp; Prausnitz 1971)

56.07 (Miller et al. 1984)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.426 (mp at  $62.8^{\circ}C$ )0.413 ( $25^{\circ}C$ , Suntio et al. 1988b)

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

25.03 (Tsonopoulos &amp; Prausnitz 1971)

6.59 (shake flask-UV, Yalkowsky et al. 1979)

5.87 (shake flask-GC, Könnemann 1981)

6.61 (recommended, Hovarth 1982)

4.12 (generator column-GC/ECD, Miller et al. 1984, 1985)

6.01 (shake flask-HPLC, Banerjee 1984)

10.6 (shake flask-GC, Chiou 1985)

6.53 (recommended, IUPAC Solubility Data Series, Horvath &amp; Getzen 1985)

 $8.46^* \pm 0.26$  (generator column-GC/ECD, measured range  $5$ – $45^{\circ}C$ , Shiu et al. 1997)

2.40 (shake flask-GC, Boyd et al. 1998)

 $\ln x = -5.083768 - 2650.68/(T/K)$ , temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

666.6\* ( $63.8^{\circ}C$ , summary of literature data, temp range  $63.8$ – $208.4^{\circ}C$ , Stull 1947)

77 (extrapolated-Antoine eq., supercooled liquid, Weast 1972–73)

 $\log(P/mmHg) = [-0.2185 \times 11211.0/(T/K)] + 7.977218$ ; temp range  $63.8$ – $208.4^{\circ}C$  (Antoine eq., Weast 1972–73)

30.23 (gas saturation, interpolated from reported graph, Rordorf 1985)

24.4 (solid, extrapolated-Antoine eq.-I, Stephenson &amp; Malanowski 1987)

$\log (P_s/\text{kPa}) = 8.301 - 2956/(T/\text{K})$ ; temp range 282–301 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.43345 - 1932.26/(-45.268 + T/\text{K})$ ; temp range 336–482 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

124.4 (GC-RT correlation, Watanabe & Tatsukawa 1989)

62.4; 74.9 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; quoted lit., Spieksma et al. 1994)

$\log (P/\text{mmHg}) = 19.2854 - 4.4976 \times 10^3/(T/\text{K}) - 3.6158 \cdot \log (T/\text{K}) - 5.2495 \times 10^{-9} \cdot (T/\text{K}) + 1.5596 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 398–748 K (Yaws 1994)

12.4, 20.44\* (20.35°C pressure gauge measurement, 25°C interpolated from reported Antoine eq. based on exptl. data, Polednicek et al. 1996)

$\ln (P_s/\text{Pa}) = 32.5109 - 8909.70/[(T/\text{K}) + 3.94116]$ ; temp range 273–333 K (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)

$\ln (P_L/\text{Pa}) = 21.1215 - 3939.96/[(T/\text{K}) - 71.2907]$ ; temp range 343–442 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)

12.5 (20°C, recommended, summary of literature data, temp range 233.15–483.15 K, Roháč et al. 1999)

$\ln [(P_s/\text{Pa})/565.0] = [1 - (T/\text{K})/337.0] \cdot \exp\{3.305508 - 2.3049477 \times 10^{-4} \cdot (T/\text{K})\}$ ; temp range 273–333 K (Cox eq., solid, recommended, Roháč et al. 1999)

$\ln [(P_L/\text{Pa})/547.0] = [1 - (T/\text{K})/336.6] \cdot \exp\{3.190854 - 1.0710853 \times 10^{-3} \cdot (T/\text{K}) + 7.5659237 \times 10^{-7} \cdot (T/\text{K})^2\}$ ; temp range 343–442 K (Cox eq., liquid, recommended, Roháč et al. 1999)

32.3\* (29.33°C, static method-diaphragm manometer, measured range 29–142°C, Blok et al. 2001)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at 25°C):

192.5 (20°C, batch stripping-GC, Oliver 1985)

192 (gas stripping-GC/ECD, ten Hulscher et al. 1992)

Octanol/Water Partition Coefficient,  $\log K_{ow}$  or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated \* are compiled at the end of this section:

4.02 (Leo et al. 1971; Hansch & Leo 1979)

4.15 (shake flask-GC, HPLC- $k'$  correlation, Könemann et al. 1979)

4.17 (shake flask-GC, Watarai et al. 1982)

4.17 (HPLC- $k'$  correlation, Hammers et al. 1982)

4.02 (generator column-GC/ECD, Miller et al. 1984; 1985)

4.18 (HPLC-RV correlation, Garst 1984)

4.31 (shake flask-GC, Chiou 1985)

4.49 (Hansch & Leo 1985)

4.32\* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)

4.31 (shake flask-GC, Pereira et al. 1988)

4.189 (slow stirring-GC, De Bruijn et al. 1989)

4.15 (recommended, Sangster 1993)

4.19 (recommended, Hansch et al. 1995)

4.34\*  $\pm 0.04$  (shake flask-GC/ECD, Bahadur et al. 1997)

$\log K_{ow} = 1.1228 - 18200/[2.303 \cdot R(T/\text{K})]$ ; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)

4.44 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

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:

4.85 (calculated- $S_{oct}$  and vapor pressure  $P$ , Abraham et al. 2001)

4.89\* (20°C HPLC- $k'$  correlation, measured range 10–50°C, Su et al. 2002)

$\log K_{OA} = 68550/(2.303 \cdot RT) - 7.368$ ; temp range 10–50°C (HPLC- $k'$  correlation, Su et al. 2002)

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

4.15 (guppy, lipid basis, Könemann & van Leeuwen 1980)

3.15–3.30 mean 3.26; 3.57–3.92 mean 3.61 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

4.34–4.67 (rainbow trout, lipid basis, Oliver & Niimi 1983)

3.26–3.61 (fish, Oliver 1984)

- 4.15 (guppy, female, 5.4% lipid, wet wt basis; lipid basis, Geyer et al. 1985)  
 2.39–2.55 (fish, normalized, Tadokoro & Tomita 1987)  
 4.14 (guppy-lipid phase, Gobas et al. 1987, 1989)  
 2.88 (fish, calculated- $C_B/C_W$  or  $k_1/k_2$ , Connell & Hawker 1988; Hawker 1990)  
 4.32, 4.35, 4.38, 4.43 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)  
 4.40, 4.45, 3.51, 4.22 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)  
 3.26, 3.61; 3.48 (*Oncorhynchus mykiss*; *Poecilia reticula*, quoted lit., flow through conditions, Devillers et al. 1996)  
 2.68 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)  
 3.26, 4.33; 3.271, 2.884 (quoted: whole fish, lipid content; calculated-MCI  $\chi$ ,  $K_{OW}$ , Lu et al. 1999)  
 3.69; 3.64 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

#### Sorption Partition Coefficient, log $K_{OC}$ :

- 5.10; 4.20 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)  
 2.85 (forest soil 0.2% OC, observed, Seip et al. 1986)  
 4.13 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)  
 3.55  $\pm$  0.47 (suspended particulates in coastal waters, Masunaga et al. 1996)  
 3.69 (soil: organic carbon OC  $\geq$  0.1%, average, Delle Site 2001)

#### Environmental Fate Rate Constants, $k$ , or Half-Lives, $t_{1/2}$ :

Volatilization:  $t_{1/2} = 4.5$  h from a model river of 1 m depth with water current 1 m/s and wind velocity 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: may be susceptible to direct photolysis by sunlight (Howard 1989)

$t_{1/2} \sim 450$  yr for sunlight photolysis at 40°N in the summer (Dulin et al. 1986)

$k = 0.003 \text{ min}^{-1}$ , measured pseudo-first-order direct photolysis reaction with  $t_{1/2} = (205.5 \pm 7.5) \text{ min}$  in aqueous solution (Peijnenburg et al. 1992)

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

$k_{OH} \sim 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

photooxidation  $t_{1/2} = 6.17$  months, based on a measured rate for the vapor phase reaction with photochemically produced hydroxyl radicals in air (Atkinson et al. 1985).

Hydrolysis: will not hydrolyze under normal environmental conditions (Howard 1989).

Biodegradation: resistant to biodegradation (Tabak et al. 1964; Howard 1989);

dechlorination pseudo-first order rate constant  $k = 0.069 \text{ d}^{-1}$  with  $t_{1/2} = 10.1 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

#### Biotransformation:

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

$k_1 = 8000 \text{ d}^{-1}$ ;  $k_2 = 0.40 \text{ d}^{-1}$  (guppy, Könemann & van Leeuwen 1980)

$k_1 = 18.0 \text{ h}^{-1}$ ;  $1/k_2 = 60 \text{ h}$  (guppy, quoted, Hawker & Connell 1985)

$k_1 = 430 \text{ d}^{-1}$  (fish, quoted, Opperhuizen 1986)

$\log k_1 = 2.63 \text{ d}^{-1}$ ;  $\log k_2 = 0.440 \text{ d}^{-1}$  (fish, quoted, Connell & Hawker 1988)

$\log k_1 = 2.48 \text{ d}^{-1}$ ;  $\log k_2 = -0.40 \text{ d}^{-1}$  (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)

$\log k_2 = -0.40 \text{ d}^{-1}$  (fish, calculated- $K_{OW}$ , Thomann 1989)

$k_1 = 7 \text{ mL g}^{-1} \text{ d}^{-1}$ ,  $k_2 = 3 \text{ d}^{-1}$  (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

#### Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in 1 d or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

Surface Water:  $t_{1/2} = 18 \text{ d}$  under field conditions in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

direct photolysis  $t_{1/2} = 206 \text{ min}$  in aqueous solution (Peijnenburg et al. 1992)

Groundwater:.

Sediment: dechlorination  $t_{1/2} = 1.8$  d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

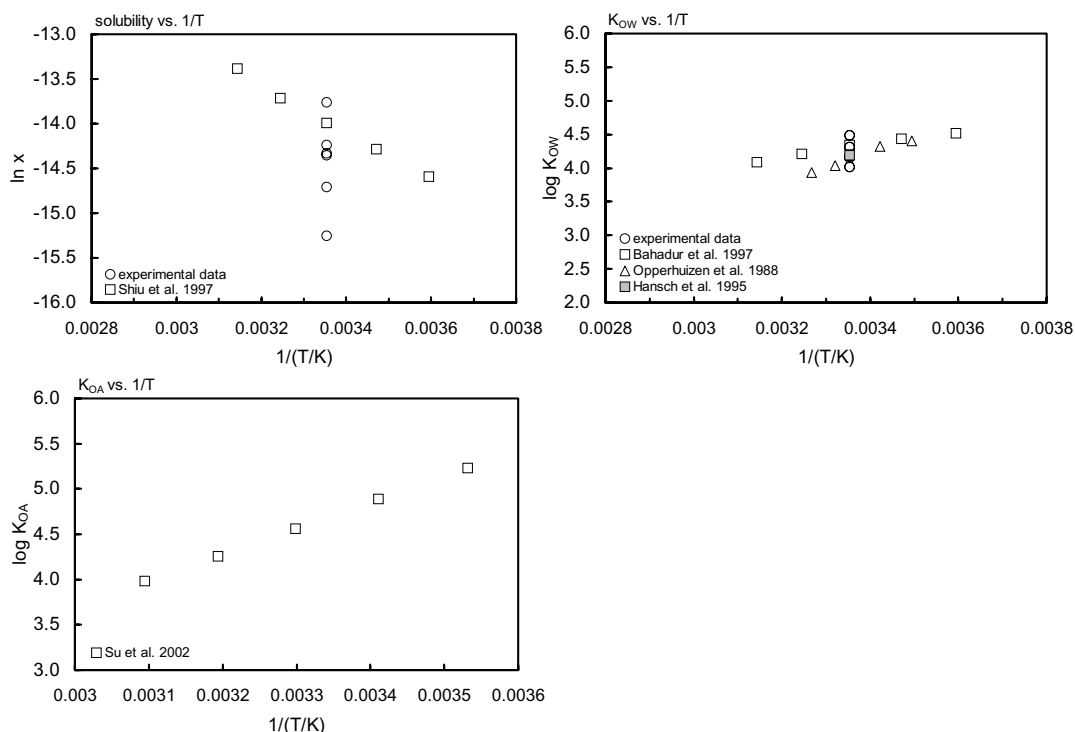
Biota: biological half-lives,  $t_{1/2} < 1$  d in trout,  $t_{1/2} = 2$  d in sunfish and  $t_{1/2} = 2$  d in guppy for trichlorobenzenes (Niimi 1987);

$t_{1/2} < 5$  d in worms at 8°C (Oliver 1987a).

**TABLE 6.1.1.7.1**

**Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,3,5-trichlorobenzene at various temperatures**

Aqueous solubility		log $K_{OW}$				log $K_{OA}$	
Shiu et al. 1997		Oppenhuizen et al. 1988		Bahadur et al. 1997		Su et al. 2002	
shake flask-GC		shake flask-GC/ECD		shake flask-GC/ECD		GC-RT correlation	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	log $K_{OW}$	$t/^{\circ}\text{C}$	log $K_{OW}$	$t/^{\circ}\text{C}$	log $K_{OA}$
5	4.62	13	4.40	5	4.52	25	5.23
15	6.29	19	4.32	15	4.43	-10	4.89
25	8.46	28	4.04	25	4.34	0	4.56
35	11.14	33	3.93	35	4.21	10	4.26
45	15.55			45	4.09	18.7	3.98
$\Delta H_{\text{sol}} = 22.04 \text{ kJ/mol}$		$\Delta H/(\text{kJ mol}^{-1}) = -21.7$		enthalpy of transfer $\Delta H/(\text{kJ mol}^{-1}) = -18.2$		$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 68.55$	
				$\log K_{OW} = A - \Delta H/2.303RT$		$\log K_{OA} = A + B/2.303RT$	
				A 1.1228		A -7.368	
				$\Delta H -18200$		B 68500	



**FIGURE 6.1.1.7.1** Logarithm of mole fraction solubility,  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for 1,3,5-trichlorobenzene.

TABLE 6.1.1.7.2

Reported vapor pressures of 1,3,5-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/(C + T/K) & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Stull 1947		Sears & Hopke 1949		Poledniecek et al. 1996			
summary of lit. data		Rodebush gauge		pressure gauge			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
63.8	666.6	measured between		0.29	solid	70.04	liquid
78.0	1333	9–28°C	solid	0.29	1.493	70.05	760.47
93.7	2666	eq. 1	P/μm	10.31	1.383	80.05	759.77
110.8	5333			10.31	4.492	88.76	126.39
121.8	7999	A	12.176	20.25	4.556	88.77	1956.9
136.0	13332	B	2956.0	20.25	12.41	89.95	1954.0
157.7	26664	mp/°C	63.45 to	30.15	12.40	90.01	2007.8
183.0	53329			30.15	34.58	99.25	2009.2
208.4	101325			30.15	34.56	99.25	3041.1
				40.09	83.96	108.75	4625.3
			63.50	40.09	83.89	118.8	6879.8
				50.09	193.4	128.8	9960.8
mp/°C	63.5			60.13	442.4	138.89	14257
				25	20.44	148.98	19754
					interpolated	159.03	27045
						169.13	36475
					solid	169.15	36355
				eq. 3a	P/Pa		
				A	32.5109		
				B	8909 70		liquid
				C	3.94116	eq. 3a	P/Pa
						A	21.1215
						B	3939.56
						C	–71.2907

2.

Blok et al. 2001					
torsion, mass-loss effusion		static-diaphragm manometer		static-diaphragm manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
	solid		solid	series I	liquid
–17.65	0.167	29.33	32.3	65.7	586
–15.65	0.218	29.34	32.3	68.1	669
–14.15	0.265	32.38	43.2	70.0	740
–12.15	0.343	32.38	43.6	72.17	828
–10.65	0.416	35.37	56.9	75.06	963
–9.15	0.502	38.38	74.0	77.84	1110
–7.15	0.643	38.39	74.4	79.57	1200

TABLE 6.1.1.7.2 (Continued)

Blok et al. 2001					
torsion, mass-loss effusion		static-diaphragm manometer		static-diaphragm manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-5.15	0.822	41.43	95.4	81.90	1350
-3.65	0.984	44.47	122	83.47	1460
-0.65	1.40	47.57	157	series II	
		50.51	197	76.43	1050
		53.61	254	84.40	1550
		57.47	253	91.37	2140
		57.48	338	98.34	2920
		57.48	344	105.31	3940
		57.48	342	112.28	5230
		57.48	341	119.25	6880
		57.49	340	123.23	7990
				127.21	9240
				131.18	10600
				135.16	12200
				139.14	13900
				142.12	15200
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 70.74$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 50.27$	
		at 298.15 K		at 375 K	

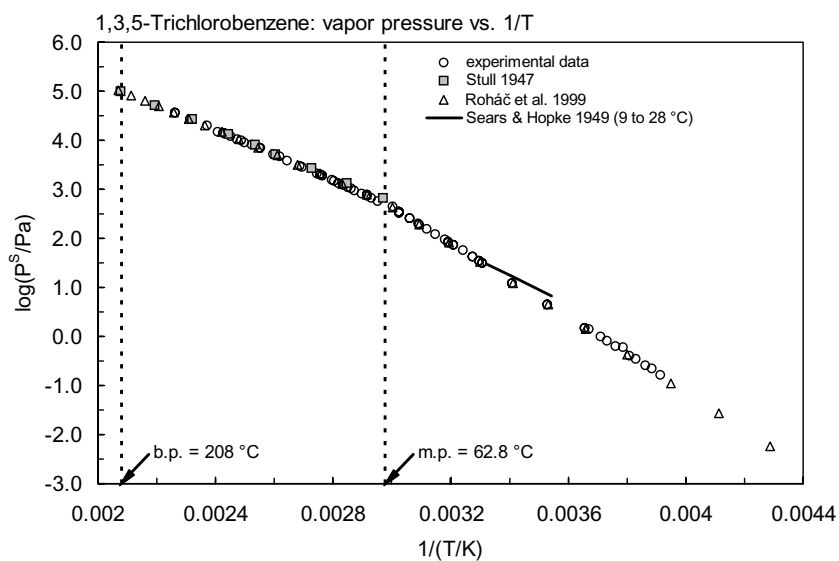
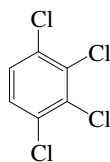


FIGURE 6.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trichlorobenzene.

## 6.1.1.8 1,2,3,4-Tetrachlorobenzene



Common Name: 1,2,3,4-Tetrachlorobenzene

Synonym:

Chemical Name: 1,2,3,4-tetrachlorobenzene

CAS Registry No: 634-66-2

Molecular Formula:  $C_6H_2Cl_4$

Molecular Weight: 215.892

Melting Point ( $^{\circ}C$ ):

47.5 (Weast 1972–73; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

254 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

142 (calculated-density, liquid molar volume, Chiou 1985)

179.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

17.0 (Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)

16.95 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

53.14 (Miller et al. 1984)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 156$  J/mol K), F: 0.602 (mp at  $47.5^{\circ}C$ )

0.608 ( $25^{\circ}C$ , Suntio et al. 1988b)

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

4.31 (shake flask-UV, Yalkowsky et al.)

3.42 (shake flask-GC, Könemann 1981)

4.32 (recommended, Horvath 1982)

3.50 ( $22^{\circ}C$ , Verschueren 1983)

12.2 (generator column-GC/ECD, Miller et al. 1984, 1985)

7.18 ( $23^{\circ}C$ , shake flask-GC, Chiou 1985)

5.92 (shake flask-HPLC, Banerjee et al. 1984)

4.33 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

12.2 (generator column-GC, Doucette & Andren 1988)

3.27 (shake flask-GC/ECD, Kim & Saleh 1990)

12.0 (shake flask-GC, Boyd et al. 1998)

1.40, 2.11, 2.80, 5.25 (5, 15, 25,  $35^{\circ}C$ , estimated- RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

133.3\* ( $68.5^{\circ}C$ , summary of literature data, temp range  $68.5$ – $254.0^{\circ}C$ , Stull 1947)

8.76 (extrapolated-Antoine eq., supercooled liquid  $P_L$ , Weast 1972–73)

5.21 (calculated-Antoine eq. from Weast 1972–73, converted to solid  $P_s$ ; Mackay & Shiu 1981)

$\log(P/mmHg) = [-0.2185 \times 12872.5/(T/K)] + 8.251056$ ; temp range  $68.5$ – $254^{\circ}C$  (Antoine eq., Weast 1972–73)

4.017, 3.49 ( $P_{GC}$  by GC-RT correlation with different GC columns, Bidleman 1984)

8.0 (supercooled liquid  $P_L$ , converted from literature  $P_s$  with  $\Delta S_{fus}$ , Bidleman 1984)

6.285 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)

2.44 (supercooled liquid  $P_L$ , extrapolated-Antoine eq., Stephenson & Malanowski 1987)



$\log (P_L/\text{kPa}) = 5.7082 - 1517.2/(-117.384 + T/\text{K})$ ; temp range 331–527 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

5.60 (selected, supercooled liquid  $P_L$ , Suntio et al. 1988b; quoted, Ballschmiter & Wittlinger 1991)

8.0 (supercooled  $P_L$ , converted from literature  $P_S$  with  $\Delta S_{\text{fus}}$ , Hinckley et al. 1990)

4.02 ( $P_{\text{GC}}$  by GC-RT correlation, Hinckley et al. 1990)

12.1 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; Spijksma et al. 1994)

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

70 (gas stripping-GC, Oliver 1985)

62.0\* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)

289 (modified EPICS method-GC, Ryu & Park 1999)

58.5 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 5.014 - 1945/(T/\text{K})$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient,  $\log K_{\text{OW}}$  or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated \* are compiled at the end of this section.:

4.72 (Leo et al. 1971)

4.46 (shake flask-GC, HPLC- $k'$  correlation, Könemann et al. 1979)

4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)

4.37 (shake flask-GC, Watarai et al. 1982)

4.94 (TLC-RT correlation, Bruggeman et al. 1982)

4.75 (shake flask-GC, Bruggeman et al. 1982)

4.41 (HPLC- $k'$  correlation, Hammers et al. 1982)

4.55 (generator column-GC, Miller et al. 1984)

4.60 (shake flask-GC, Chiou 1985)

4.65 (HPLC-RV/MS, Burkhard & Kuehl 1986)

4.61\* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)

4.60 (shake flask-GC, Pereira et al. 1988)

4.635 (shake flask/slow stirring-GC, De Bruijn et al. 1989)

4.54 (recommended, Sangster 1993)

4.64 (recommended, Hansch et al. 1995)

$4.41 \pm 0.06^*$  (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)

$\log K_{\text{OW}} = 0.6978 - 21100/[2.303 \cdot R(T/\text{K})]$ , temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)

4.30\* (estimated RP-HPLC- $k'$  correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient,  $\log K_{\text{OA}}$  at 25°C and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section:

5.64\*; 5.74 (generator column-GC; measured range –10 to 20°C, calculated, Harner & Mackay 1995)

$\log K_{\text{OA}} = -5.3 + 3254/(T/\text{K})$ ;  $\Delta H_{\text{OA}} = 62.3 \text{ kJ/mol}$  (Harner & Mackay 1995)

5.64 (calculated- $S_{\text{oct}}$  and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor,  $\log \text{BCF}$  at 25°C or as indicated:

4.86 (guppy, lipid basis, Könemann & van Leeuwen 1980)

3.25 (Briggs 1981)

3.36–3.75 mean 3.72; 4.00–4.15 mean 4.08 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

4.80–5.13 (rainbow trout, lipid basis, Oliver & Niimi 1983)

3.72–4.08 (fish, Oliver 1984)

3.70 (15°C, rainbow trout, Banerjee et al. 1984)

3.41–3.93 mean 3.80; 3.49–4.00 mean 3.91 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

3.72; .89 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)

3.38 (fathead minnow, Carlson & Kosian 1987)

4.9–5.4, 5.1; 4.1 (Niagara River plume, range, mean; calculated- $K_{\text{OW}}$ , Oliver 1987b)

- 4.70, 4.74, 4.75, 4.84 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)  
 3.36 (guppy, Van Hoogan & Opperhuizen 1988)  
 5.46, 5.70, 4.68, 5.30 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)  
 3.68; 3.79 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)  
 3.40 (guppy, steady-state conditions, rate const. ratio  $k_1/k_2$ , 96-h exposure, Sijm et al. 1993)  
 4.70 (guppy, lipid normalized BCF, Sijm et al. 1993)  
 3.72–4.08; 3.82 (*Oncorhynchus mykiss*; *Poecilia reticulata*, flow through conditions, Devillers et al. 1996)  
 3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)  
 4.28 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)  
 3.96; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

#### Sorption Partition Coefficient, log $K_{OC}$ :

- 3.49 (soil, sorption isotherm, converted from reported log  $K_{OM}$  of 3.25, Briggs 1981)  
 3.27 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)  
 3.16–4.42 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)  
 5.00; 4.90 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)  
 4.1–6.0, 5.2 (suspended sediment, average, Oliver 1987c)  
 3.52, 3.91, 3.75, 3.48, 3.52 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)  
 3.48–3.91 (soil, batch-equilibration, Kishi et al. 1990)  
 4.28 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)  
 4.26 (sediment 3.86% OC, batch sorption equilibrium, Koelmans & Lijkelma 1992)  
 4.39 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)  
 3.70, 3.64, 3.84 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)  
 4.14 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

#### Sorption Partition Coefficient, log $K_{OM}$ :

- 3.25 (soil, sorption isotherm, shake flask-GC, soil organic matter, Briggs 1981)  
 4.90 (Niagara River-organic matter, Oliver & Charlton 1984)  
 4.90–5.40; 5.10; 4.10; 4.50 (Niagara-River plume: range; average; calculated- $K_{OW}$ , algae > 50 µm, Oliver 1987b)

#### Environmental Fate Rate Constants, $k$ , or Half-Lives, $t_{1/2}$ :

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: dechlorination pseudo-first order rate constant  $k = 1.455 \text{ d}^{-1}$  with  $t_{1/2} = 0.5 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

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

$k_1 = 140 \text{ h}^{-1}$ ;  $k_2 = 0.021 \text{ h}^{-1}$  (rainbow trout, 15°C, Banerjee et al. 1984)

$k_1 = 670 \text{ mL g}^{-1} \text{ d}^{-1}$ ;  $k_2 = 0.29 \text{ d}^{-1}$  (guppy, van Hoogan & Opperhuizen 1988)

$k_1 = 670 \pm 180 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 0.29 \pm 0.06 \text{ d}^{-1}$  (guppies, 96-h exposure, Sijm et al. 1993)

$k_1 = 1807.8 \text{ h}^{-1}$ ;  $k_2 = 0.304 \text{ h}^{-1}$  (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)

$k_1 = 141 \text{ mL g}^{-1} \text{ d}^{-1}$ ,  $k_2 = 1.5 \text{ d}^{-1}$  (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

#### Half-Lives in the Environment:

Air:

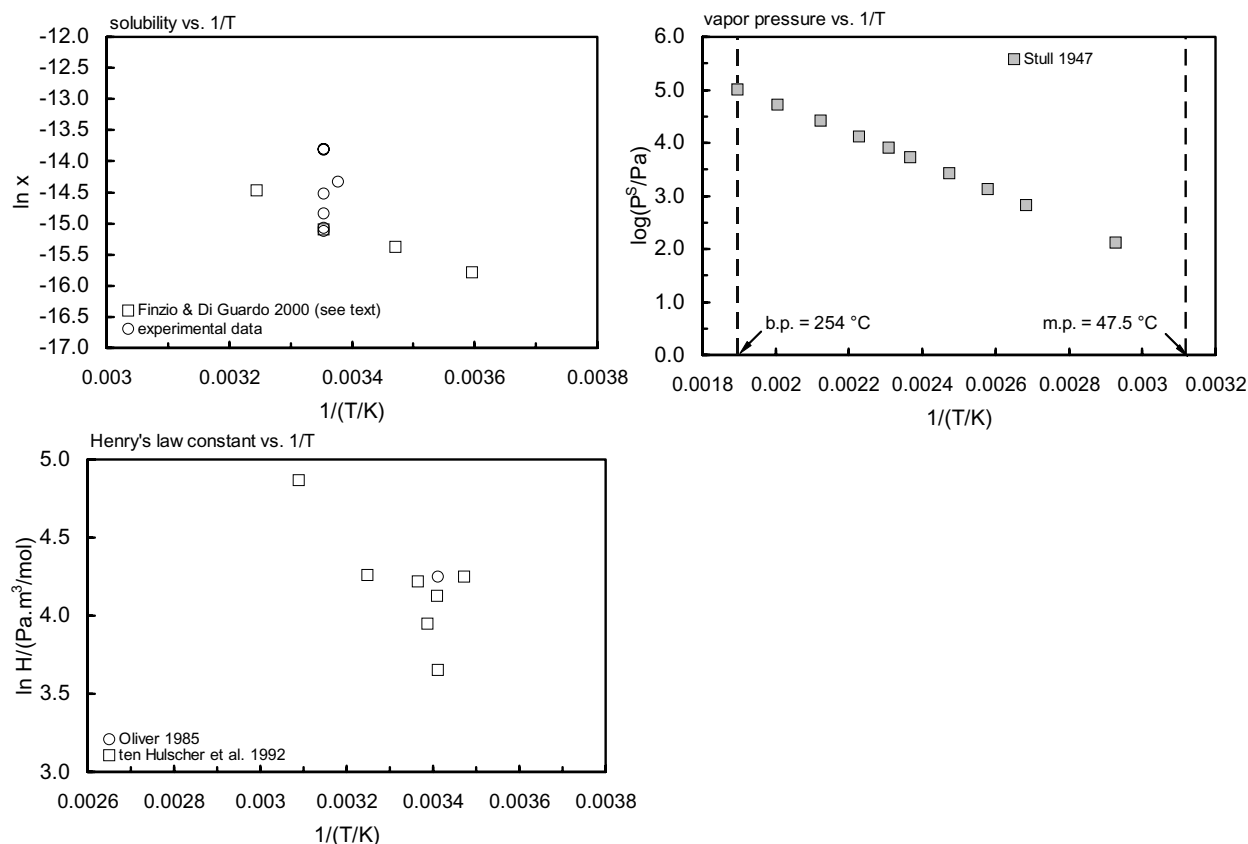
Surface Water:

Groundwater:

Sediment: dechlorination  $t_{1/2}$  = 1.8 d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).  
Soil:  
Biota: biological half-lives,  $t_{1/2}$  = 3 d in sunfish and  $t_{1/2}$  = 2 d in guppy for tetrachlorobenzenes (Niimi 1987);  
 $t_{1/2}$  < 5 d in worms at 8°C (Oliver 1987a).

**TABLE 6.1.1.8.1**  
**Reported vapor pressures and Henry’s law constants of 1,2,3,4-tetrachlorobenzene 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)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<b>Vapor pressure</b>		<b>Henry's law constant</b>	
<b>Stull 1947</b>		<b>ten Hulscher et al. 1992</b>	
<b>summary of literature data</b>		<b>gas stripping-GC</b>	
<b>t/°C</b>	<b>P/Pa</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>
68.5	133.3	14.8	48.5
99.6	666.6	20.0	62.0
114.7	1333	20.1	52.0
131.2	2666	22.1	68.1
149.2	5333	24.1	70.9
160.0	7999	34.8	129.9
175.7	13332	50.0	276.2
198.0	26664		
225.5	53329	temp dependence eq.	
254.0	101325	$\ln K_{\text{AW}} = A - B/(T/K)$	
		A	22.156
mp/°C	46.5	B	5532.84



**FIGURE 6.1.1.8.1** Logarithm of mole fraction solubility, vapor pressure and Henry's law constant versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.

**TABLE 6.1.1.8.2**

**Reported octanol-water and octanol-air partition coefficients of 1,2,3,4-tetrachlorobenzene at various temperatures**

log K <sub>OW</sub>				log K <sub>OA</sub>			
Opperhuizen et al. 1988		Bahadur et al. 1997		Finizio & Di Guardo 2001		Harner & Mackay 1995	
shake flask-GC/ECD		shake flask-GC/ECD		GC-RT correlation		generator column-GC	
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
13	4.83	5	4.65	5	4.52	25	5.64
19	4.61	15	4.53	15	4.4	-10	7.076
28	4.37	25	4.41	25	4.30	0	6.64
33	4.66	35	4.28	35	4.11	9.88	6.213
		45	4.15			19.85	5.818
$\Delta H/(\text{kJ mol}^{-1}) = -26.3$		enthalpy of transfer				$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 62.03$	
		$\Delta H/(\text{kJ mol}^{-1}) = -21.1$					
		$\log K_{\text{OW}} = A - \Delta H/2.303RT$				$\log K_{\text{OA}} = A + B/T$	
		A	0.6978			A	-5.3
		$\Delta H$	-21100			B	3254

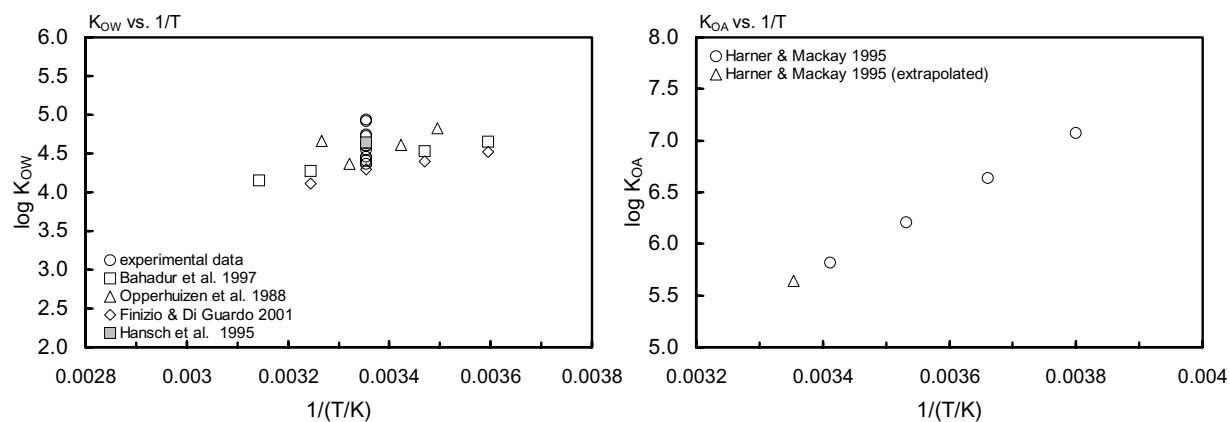
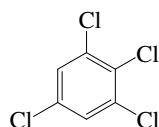


FIGURE 6.1.1.8.2 Logarithm of  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.

## 6.1.1.9 1,2,3,5-Tetrachlorobenzene



Common Name: 1,2,3,5-Tetrachlorobenzene

Synonym:

Chemical Name: 1,2,3,5-tetrachlorobenzene

CAS Registry No: 634-90-2

Molecular Formula:  $C_6H_2Cl_4$

Molecular Weight: 215.892

Melting Point ( $^{\circ}C$ ):

54.5 (Weast 1972–73; 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

246 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

179.6 (calculated-Le Bas method at normal boiling point)

141.0 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

19.0 (Miller et al. 1984; Chickos et al. 1999)

19.32 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

58.576 (Miller et al. 1984)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.514 (mp at  $54.5^{\circ}C$ )

0.556 (Suntio et al. 1988b)

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

3.50 (shake flask-UV, Yalkowsky et al. 1979)

4.02 (shake flask-LSC, Banerjee et al. 1980)

4.11, 17.1 (LSC- $^{14}C$ , calculated- $K_{ow}$ , Veith et al. 1980)

2.48 (shake flask-GC, Könemann 1981)

3.51 (recommended, Horvath 1982)

2.40 ( $22^{\circ}C$ , Verschueren 1983)

5.10 (shake flask-HPLC, Banerjee 1984)

2.89 (generator column-GC/ECD, Miller et al. 1984, 1985)

3.23 (shake flask-GC, Chiou 1985)

3.46 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

4.32 (generator column-GC, Doucette & Andren 1988)

4.32 (shake flask-GC/ECD, Kim & Saleh 1990)

4.52 (shake flask-GC/ECD, Tam et al. 1996)

$3.44 \pm 0.15^*$ ,  $3.79 \pm 0.23$  (generator column-GC/ECD, shake flask-GC at  $27^{\circ}C$ , Shiu et al. 1997)

$\ln x = -4.4222 - 3162.74/(T/K)$ ; temp range  $5-50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

133.3\* ( $58.2^{\circ}C$ , summary of literature data, temp range  $58.2-246^{\circ}C$ , Stull 1947)

18.6 (extrapolated-supercooled liquid  $P_L$ , Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 11982.1/(T/K)] + 7.925176$ ; temp range  $58.2-246^{\circ}C$  (Antoine eq., Weast 1972–73)

9.80 (solid  $P_s$ , calculated from extrapolated vapor pressure  $P_L$  with a fugacity ratio correction, Mackay & Shiu 1981)

- 5.085 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)  
 17.2; 9.56 (extrapolated-Antoine eq., supercooled liquid  $P_L$ , converted to  $P_S$ , Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.7756 - 2394/(-17.85 + T/K)$ ; temp range 331–519 K (liquid, Antoine eq., Stephenson & Malanowski 1987)  
 15.1 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; Spieksma et al. 1994)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at 25°C):

- 159 (batch stripping-GC, Mackay & Shiu 1981)  
 99 (20°C, gas stripping-GC, ten Hulscher et al. 1992)  
 160 (gas stripping-GC, Shiu & Mackay 1997)

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

Additional data at other temperatures designated \* are compiled at the end of this section.:

- 4.50, 4.92 (shake flask-GC, HPLC-k' correlation, Könemann et al. 1979)  
 4.46 (HPLC-RT correlation, Veith et al. 1979b)  
 4.46, 5.0 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)  
 4.52 (shake flask-LSC, Banerjee et al. 1980)  
 5.05 (head-space GC, Hutchinson et al. 1980)  
 4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)  
 4.56 (shake flask-GC, Watarai et al. 1982)  
 4.53 (HPLC-k' correlation, Hammers et al. 1982)  
 4.51 (generator-column-GC/ECD, Miller et al. 1984; 1985)  
 4.61–4.73 (HPLC-RV correlation, Garst 1984)  
 4.59 (shake flask-GC, Chiou 1985)  
 4.59 (shake flask-GC, Pereira et al. 1988)  
 4.658 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 4.63 (recommended, Sangster 1993)  
 4.66 (recommended, Hansch et al. 1995)  
 4.55\*  $\pm$  -0.02 (shake flask-GC/ECD, Bahadur et al. 1997)  
 $\log K_{OW} = 1.0159 - 20200/[2.303 \cdot R(T/K)]$ ; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)

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:

- 5.55 (calculated- $S_{oct}$  and vapor pressure  $P$ , Abraham et al. 2001)  
 5.78\* (20°C, HPLC-k' correlation, measured range 10–50°C, Su et al. 2002)  
 $\log K_{OA} = 66320/(2.303 \cdot RT) - 6.086$ ; temp range 10–50°C (HPLC-k' correlation, Su et al. 2002)

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

- 3.26 (fathead minnow, Veith et al. 1979b)  
 4.86 (guppy-lipid basis, Könemann et al. 1979)  
 4.15, 4.86 (guppy-lipid basis, Könemann & van Leeuwen 1980)  
 3.26 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)  
 4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)  
 3.46 (22°C, bluegill sunfish, Banerjee et al. 1984)  
 3.59 (fish, calculated-concentration ratio  $C_A/C_W$  or  $k_1/k_2$ , Connell & Hawker 1988; Hawker 1990)  
 4.73 (guppy-lipid phase, 12 to 31-d exposure studies, Gobas et al. 1989)  
 5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)  
 3.64–4.89 (*Poecilia reticulata*, quoted lit., flow through conditions, Devillers et al. 1996)  
 3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)  
 4.27 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)  
 4.11; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient,  $\log K_{OC}$ :

- 3.49 (soil, sorption isotherm, converted from reported  $\log K_{OM}$  of 3.25, Briggs 1981)

- 3.20 (Koch 1983)  
 4.25 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)  
 $3.94 \pm 0.33$  (suspended particulates in coastal waters, Masunaga et al. 1996)

Sorption Partition Coefficient,  $\log K_{OM}$ :

- 3.20, 2.98 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: dechlorination pseudo-first order rate constant  $k = 0.639 \text{ d}^{-1}$  with  $t_{1/2} = 1.1 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

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

$k_1 = 15000 \text{ d}^{-1}$ ;  $k_2 = 0.26 \text{ d}^{-1}$  (guppy, Könemann & van Leeuwen 1980)

$k_1 = 74 \text{ h}^{-1}$ ;  $k_2 = 0.026 \text{ h}^{-1}$  (bluegill sunfish, Banerjee et al. 1984)

$k_1 = 33.8 \text{ h}^{-1}$ ;  $1/k_2 = 92.0 \text{ h}$  (guppy, Hawker & Connell 1985)

$k_1 = 810 \text{ d}^{-1}$  (fish quoted, Opperhuizen 1986)

$\log k_1 = 2.91 \text{ d}^{-1}$ ;  $\log 1/k_2 = -0.42 \text{ d}$  (guppy, quoted, Connell & Hawker 1988)

$\log k_1 = 3.00 \text{ d}^{-1}$ ;  $\log k_2 = -0.59 \text{ d}^{-1}$  (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)

$\log k_2 = -0.58 \text{ d}^{-1}$  (fish, calculated- $K_{OW}$ , Thomann 1989)

$k_1 = 1807.8 \text{ h}^{-1}$ ;  $k_2 = 0.304 \text{ h}^{-1}$  (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)

$k_1 = 131 \text{ mL g}^{-1} \text{ d}^{-1}$ ,  $k_2 = 1.4 \text{ d}^{-1}$  (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air:

Surface Water:

Groundwater:

Sediment: dechlorination  $t_{1/2} = 1.8 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota:  $t_{1/2} = 2\text{--}4 \text{ d}$  in fish (Veith et al. 1980);

$2 < t_{1/2} < 4 \text{ d}$  in bluegill sunfish (Barrows et al. 1980).



TABLE 6.1.1.9.1

Reported aqueous solubilities, vapor pressures, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3,5-tetrachlorobenzene at various temperatures

Aqueous solubility		Vapor pressure		log K <sub>OW</sub>		log K <sub>OA</sub>	
Shiu et al. 1997		Stull 1947		Bahadur et al. 1997		Su et al. 2002	
shake flask-GC		summary of literature data		shake flask-GC/ECD		GC-RT correlation	
t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
5	1.7	58.2	133.3	5	4.8	10	6.15
15	2.43	89	666.6	15	4.67	20	5.78
25	3.44	104.1	1333	25	4.55	30	5.43
35	5.08	121.6	2666	35	4.42	40	5.11
45	7.03	140	5333	45	4.33	50	4.8
$\Delta H_{\text{sol}} = 26.3 \text{ kJ/mol}$		142	7999	enthalpy of transfer $\Delta H/(\text{kJ mol}^{-1}) = -20.2$		$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 66.32$	
		168	13332			$\log K_{\text{OA}} = A + B/2.303RT$	
		193.7	26664			A	-6.086
		220	53329	$\log K_{\text{OW}} = A - B/2.303RT$		B	66320
		246	101325	A		1.0195	
		mp/°C	54.5	$\Delta H$		-20200	

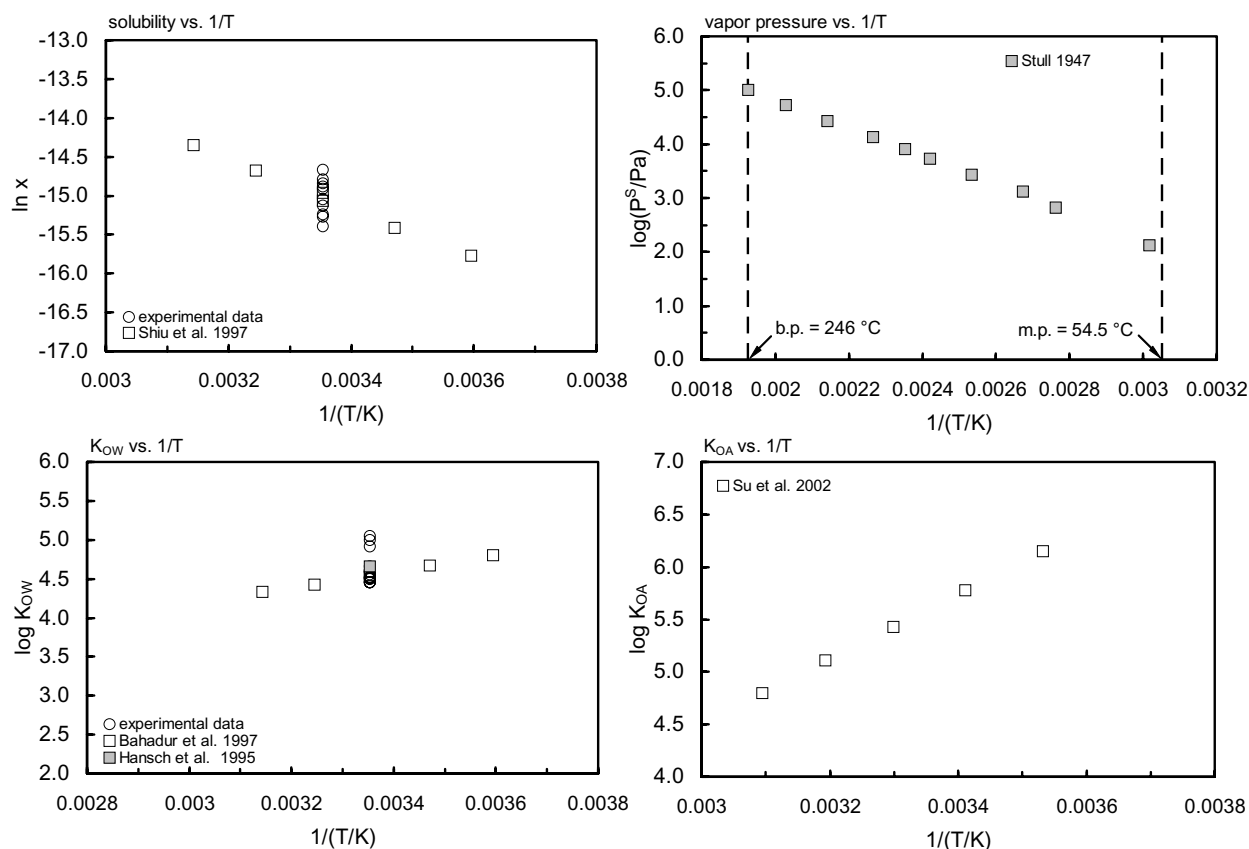
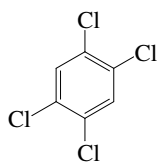


FIGURE 6.1.1.9.1 Logarithm of mole fraction solubility, vapor pressure, K<sub>OW</sub> and K<sub>OA</sub> versus reciprocal temperature for 1,2,3,5-tetrachlorobenzene.

## 6.1.1.10 1,2,4,5-Tetrachlorobenzene



Common Name: 1,2,4,5-Tetrachlorobenzene

Synonym:

Chemical Name: 1,2,4,5-tetrachlorobenzene

CAS Registry No: 95-94-3

Molecular Formula:  $C_6H_2Cl_4$

Molecular Weight: 215.892

Melting Point ( $^{\circ}C$ ):

139.5 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

244.5 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.858 ( $22^{\circ}C$ , Weast 1972–1973; Horvath 1982; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

116.2 ( $22^{\circ}C$ , calculated-density)

179.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

23.64 (Miller et al. 1984)

24.10 (Ruelle & Kesselring 1993; Chickos et al. 1999)

29.94 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

58.576 (Miller et al. 1984)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.0753 (mp at  $139.5^{\circ}C$ )

0.073 (Suntio et al. 1988b)

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

0.595 (shake flask-UV, Yalkowsky et al. 1979)

0.29 (shake flask-GC, Könemann 1981)

0.596 (recommended, Horvath 1982)

0.30 ( $22^{\circ}C$ , quoted, Verschueren 1983)

2.35 (generator column-GC/ECD, Miller et al. 1984, 1985)

0.465 (shake flask-HPLC, Banerjee 1984)

0.606 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

0.56 (shake flask-GC/ECD, Kim & Saleh 1990)

$0.528^* \pm 0.018$ ,  $0.543 \pm 0.016$  (generator column-GC/ECD, shake flask-GC at  $27^{\circ}C$ , Shiu et al. 1997)

2.20 (shake flask-GC, Boyd et al. 1998)

$\ln x = -4.529 - 3708.6/(T/K)$ ; temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

$5333^*$  ( $146.0^{\circ}C$ , summary of literature data, temp range  $146.0$ – $245^{\circ}C$ , Stull 1947)

10.1 (extrapolated-Antoine eq., supercooled liquid  $P_L$ , Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 12828.8/(T/K)] + 8.282213$ ; temp range  $146$ – $245^{\circ}C$  (Antoine eq., Weast 1972–73)

0.72 ( $P_S$  converted from  $P_L$  of Weast 1972–73, Mackay & Shiu 1981)

0.20 (evaporation rate, Dobbs & Cull 1982)

2.163 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)

- 2.98, 0.22 (supercooled liquid  $P_L$ , solid  $P_S$ , Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 9.1357 - 4642.36/(132.952 + T/\text{K})$ ; temp range 419–518 K (liquid, Antoine eq., Stephenson & Malanowski 1987)  
 7.497 (GC-RT correlation, Watanabe & Tatsukawa 1989)  
 0.615 (calculated-UNIFAC activity coefficients, Banerjee et al. 1990)  
 15.1; 12.5 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; quoted lit., Spijksma et al. 1994)  
 0.392\* (24.65°C, torsion, mass-loss effusion, measured range 17–32.5°C, Blok et al. 2001)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at 25°C):

- 101 (gas stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section:

- 4.72 (Leo et al. 1971)  
 4.82, 4.56 (shake flask-GC, HPLC- $k'$  correlation, Könemann et al. 1979)  
 4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)  
 4.46 (shake flask-GC, Watarai et al. 1982)  
 4.52 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 4.51 (generator column-GC/ECD, Miller et al. 1984, 1985)  
 4.70 (shake flask-GC, Chiou 1985)  
 4.60 (HPLC- $k'$  correlation, Mailhot 1987)  
 5.16 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)  
 4.604 (slow stirring-GC, De Bruijn et al. 1989)  
 5.16 (calculated-fragment const., De Bruijn et al. 1989)  
 4.70 (shake flask-GC, Pereira et al. 1988)  
 4.63 (recommended, Sangster 1993)  
 4.70 (recommended, Hansch et al. 1995)  
 4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)  
 4.44\* (estimated- RP-HPLC- $k'$  correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C and the reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.:

- 5.63\*; 5.81 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)  
 $\log K_{OA} = -5.0 + 3176/(T/\text{K})$ ;  $\Delta H_{OA} = 60.8 \text{ kJ/mol}$  (Harner & Mackay 1995)  
 5.62, 5.63 (calculated- $S_{oct}$  and vapor pressure  $P$ , quoted lit., Abraham et al. 2001)

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

- 0.20 (rats, adipose tissue, Geyer et al. 1980)  
 3.65 (fish, flowing water, Kenaga & Goring 1980; Kenaga)  
 3.36–3.79 mean 3.72; 4.04–4.18 mean 4.11 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)  
 4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)  
 3.72–4.11 (fish, Oliver 1984)  
 2.80 (Tadokoro & Tomita 1987)  
 3.89 (green algae, Mailhot 1987)  
 4.08 (guppy, concn ratio of  $C_{fish}/C_{water}$ , Opperhuizen & Voors 1987)  
 5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)  
 2.76 (*picea omorika*, Reischl et al. 1989)  
 3.61, 4.70 (American flagfish: whole fish, fish lipid, Smith et al. 1990)  
 3.20 (fish, calculated, Figueroa & Simmons 1991)  
 3.72–4.11; 3.61 (*Oncorhynchus mykiss*; *Jordanella floridae*, quoted lit., flow through conditions, Devillers et al. 1996)  
 3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)  
 3.72, 4.80; 3.517, 3.417 (quoted: whole fish, lipid content; calculated-MCI  $\chi$ , calculated- $K_{OW}$ , Lu et al. 1999)

3.89; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

#### Sorption Partition Coefficient, log $K_{OC}$ :

3.20 (Kenaga 1980a)  
 3.49 (soil, sorption isotherm, converted from reported log  $K_{OM}$  of 3.25, Briggs 1981)  
 3.36 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)  
 3.24–4.50 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)  
 5.10; 4.70 (field data of sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)  
 2.79 (McLaurin sandy loam, OC 0.66%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)  
 3.94 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)  
 3.48 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

#### Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation:  $t_{1/2}$  = 763.1–7631 h, based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: base rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  at 25°C with a calculated  $t_{1/2} > 900 \text{ yr}$  at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)  
 first order hydrolysis  $t_{1/2} > 879 \text{ yr}$  (Howard et al. 1991)

Biodegradation:  $t_{1/2}$ (aerobic) = 672–4320 h, based on unacclimated aerobic screening test data;  $t_{1/2}$ (anaerobic) = 2880–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

dechlorination pseudo-first order  $k = 0.037 \text{ d}^{-1}$  with  $t_{1/2} = 18.7 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

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

$k_1 = 1490 \text{ mL g}^{-1} \text{ d}^{-1}$ ;  $k_2 = 0.14 \text{ d}^{-1}$  (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

$k_1 = 1630 \text{ d}^{-1}$ , 171000  $\text{d}^{-1}$ ;  $k_2 = 0.4 \text{ d}^{-1}$ , 0.34  $\text{d}^{-1}$  (American flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 0.4 \text{ d}^{-1}$ , 2.35  $\text{d}^{-1}$  (American flagfish: bioconcentration data, toxicity data, Smith et al. 1990)

$k_1 = 1807.8 \text{ h}^{-1}$ ;  $k_2 = 0.304 \text{ h}^{-1}$  (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)

#### Half-Lives in the Environment:

Air:  $t_{1/2}$  = 763.1–7631 h, based on photooxidation half-life in air (Howard et al. 1991)

Surface Water: hydrolysis  $t_{1/2} > 900 \text{ yr}$  at pH 7 and 25°C (Ellington et al. 1988)

$t_{1/2}$  = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater:  $t_{1/2}$  = 1344–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment: dechlorination  $t_{1/2} = 18.7 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:  $t_{1/2}$  = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota:  $t_{1/2} < 5 \text{ d}$  in worms at 8°C (Oliver 1987a);

biological  $t_{1/2} = 3 \text{ d}$  in sunfish,  $t_{1/2} = 2 \text{ d}$  in guppy for tetrachlorobenzenes (Niimi 1987);

$t_{1/2} = 33 \text{ d}$  in *Picea omorika* (Reischl et al. 1989);

$t_{1/2} = 1.72 \text{ d}$  clearance from American flagfish (Smith et al. 1990);

elimination  $t_{1/2} = 2.01 \text{ d}$  from earthworm in water (Belfroid et al. 1993);

elimination  $t_{1/2} = 0.204 \text{ d}$  and 2.63 d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994).

TABLE 6.1.1.10.1

Reported aqueous solubilities and vapor pressures of 1,2,4,5-tetrachlorobenzene 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)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Aqueous solubility		Vapor pressure					
Shiu et al. 1997	Stull 1947	Blok et al. 2001					
shake flask-GC	summary of literature data	torsion, mass loss effusion	static-diaphragm manometer				
t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
5	0.298	146.0	5333	16.85	0.155	99.74	328
15	0.322	157.7	7999	19.45	0.212	104.82	461
25	0.528	173	13332	22.05	0.289	108.83	612
35	0.739	196	26664	24.65	0.392	113.82	844
45	1.127	220.5	53329	27.25	0.528	117.74	1100
		245	101325	29.85	0.707	121.82	1140
$\Delta H_{\text{sol}} = 30.8 \text{ kJ/mol}$				32.45	0.943	125.84	1820
	mp/°C					129.82	2310
				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 82.10$		132.79	2770
				at 353 K		136.82	3500

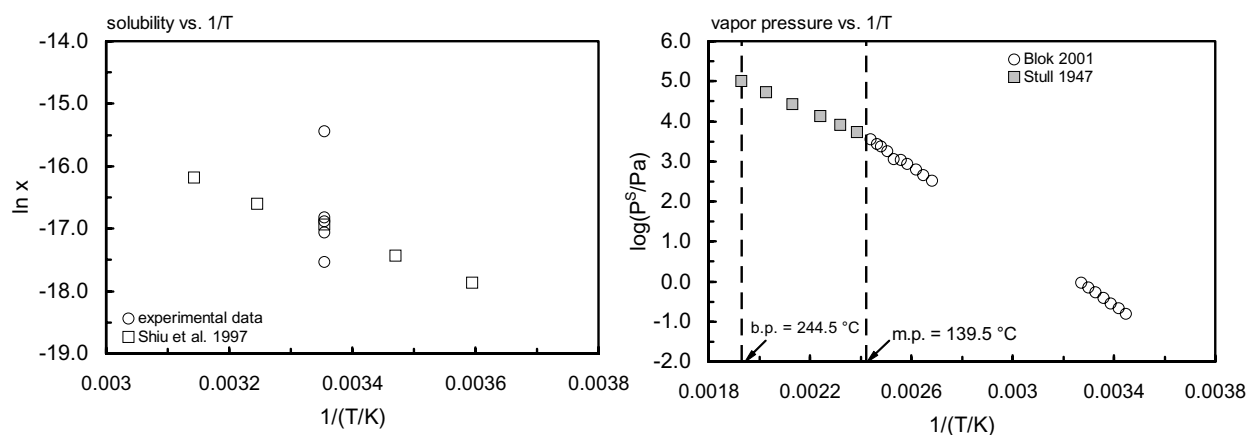


FIGURE 6.1.1.10.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.

TABLE 6.1.1.10.2

Reported octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4,5-tetrachlorobenzene at various temperatures

log K <sub>OW</sub>		log K <sub>OA</sub>	
Finizio & Di Guardo 2001		Harner & Mackay 1995	
GC-RT correlation		generator column-GC	
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
5	4.63	25	5.63
15	4.54	-10	7.056
25	4.44	0	6.622
35	4.26	9.88	6.204
		19.85	5.829
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 60.8$	
		$\log K_{OA} = A + B/T$	
		A	-5.0
		B	3176

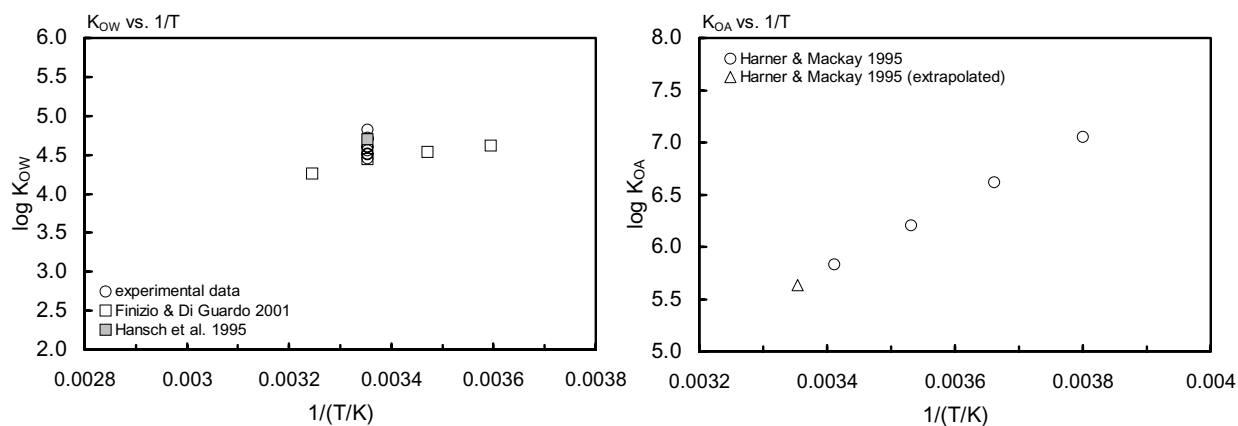
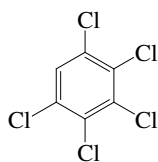


FIGURE 6.1.1.10.2 Logarithm of K<sub>OW</sub> and K<sub>OA</sub> versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.

## 6.1.1.11 Pentachlorobenzene



Common Name: Pentachlorobenzene

Synonym:

Chemical Name: Pentachlorobenzene

CAS Registry No: 608-93-5

Molecular Formula:  $C_6HCl_5$

Molecular Weight: 250.337

Melting Point ( $^{\circ}C$ ):

86 (Weast 1972–73; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

277 (Weast 1972–72; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.8342 (16.5 $^{\circ}C$ , Weast 1972–73; Horvath 1982)

Molar Volume ( $cm^3/mol$ ):

136.5 (16.5 $^{\circ}C$ , calculated-density, Weast 1972–73; Horvath 1982)

166 (liquid molar volume, Chiou 1985)

200.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

20.585 (Miller et al. 1984)

20.60 (Ruelle et al. 1993; Chickos et al. 1999)

20.1 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

57.74 (Miller et al. 1984)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K.), F: 0.252 (mp at  $86^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

0.56 (shake flask-UV, Yalkowsky et al. 1979)

1.33 (shake flask-LSC, Banerjee et al. 1980)

0.135 (Kenaga & Goring 1980; Kenaga 1980a)

1.34 (shake flask-LSC- $^{14}C$ , Veith et al. 1980)

0.24 (shake flask-GC, Könnemann 1981)

0.562 (recommended, Horvath 1982)

0.831 (generator column-GC/ECD, Miller et al. 1984, 1985)

0.385 (23 $^{\circ}C$ , shake flask-GC, Chiou 1985)

0.180 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.552 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

3.46 (calculated- $K_{ow}$  and HPLC-RT correlation, Chin et al. 1986)

$0.419^* \pm 0.018$ ,  $0.447 \pm 0.014$  (generator column-GC/ECD, shake flask-GC/ECD at  $27^{\circ}C$ , Shiu et al. 1997)

0.87 (shake flask-GC, Boyd et al. 1998)

$\ln x = -3.61482 - 4093.10/(T/K)$ ; temp range 5–50 $^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

2.75, 3.50 (supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

133\* (98.6 $^{\circ}C$ , summary of literature data, temp range 98.6–276 $^{\circ}C$ , Stull 1947)

- 0.889 (extrapolated-Antoine eq., supercooled liquid  $P_L$ , Weast 1972–73)  
 0.219 ( $P_S$  calculated from  $P_L$  of Weast 1972–73; Mackay & Shiu 1981)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 15124.2/(T/K)] + 8.907497$ ; temp range 98.6–276°C (Antoine eq., Weast 1972–73)  
 1.44 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)  
 1.08, 0.28 (supercooled liquid  $P_L$ , solid  $P_S$ , Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 8.00795 - 3325.33/(4.814 + T/K)$ ; temp range 371–549 K (liquid, Antoine eq., Stephenson & Malanowski 1987)  
 1.718 (GC-RT correlation, Watanabe & Tatsukawa 1989)  
 2.49; 2.19 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; quoted lit., Spijksma et al. 1994)  
 0.212; 0.39\* (25°C extrapolated; 30.3°C, static method-pressure gauge, measured range 30.3–179°C, Polednicek et al. 1996)  
 $\ln (P_S/\text{Pa}) = 30.4445 - 8654.67/[(T/K) - 27.6534]$ ; temp range 303.45–353.17 K (solid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)  
 $\ln (P_L/\text{Pa}) = 23.4783 - 6188.33/[(T/K) - 34.6922]$ ; temp range 371.8–452.29 K (liquid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)  
 0.11\* (20°C, recommended, summary of literature data, temp range 233.15–503.15 K, Roháč et al. 1999)  
 $\ln [(P_S/\text{Pa})/67.0] = [1 - (T/K)/357.0] \cdot \exp\{3.431590 - 1.8864070 \times 10^{-4} \cdot (T/K)\}$ ; temp range 300–353 K (Cox eq., solid, recommended, Roháč et al. 1999)  
 $\ln [(P_L/\text{Pa})/67.0] = [1 - (T/K)/357.0] \cdot \exp\{3.419638 - 1.1673259 \times 10^{-3} \cdot (T/K) + 7.7842905 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range 365–452 K (Cox eq., liquid recommended, Roháč et al. 1999)  
 $\log (P/\text{kPa}) = 15.6174 - 4831.4/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)  
 1.2, 1.0 (supercooled liquid  $P_L$ : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)  
 $\log (P_L/\text{Pa}) = -3220/(T/K) + 10.87$  (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

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

- 71.9 (gas stripping-GC, Oliver 1985)  
 59.0\* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)  
 52.6 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 5.607 - 2132/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)  
 74, 70 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)  
 $\log K_{AW} = -2026/(T/K) + 5.27$  (LDV linear regression of literature data, Shen & Wania 2005)

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

- 5.79 (calculated-fragment const., Yalkowsky et al. 1979)  
 4.88, 5.52 (shake flask-GC, HPLC- $k'$  correlation, Könnemann et al. 1979)  
 4.94 (shake flask-LSC, Banerjee et al. 1980)  
 4.94, 5.29 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)  
 5.17 (shake flask-GC, Watarai et al. 1982)  
 5.06 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 5.69 (HPLC-RT correlation, Bruggeman et al. 1982)  
 5.03 (generator column-GC/ECD, Miller et al. 1984; 1985)  
 5.17 (shake flask-HPLC, Banerjee 1984)  
 5.11–5.21 (HPLC-RV correlation, Garst 1984)  
 5.20 (shake flask-GC, Chiou 1985)  
 4.97 (calculated- $K_{OW}$  and HPLC-RT correlation, Chin et al. 1986)  
 6.12 (HPLC- $k'$  correlation, De Kock & Lord 1987)  
 5.47 (HPLC-RT correlation, Doucette & Andren 1988)  
 5.20 (shake flask-GC, Pereira et al. 1988)  
 5.05\* (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)  
 5.183 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 5.17 (recommended, Sangster 1993)  
 5.18 (recommended, Hansch et al. 1995)  
 4.94\*  $\pm 0.03$  (shake flask-GC/ECD, Bahadur et al. 1997)



$\log K_{OW} = 0.9255 - 22800/[2.303 \cdot R(T/K)]$ ; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)  
 5.67–5.78 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)  
 5.08, 5.19 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

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:

6.27\*; 6.46 (generator column-GC, measured range –10 to 20°C, calculated, Harner & Mackay 1995)  
 7.93, 7.418, 6.931, 6.539 (–10, 0, 10, 18.7°C, generator column-GC, Harner & Mackay 1995)  
 $\log K_{OA} = -6.2 + 3722.3/(T/K)$ ; temp range –10 to 20°C,  $\Delta H_{OA} = 72.3$  kJ/mol (generator column-GC, Harner & Mackay 1995)  
 6.50 (calculated- $K_{OW}/K_{AW}$ , Wania & Mackay 1996)  
 6.49, 6.27 (calculated- $S_{oct}$  and vapor pressure P, quoted lit., Abraham et al. 2001)  
 6.90, 6.73 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

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

3.89 (trout muscle, Neely et al. 1974)  
 3.70 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980a)  
 5.40 (guppy, lipid content, Könemann et al. 1979)  
 3.53 (bluegill sunfish, Veith et al. 1980)  
 3.53 (bluegill sunfish, whole body, flow system, Barrows 1980)  
 5.41 (guppy, lipid basis, Könemann & van Leeuwen 1980)  
 3.84 (fish, flowing water, Garten & Trabalka 1983)  
 3.46–4.15 mean 4.11; 4.26–4.36 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)  
 5.19–5.36 (rainbow trout, lipid basis, Oliver & Niimi 1983)  
 4.11–4.30 (rainbow trout, Oliver 1984)  
 3.71 (22°C, bluegill sunfish, 1.5% lipid, Banerjee et al. 1984)  
 3.65; 3.86 (15°C, rainbow trout, 1.8% lipid; guppy, 2.8% lipid, Banerjee et al. 1984)  
 3.60; 3.49 (algae: exptl.; calculated, Geyer et al. 1984)  
 3.65 (algae, Freitag et al. 1984; Halfon & Reggiani 1986)  
 3.48 (fish, Freitag et al. 1984; Halfon & Reggiani 1986)  
 3.48, 3.65, 4.16 (fish, algae, activated sludge, Freitag et al. 1985)  
 4.23 (guppy, calculated-rate constants ratio  $k_1/k_2$ , Opperhuizen et al. 1985)  
 3.92 (fathead minnow, Carlson & Kosian 1987)  
 2.83, 2.65 (human fat, Geyer et al. 1987)  
 4.28, 4.30 (worm, fish, Oliver 1987a)  
 3.36–3.42 (fish, Tadokoro & Tomita 1987)  
 5.46 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1989)  
 3.87 (*picea omorika*, Reischl et al. 1989)  
 5.33 (fish, calculated- $K_{OW}$ , Thomann 1989)  
 4.14, 2.96, 4.23 (fish, Connell & Hawker 1988; Hawker 1990)  
 5.11, 5.18, 5.20, 5.28 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)  
 3.67 (guppy, Van Hoogan & Opperhuizen 1988)  
 5.93, 6.12, 4.96, 5.57 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)  
 4.22 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption, Koelmans et al. 1993)  
 3.70 (guppy, steady-state conditions, rate const. ratio  $k_1/k_2$ , 96-h exposure, Sijm et al. 1993)  
 5.00 (guppy, lipid normalized BCF, Sijm et al. 1993)  
 4.11–4.30; 2.94–4.36; 3.53 (*Oncorhynchus mykiss*; *Poecilia reticulata*; *Lepomis macrochirus*, quoted lit., flow through conditions, Devillers et al. 1996)  
 5.22–5.50 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)  
 4.11, 5.19; 3.797, 3.877 (quoted: whole fish, lipid content; calculated-MCI  $\chi$ , calculated- $K_{OW}$ , Lu et al. 1999)  
 4.09; 3.96 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient,  $\log K_{OC}$ :

- 4.11 (Kenaga 1980a)
- 5.30; 5.40 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
- 4.60 (bottom sediment, Karickhoff & Morris 1985)
- 4.9–6.2, 5.8 (suspended sediment, average, Oliver 1987c)
- 5.7 (algae > 50  $\mu\text{m}$ , Oliver 1987c)
- 5.50–5.90, 5.70 (Niagara River plume: range, average, Oliver 1987b)
- 4.49 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
- 4.68 (lake sediment 2.5% OC, batch sorption equilibrium, Schrap et al. 1994)
- 4.59  $\pm$  0.41 (suspended particulates in coastal waters, Masunaga et al. 1996)
- 4.91 (sediment: organic carbon OC  $\geq$  0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation:  $t_{1/2} = 1088\text{--}10877$  h, based on estimated rate constant for the vapor phase reaction with OH radicals in air (Howard et al. 1991)

Hydrolysis: base rate constant  $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$  at 25°C with a calculated  $t_{1/2} > 900$  yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)  
first order  $t_{1/2} > 879$  yr (Howard et al. 1991)

Biodegradation:  $t_{1/2}(\text{aerobic}) = 4656\text{--}8280$  h, based on estimated unacclimated aerobic soil grab sample data;  
 $t_{1/2}(\text{anaerobic}) = 18642\text{--}33120$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

dechlorination pseudo-first order rate constant  $k = 0.557 \text{ d}^{-1}$  with  $t_{1/2} = 1.2$  d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

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

- $k_1 = 18.76 \text{ h}^{-1}$ ;  $k_2 = 0.00238 \text{ h}^{-1}$  (trout, Neely et al. 1974)
- $k_1 = 22000 \text{ d}^{-1}$ ;  $k_2 = 0.14 \text{ d}^{-1}$  (guppy, Könemann & van Leeuwen 1980)
- $k_1 = 130 \text{ d}^{-1}$ ;  $k_2 = 0.15 \text{ d}^{-1}$  (guppy, Bruggeman et al. 1984)
- $k_1 = 110 \text{ h}^{-1}$ ;  $k_2 = 0.021 \text{ h}^{-1}$  (22°C, bluegill sunfish, Banerjee et al. 1984)
- $k_1 = 170 \text{ h}^{-1}$ ;  $k_2 = 0.036 \text{ h}^{-1}$  (15°C, rainbow trout, Banerjee et al. 1984)
- $k_1 = 98 \text{ h}^{-1}$ ;  $k_2 = 0.014 \text{ h}^{-1}$  (15°C, guppy, Banerjee et al. 1984)
- $k_1 = 5.4 \text{ h}^{-1}$ ;  $1/k_2 = 160 \text{ h}$  (guppy, quoted, Hawker & Connell 1985)
- $k_1 = 1400 \text{ d}^{-1}$ ;  $k_2 = 0.078 \text{ d}^{-1}$  (guppy, Opperhuizen et al. 1985)
- $k_1 = 1200 \text{ d}^{-1}$  (fish, quoted, Opperhuizen 1986)
- $k_2 = 0.00309, 0.00402 \text{ d}^{-1}$  (rainbow trout, calc-fish mean body weight, Barber et al. 1988)
- $\log k_1 = 3.08 \text{ d}^{-1}$ ;  $\log 1/k_2 = 0.96 \text{ d}$  (fish, quoted, Connell & Hawker 1988)
- $k_1 = 710 \text{ mL g}^{-1} \text{ d}^{-1}$ ;  $k_2 = 0.15 \text{ d}^{-1}$  (guppy, Van Hoogan & Opperhuizen 1988)
- $\log k_1 = 3.24 \text{ d}^{-1}$ ;  $\log k_2 = -0.96 \text{ d}^{-1}$  (guppy, 12 to 31-d exposure studies, Gobas et al. 1989a)
- $k_1 = 0.049 \text{ h}^{-1}$ ;  $k_2 = 0.027 \text{ h}^{-1}$  (mayfly-sediment model II, Gobas et al. 1989b)
- $\log k_2 = -0.82 \text{ d}^{-1}$ ;  $-0.96 \text{ d}^{-1}$  (fish, calculated- $K_{OW}$ , Thomann 1989)
- $1/k_2 = 9.12, 12.9 \text{ d}$  (guppy, Clark et al. 1990)
- $k_1 = 710 \pm 290 \text{ L kg}^{-1} \text{ d}^{-1}$ ;  $k_2 = 0.15 \pm 0.04 \text{ d}^{-1}$  (guppies, 96-h exposure., Sijm et al. 1993)
- $k_2 = 0.00116 \text{ d}^{-1}$  (18°C earthworm in field-contaminated soil, Belfroid et al. 1995)
- $k_1 = (240\text{--}290) \text{ mL g}^{-1} \text{ d}^{-1}$ ,  $k_2 = (0.3\text{--}0.19) \text{ d}^{-1}$  (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

## Half-Lives in the Environment:

Air:  $t_{1/2} = 1088\text{--}10877$  h, based on estimated rate constant for the vapor phase reaction with OH radicals (Howard et al. 1991)

Surface Water:  $t_{1/2} = 4656\text{--}8280$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater:  $t_{1/2} = 9312\text{--}16560$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment: dechlorination  $t_{1/2} = 1.20$  d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:  $t_{1/2} = 4656\text{--}8280$  h, based on estimated unacclimated aerobic soil grab sample data (Howard et al. 1991)

Biota:  $t_{1/2} > 7$  d in fish (Veith et al. 1980);

$t_{1/2} > 7$  d in bluegill sunfish (Barrows et al. 1980);

$t_{1/2} = 4.6$  d in guppy (Bruggeman et al. 1984);

$t_{1/2} = 8.9$  d in guppy (Opperhuizen et al. 1985);

$t_{1/2} < 5$  d in worms at  $8^\circ\text{C}$  (Oliver 1987a);

biological half-lives,  $t_{1/2} > 7$  d in sunfish,  $t_{1/2} = 4, 5$  and  $< 5$  d in guppy (Niimi 1987);

$t_{1/2} = 27$  d in *picea omorika* (Reischl et al. 1989);

elimination  $t_{1/2} = 5.46$  d from earthworm in water (Belfroid et al. 1993);

elimination  $t_{1/2} = 0.53$  d and  $5.9$  d in a two-phase kinetics from earthworm in OECD soil (Belfroid et al. 1994);

elimination  $t_{1/2} = 0.60$  d from earthworm in Volgermeerpolder soil (Belfroid et al. 1995).

**TABLE 6.1.1.11.1**

**Reported aqueous solubilities of pentachlorobenzene at various temperatures**

Shiu et al. 1997	
generator column-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
5	0.145
15	0.254
25	0.419
35	0.618
45	0.856
shake flask-GC	
27	0.447
$\Delta H_{\text{sol}} = 32.9$ kJ/mol	

**TABLE 6.1.1.11.2**

**Reported vapor pressures of pentachlorobenzene at various temperatures and the coefficients for the vapor pressure equations**

$$\log (P/\text{Pa}) = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^\circ\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^\circ\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3) \quad \ln (P/\text{Pa}) = A - B/(C + T/K) \quad (3a)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

$$\ln (P/P_0) = (1 - T/T_0) \cdot \exp[\Sigma A_i T^i] \quad (5) - \text{Cox eq.}$$

1.

Stull 1947		Polednicek et al. 1996				Roháč et al. 1999	
summary of lit. data		pressure gauge				recommended	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	T/K	P/Pa
			solid		liquid		solid
98.6	133	30.3	0.385	98.65	167.99	233.15	0.00001
129.7	666.6	30.3	0.401	98.69	167.56	243.15	0.000066
144.3	1333	40.26	1.163	108.65	285.2	253.15	0.00037
160	2666	40.27	1.167	108.68	284.76	263.15	0.0019
178.5	5333	50.27	3.227	118.82	470.83	273.15	0.0081

(Continued)

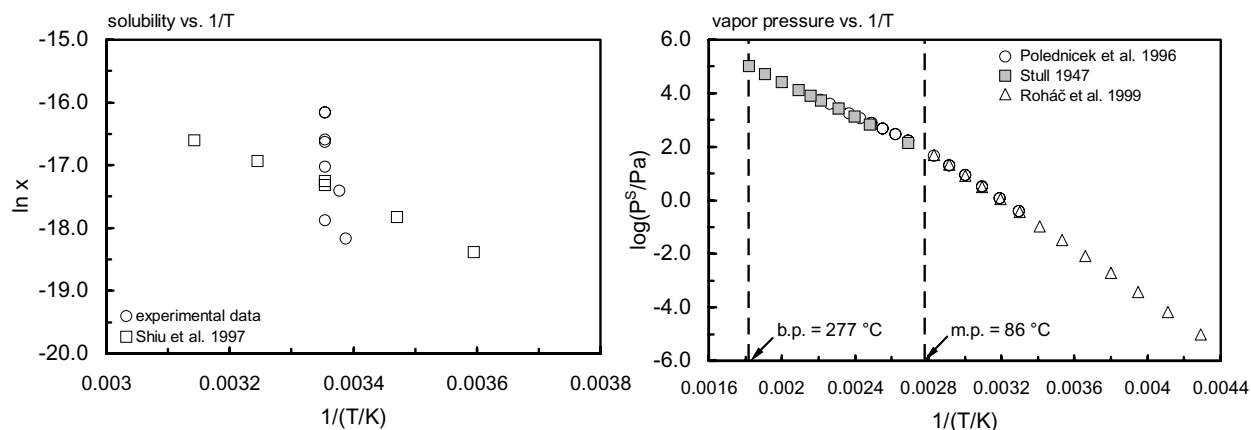
TABLE 6.1.1.11.2 (Continued)

Stull 1947		Polednicek et al. 1996				Roháč et al. 1999	
summary of lit. data		pressure gauge				recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
190.1	7999	50.27	3.209	118.84	471.55	283.15	0.032
205.5	13332	60.14	8.473	128.85	756.41	293.15	0.11
227	26664	60.16	8.480	128.85	755.7	303.15	0.37
251.5	53329	70.05	20.35	138.9	1189.2	313.15	1.10
276	101325	70.05	20.39	149.01	1820.6	232.15	3.20
		80.02	47.29	159.06	2731.2	333.15	8.40
mp/°C	85.5	25	0.212	169.11	4009.9	343.25	20.8
			extrapolated	179.14	5750.8	353.15	48.9
			solid		liquid	Cox eq.	
		eq. 3a	P/Pa	eq. 3a	P/Pa	eq. 5	P/Pa
		A	30.4445	A	22.4783	A <sub>0</sub>	3.431590
		B	8654.67	B	6188.33	10 <sup>-4</sup> A <sub>1</sub>	-1.8864070
		C	-27.6534	C	-34.6922	A <sub>2</sub>	0
						T <sub>0</sub> /K	357.0
						P <sub>0</sub> /Pa	67.0
						bp/K	558.42
						for temp range 300–353 K	

2.

Roháč et al. 1999

recommended					
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
continued	liquid				
363.15	97.5	473.15	11440	Cox eq.	
373.15	173.9	483.15	15500	eq. 5	P/Pa
383.15	298.8	493.15	20700	A <sub>0</sub>	3.419638
393.15	486.4	503.15	27250	10 <sup>-3</sup> A <sub>1</sub>	-1.1673259
403.15	799.8	513.15	35430	10 <sup>-7</sup> A <sub>2</sub>	7.7842905
413.15	1253	523.15	45510	T <sub>0</sub> /K	357.0
423.15	1912	533.15	57820	P <sub>0</sub> /Pa	67.0
433.15	2848	543.15	72710	bp/K	558.42
443.15	4151	553.15	90570	for temp range 365–452 K	
453.15	5927	563.15	111800		
463.15	8306				

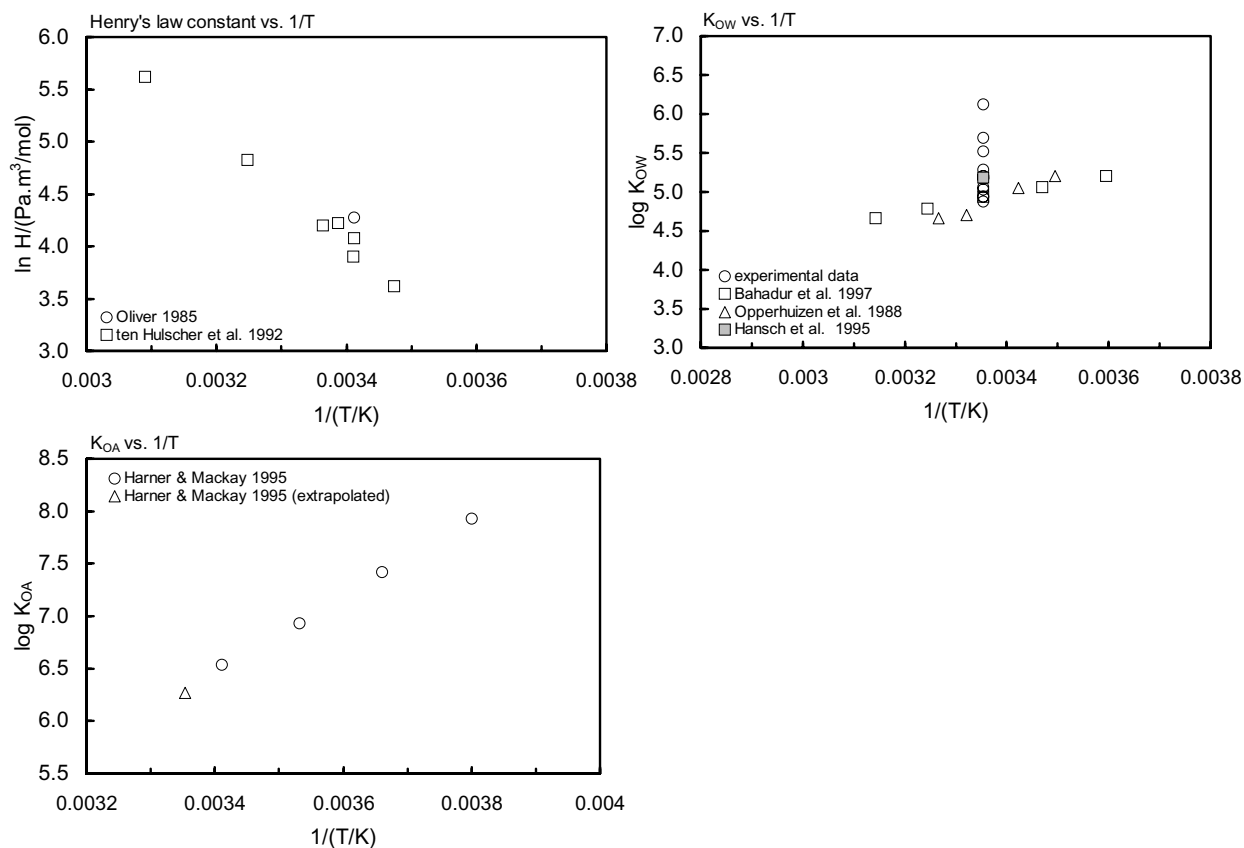


**FIGURE 6.1.1.11.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for pentachlorobenzene.

**TABLE 6.1.1.11.3**

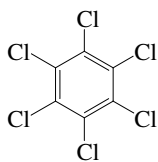
Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of pentachlorobenzene at various temperatures

Henry's law constant		log K <sub>OW</sub>				log K <sub>OA</sub>	
Ten Hulscher et al. 1992		Opperhuizen et al. 1988		Bahadur et al. 1997		Harner & Mackay 1995	
gas stripping-GC		shake flask-GC/ECD		shake flask-GC/ECD		generator column-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
14.8	37.4	13	5.2	5	5.2	25	5.64
20	59.0	19	5.05	15	5.06	−10	7.93
20.1	49.4	28	4.70	25	4.94	0	7.418
22.1	68.1	33	4.66	35	4.79	10	6.931
24.1	66.7			45	4.66	18.7	6.539
34.8	124.1						
50.5	276.2	ΔH/(kJ mol <sup>−1</sup> ) = −30.8		enthalpy of transfer ΔH/(kJ mol <sup>−1</sup> ) = −22.8		ΔH <sub>OA</sub> /(kJ mol <sup>−1</sup> ) = 62.03	
ln H = A − B/(T/K)				log K <sub>OW</sub> = A −ΔH/2.303RT		log K <sub>OA</sub> = A + B/T	
	H/(Pa m <sup>3</sup> /mol)			A	0.9255.	A	−6.2
A	21.4142			ΔH	−22800	B	3722.3
B	5108						



**FIGURE 6.1.11.2** Logarithm of Henry's law constant,  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for pentachlorobenzene.

## 6.1.1.12 Hexachlorobenzene



Common Name: Hexachlorobenzene

Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride

Chemical Name: hexachlorobenzene

CAS Registry No: 118-74-1

Molecular Formula:  $C_6Cl_6$

Molecular Weight: 284.782

Melting Point ( $^{\circ}C$ ):

228.83 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

325 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.5691 ( $23.6^{\circ}C$ , Weast 1972–73; Horvath 1982)

2.004 ( $23^{\circ}C$ , Lide 2003)

Molar Volume ( $cm^3/mol$ ):

181.5 ( $23.6^{\circ}C$ , calculated-density, Weast 1972–73; Horvath 1982)

221.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

23.85 (Plato & Glasgow 1969; Ruelle et al. 1993; Chickos et al. 1999)

28.74 (Tsonopoulos & Prausnitz 1971)

22.40 (Miller et al. 1984)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

57.32 (Tsonopoulos & Prausnitz 1971)

44.77 (Miller et al. 1984)

47.1 (Hinckley et al. 1990; quoted, Passivirta et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ),  $F$ : 0.01 (mp at  $228.83^{\circ}C$ )

0.009 (Miller et al. 1985; Suntio et al. 1988b)

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

0.005 (generator column-GC/ECD, Weil et al. 1974)

0.006 (shake flask-LSC/ $^{14}C$ , Lu & Metcalf 1975)

0.11 (shake flask-nephelometric spectrophotofluorometry, Hollifield 1979)

0.005 (shake flask-UV, Yalkowsky et al. 1979)

0.0039 (shake flask-GC, Könnemann 1981)

0.00921, 0.00996 (15,  $25^{\circ}C$ , generator column/elution method, average values of 6–7 labs., OECD 1981)

0.0054 (generator column-GC/ECD, Hashimoto et al. 1982)

0.0012–0.014 (shake flask-GC/ECD, Hashimoto et al. 1982)

0.005 (recommended, Horvath 1982)

0.047 (generator column-GC/ECD, Miller et al. 1984; 1985)

0.005 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$0.00544 \pm 0.00018$  (generator column-GC/ECD, measured range  $5$ – $45^{\circ}C$ , Shiu et al. 1997)

0.38 (shake flask-GC, Boyd et al. 1998)

$0.0050 \pm 0.00002$  (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)

$\log [S_L/(mol/L)] = 0.450 - 1212/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$\ln x = -8.22956 - 4037.26/(T/K)$ ; temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

0.010\* (generator column-GC/ECD, measured range  $15$ – $55^{\circ}C$ , Oleszek-Kudlak et al. 2004)

0.0273, 0.398 (supercooled liquid: derivation of literature-derived value FAV, final-adjusted value FAV, Shen & Wania 2005)

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\* (114.1°C, summary of literature data, temp range 114.1–309.4°C, Stull 1947)  
 0.00028 (extrapolated from Antoine eq., Sears & Hopke 1949)  
 $\log(P/\text{mmHg}) = 11.397 - 4197.3/(T/K)$ ; temp range 96–124°C (Rodebush gauge, Sears & Hopke 1949)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 15199.1/(T/K)] + 8.550497$ ; temp range 114.4–309.4°C (Antoine eq., Weast 1972–73)  
 0.0015 (Callahan et al. 1979)  
 0.0026 (OECD 1979)  
 0.00145 (20°C, Kiltzer et al. 1979)  
 0.0023\* (gas saturation, measured range 15–45°C, Farmer et al. 1980)  
 $\log P/\text{mmHg} = 12.94 - 5279/(T/K)$ ; temp range 15–45°C (gas saturation, Farmer et al. 1980)  
 0.000453; 0.000167 (Klein et al. 1981)  
 0.0019\* (gas saturation, measured range 10–50°C, OECD 1981)  
 $\log(P/\text{mmHg}) = 12.237 - 5152.1/(T/K)$ ; temp range 10–50°C (gas saturation, OECD 1981)  
 0.00046 (evaporation rate, Dobbs & Cull 1982)  
 0.00121 (extrapolated-Antoine eq., Gückel et al. 1982)  
 0.0006 (20°C, evaporation rate and gravimetric method, Gückel et al. 1982)  
 0.159, 0.122 ( $P_{GC}$  by GC-RT correlation with different GC columns, Bidleman 1984)  
 0.303 (supercooled liquid  $P_L$ , converted from literature  $P_S$  with  $\Delta S_{fus}$ , Bidleman 1984)  
 0.00332 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)  
 0.00205\* (41.05°C, gas saturation-GC, measured range 41–100°C, Rordorf 1985)  
 $\log(P/\text{Pa}) = 12.3243 - 4336.95/(T/K) - 41.1905$ ; temp range 41–100°C (gas saturation, Rordorf 1985)  
 0.00147, 0.187 (20°C, quoted: solid  $P_S$ , supercooled liquid  $P_L$ , Bidleman & Foreman 1987)  
 $\log(P_S/\text{kPa}) = 7.00706 - 2831.85/(-28.25 + T/K)$ ; temp range 387–502 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 7.35248 - 2786.78/(-61.33 + T/K)$ ; temp range 502–589 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)  
 0.245 (supercooled liquid  $P_L$ , Suntio et al. 1988b)  
 0.303, 0.127 (supercooled  $P_L$ , converted from literature  $P_S$  with different  $\Delta S_{fus}$  values, Hinckley et al. 1990)  
 0.159, 0.119 ( $P_{GC}$  by GC-RT correlation with different reference standards, Hinckley et al. 1990)  
 $\log(P_L/\text{Pa}) = 11.11 - 3582/(T/K)$  (supercooled liquid  $P_L$ , GC-RT correlation, Hinckley et al. 1990)  
 0.00311\* (gas saturation, measured range –15 to 40°C, Dickhut et al. 1994)  
 0.001092\* (20°C, gas saturation-GC/ECD, measured range –30 to 40°C, Wania et al. 1994)  
 $\log(P_S/\text{Pa}) = 10.83 - 4044/(T/K)$ ; temp range –30 to 40°C (derived from gas saturation data, Wania et al. 1994)  
 0.367; 0.344 (supercooled liquid  $P_L$ , GC-Kovács retention indices correlation; quoted lit., Spijksma et al. 1994)  
 $\log(P/\text{mmHg}) = -134.3625 - 1.5459 \times 10^3/(T/K) + 61.748 \cdot \log(T/K) - 6.5123 \times 10^{-2} \cdot (T/K) + 2.0872 \times 10^{-5} \cdot (T/K)^2$ ;  
 temp range 502–825 K (Yaws 1994)  
 0.0339;  $1.46 \times 10^{-3}$ , 0.141 (liquid  $P_L$  from GC-RT correlation; quoted solid  $P_S$ , converted to  $P_L$ , Donovan 1996)  
 $(4.6-26) \times 10^{-4}$ ,  $(1.11-5.40) \times 10^{-3}$  (quoted exptl. solid  $P_S$  ranges: 20°C, Delle Site 1997)  
 0.271; 0.00821 ( $P_L$  supercooled liquid, GC-RT correlation; solid  $P_S$ , Passivirta et al. 1999)  
 $\log(P_L/\text{Pa}) = 8.42 - 2834/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 0.14, 0.094 (supercooled liquid  $P_L$ : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)  
 $\log(P_L/\text{Pa}) = -3530/(T/K) + 10.97$  (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa m<sup>3</sup>/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):

- 131.3 (gas stripping-GC, Atlas et al. 1982)  
 48.6 (gas stripping-GC, Oliver 1985)  
 172 (gas stripping-GC, Warner et al. 1987)  
 41756 (computer value, Yaws et al. 1991)  
 41.0\* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)



$\ln [H/(\text{Pa m}^3/\text{mol})] = 22.7994 - 5630.6/(T/K)$ , temp range 14–50°C (gas stripping-GC, ten Hulscher et al. 1992)  
 26243, 29587 (26.0, 46.0°C, EPICS-GC, Hansen et al. 1993)  
 $\log [H/(\text{Pa m}^3/\text{mol})] = 7.97 - 1622/(T/K)$  (Passivirta et al. 1999)  
 35.1 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 6.266 - 2377/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)  
 52, 65 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient,  $\log K_{\text{OW}}$  or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated \* are compiled at the end of this section:

6.18 (Neely et al. 1974)  
 4.13 (radioisotope tracer- $^{14}\text{C}$ , Lu & Metcalf 1975)  
 6.51 (calculated-fragment constant, Rekker 1977)  
 4.13 (Hansch & Leo 1979)  
 5.0, 6.27 (shake flask-GC, HPLC- $k'$  correlation, Könemann et al. 1979)  
 5.23 (HPLC-RT correlation, Veith et al. 1979b)  
 6.18 (HPLC-RT correlation, Veith et al. 1979a)  
 5.44 (shake flask-GC, Briggs 1981)  
 6.22 (HPLC-RT correlation, McDuffie 1981)  
 5.56, 5.04–5.92 (shake flask method: mean, range of mean values, OECD 1981)  
 5.50 (shake flask-GC, Chiou et al. 1982; Chiou 1985)  
 5.66 (HPLC-RT correlation, Hammers et al. 1982)  
 5.40 (shake flask-GC, Watarai et al. 1982)  
 6.13–6.27, 5.66 (range, mean, shake flask method, Eadsforth & Moser 1983)  
 6.27–6.48, 6.38 (range, mean, HPLC method, Eadsforth & Moser 1983)  
 5.46, 5.26; 5.47 (Review of HPLC methods; OECD/EEC shake-flask method, Harnisch et al. 1983)  
 5.47 (generator column-GC/ECD, Miller et al. 1984; 1985)  
 5.70–5.79 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)  
 6.86 (HPLC/MS correlation, Burkhard et al. 1985)  
 5.75; 5.60, 5.90 (selected OECD value; HPLC-RV correlation, Brooke et al. 1986)  
 6.92 (HPLC- $k'$  correlation, De Kock & Lord 1987)  
 5.64 (HPLC- $k'$  correlation, Mailhot 1987)  
 6.22 (HPLC-RT correlation, Doucette & Andren 1988)  
 5.7\* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)  
 5.50 (shake flask-GC, Pereira et al. 1988)  
 5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)  
 5.44 (recommended, Sangster 1993)  
 5.73 (recommended, Hansch et al. 1995)  
 5.46\*  $\pm$  0.02 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)  
 $\log K_{\text{OW}} = 1.1806 - 24.4/[2.303R(T/K)]$ ; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)  
 5.845 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)  
 5.55 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)  
 5.52, 5.64 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

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

6.90\*; 6.78 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)  
 $\log K_{\text{OA}} = -6.30 + 3928/(T/K)$ ; temp range –10 to 20°C,  $\Delta H_{\text{OA}} = 75.2 \text{ kJ/mol}$  (Harner & Mackay 1995)  
 6.80 (calculated- $K_{\text{OW}}/K_{\text{AW}}$ , Wania & Mackay 1996)  
 7.17, 6.90 (calculated- $S_{\text{oct}}$  and vapor pressure  $P$ , quoted lit., Abraham et al. 2001)  
 7.384\* (generator column-GC, measured range 5–25°C, Shoeib & Harner 2002)  
 7.38, 7.21 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor,  $\log \text{BCF}$  at 25°C or as indicated:

3.89 (rainbow trout, calculated-rate constant ratio  $k_1/k_2$ , Neely et al. 1974)  
 3.09 (fish, Körte et al. 1978)

- 4.27, 3.73, 4.34 (fathead minnow, rainbow trout, green sunfish, Veith et al. 1979b)  
 5.46 (guppy, lipid basis, Könemann & van Leeuwen 1980;)  
 4.27 (fish, Ciam et al. 1980)  
 1.20 (rats, adipose tissue, Geyer et al. 1980)  
 3.93, 2.46 (fish, flowing water, static water, Kenaga & Goring 1980; Kenaga 1980a)  
 4.39 (algae, Geyer et al. 1981)  
 3.38–4.08 mean 4.08; 3.88–4.30 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)  
 5.16–5.37 (15°C, rainbow trout, lipid basis, Oliver & Niimi 1983; quoted, Chiou 1985)  
 4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)  
 4.34 (sunfish; rainbow trout, 15°C, Davis & Dobbs 1984)  
 4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)  
 5.09 (green algae, dry wt basis, Geyer et al. 1985)  
 4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)  
 2.62–2.97; 2.44–2.79 (human fat: lipid basis, wet weight, Geyer et al. 1987)  
 4.41 (algae, Mailhot 1987)  
 4.34 (fathead minnow, Carlson & Kosian 1987)  
 4.38, 4.30 (worms, fish, Oliver 1987a)  
 3.48 (fish-normalized, Tadokoro & Tomita 1987)  
 5.57, 5.62, 5.66, 5.76 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)  
 6.42, 6.71, 5.96, 5.98 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)  
 –1.35, –2.07, –0.32 (beef, milk, vegetable, reported as biotransfer factor log  $B_b$ , Travis & Arms 1988)  
 5.46 (guppy-lipid base, 12 to 31-d exposure studies, Gobas et al. 1989)  
 3.53 (*picea omorika*, Reischl et al. 1989)  
 3.57 (fish, calculated, Figueroa & Simmons 1991)  
 4.73; 4.76 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)  
 3.74–4.30; 4.21; 4.34; 4.16; (*Oncorhynchus mykiss*; *Poecilia reticulata*; *Lepomis cyanellus*; *Oryzias latipes*, quoted lit., flow through conditions, Devillers et al. 1996)  
 5.62 (*Poecilia reticulata*, quoted lit., static and semi-static conditions, Devillers et al. 1996)  
 3.18, 4.39 (macrophytes *Myriophyllum spicatum*, algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)  
 5.55 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)  
 4.38, 5.08 (algae *Chlorella*: wet wt basis, dry wt basis, Geyer et al.2000)  
 3.98, 5.98 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al.2000)  
 > 3.54, > 5.54 (mussel *Mytilus edulis* 21-d non-steady state: wet wt basis, lipid wt basis, Geyer et al.2000)  
 3.69, 5.71 (golden orfe *Leuciscus idus melanotus*, 0.95% lipid: wet wt basis, lipid wt basis, Geyer et al.2000)  
 2.65, 2.83 (human, fat: wet wt basis, lipid wt basis, Geyer et al.2000)  
 3.74; 3.95 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

#### Sorption Partition Coefficient, log $K_{OC}$ :

- 3.59 (Kenaga & Goring 1980; Kenaga 1980a)  
 4.45 (Kenaga 1980a)  
 4.49 (soil, sorption isotherm, converted from reported log  $K_{OM}$  of 4.25, Briggs 1981)  
 2.56 (Speyer soil < 2.00 mm, Freundlich isotherm, Rippen et al. 1982)  
 2.70 (Alfisol, Freundlich isotherm, Rippen et al. 1982)  
 5.90; 5.50 (field data of Lake Ontario sediment trap material; Niagara River organic matter, Oliver & Charlton 1984)  
 4.90, 5.2–6.0 (bottom sediment, range, Karickhoff & Morris 1985)  
 5.2–6.7, 6.1; 5.80 (suspended sediment, average; algae > 50  $\mu$ m, Oliver 1987c)  
 6.0–6.50, 6.30; 5.10 (Niagara River plume: range, mean; calculated- $K_{OW}$ , Oliver 1987b)  
 4.77 (HPLC- $k'$  correlation, Hodson & Williams 1988)  
 4.66, 3.08, 4.91 (soil/water, soil-dextran/water, humic acid/water, batch equilibrium-sorption isotherm, Enfield et al. 1989)

- 3.23, 4.73; 4.59 (Captina silt loam OC 1.49%, McLaurie sandy loam OC 0.66%; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 5.51 (organic matter, Koelmans et al. 1993)
- 4.89 ± 0.36 (suspended particulates in coastal waters, Masunaga et al. 1996)
- 4.70; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 4.23, 3.79 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
- 5.53, 5.48 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

#### Sorption Partition Coefficient, log $K_{OM}$ :

- 4.25 (soil-organic matter, sorption isotherm, shake flask-GC, Briggs 1981)
- 5.50 (Niagara River-organic matter, Oliver & Charlton 1984)

#### Environmental Fate Rate Constants, $k$ , or Half-Lives, $t_{1/2}$ :

Volatilization/Evaporation:  $k = 3.45 \times 10^{-10} \text{ mol m}^{-2} \text{ h}^{-1}$  (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant in air,  $k = 1.44 \times 10^{-2} \text{ h}^{-1}$  (Brown et al. 1975; quoted, Mackay et al. 1985); photooxidation  $t_{1/2} = 3753\text{--}37530 \text{ h}$ , based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987).

Hydrolysis: not expected to be important, based on  $k_h = 0$  was observed after 13 d at pH 3, 7, 11, and 85°C (Ellington et al. 1987, 1988).

Biodegradation:  $t_{1/2}$ (aq. aerobic) = 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974; Howard et al. 1991);

degradation rate constant  $k = 1.9 \times 10^{-5} \text{ h}^{-1}$  in soil (Beck & Hansen 1974; selected, Mackay et al. 1985; Mackay & Paterson 1991);

not significant in an aerobic environment, and no significant degradation rate (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2}$ (aerobic) = 970 d,  $t_{1/2}$ (anaerobic) = 3900 d in natural waters (Capel & Larson 1995)

dechlorination pseudo-first order rate constant  $k = 0.282 \text{ d}^{-1}$  with  $t_{1/2} = 2.5 \text{ d}$  using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

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

$k_1 = 18.76 \text{ h}^{-1}$ ;  $k_2 = 0.00238 \text{ h}^{-1}$  (trout muscle, Neely et al. 1974)

$k_1 = 10000 \text{ d}^{-1}$  (guppy, Konemann & van Leeuwen 1980)

$k_1 = 22.5 \text{ h}^{-1}$  (guppy, quoted from Konemann & van Leeuwen 1980, Hawker & Connell 1985)

$\log k_1 = 1.35 \text{ d}^{-1}$  (fish, quoted from Konemann & Leeuwen 1980, Hawker & Connell 1985)

$k_1 = 18.8 \text{ h}^{-1}$  (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)

$\log k_1 = 1.27 \text{ d}^{-1}$  (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)

$1/k_2 = 420 \text{ h}$  (trout, quoted from Bruggeman et al. 1984, Hawker & Connell 1985)

$\log k_2 = 2.62 \text{ d}^{-1}$  (fish, quoted, Hawker & Connell 1985)

$k_1 = 540 \text{ d}^{-1}$  (fish, quoted, Opperhuizen 1986)

$k_2 = 0.00510, 0.00818, 0.00640, 0.0047 \text{ d}^{-1}$  (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)

$\log k_1 = 2.73 \text{ d}^{-1}$  (fish, quoted from Konemann & Leeuwen 1980, Connell & Hawker 1988)

$\log k_1 = 2.65 \text{ d}^{-1}$ ;  $\log 1/k_2 = 1.24 \text{ d}$  (fish, quoted from Bruggeman et al. 1984, Connell & Hawker 1988)

$\log k_2 = -1.24 \text{ d}^{-1}$  (fish, calculated- $K_{OW}$ , Thomann 1989)

$k_1 = 0.049 \text{ h}^{-1}$ ;  $k_2 = 0.023 \text{ h}^{-1}$  (mayfly-sediment model II, Gobas et al. 1989b)

$k_2 = 0.092 \text{ d}^{-1}$  with elimination  $t_{1/2} = 7.5 \text{ d}$  (earthworm, Belfroid et al. 1995)

$k_1 = 6.558 \text{ h}^{-1}$ ,  $k_2 = 0.00429 \text{ h}^{-1}$  (Macrophytes *Myrioophyllum spicatum*, Wang et al. 1996)

$k_1 = 10489 \text{ h}^{-1}$ ,  $k_2 = 0.424 \text{ h}^{-1}$  (algae *Chlorella fusca*, Wang et al. 1996)

$k_2 = 0.016 \text{ d}^{-1}$  with  $t_{1/2} = 43 \text{ d}$  and  $k_2 = 0.017 \text{ d}^{-1}$  with  $t_{1/2} = 42 \text{ d}$  for food concn of 14 ng/g and 103 ng/g respectively in a 30-d uptake followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_1 = 467 \text{ mL g}^{-1} \text{ d}^{-1}$ ,  $k_2 = 0.26 \text{ d}^{-1}$  (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

$k_1 = 8$  (food lipid mg)/(g worm lipid-d) (earthworm, Wågman et al. 2001)

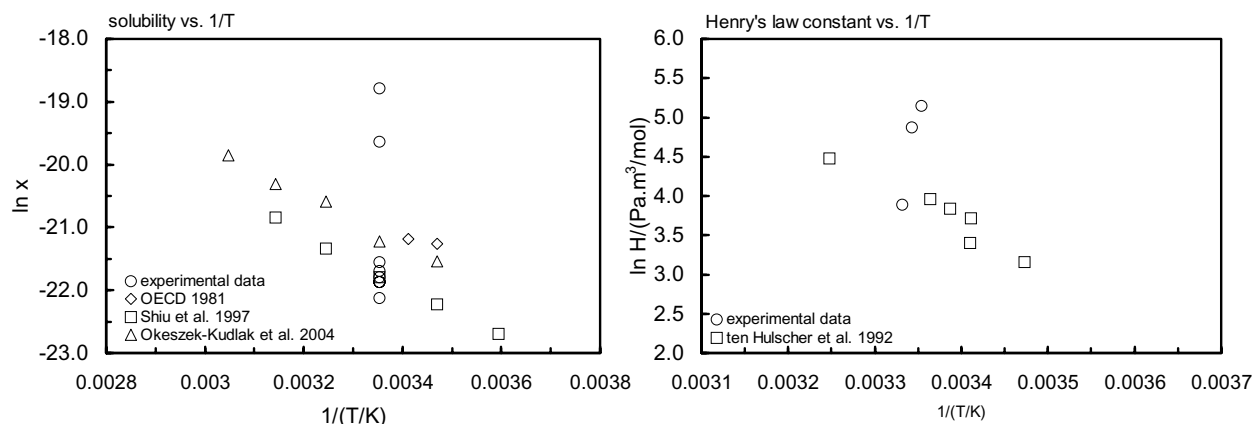
## Half-Lives in the Environment:

- Air:  $t_{1/2} = 3753\text{--}37530$  h, based on estimated photooxidation half-life (Atkinson 1987, Howard et al. 1991)  
 $t_{1/2} = 29 \pm 5.8$  yr at Eagle Harbor,  $t_{1/2} = 15 \pm 1.9$  yr at Sleeping Bear Dunes and  $t_{1/2} = 18 \pm 2.3$  yr in the Great Lakes = atmosphere at Sturgeon Point (Buehler et al. 2004).
- Surface Water:  $t_{1/2} = 1.4\text{--}50$  d estimated,  $t_{1/2} = 0.3\text{--}3$  d for river water and  $t_{1/2} = 30\text{--}300$  d for lakes, estimated from persistence (Zoeteman et al. 1980)  
 $t_{1/2} = 23256\text{--}50136$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)  
 $t_{1/2}(\text{aerobic}) = 970$  d,  $t_{1/2}(\text{anaerobic}) = 3900$  d in natural waters (Capel & Larson 1995)
- Groundwater:  $t_{1/2} = 30\text{--}300$  d, estimated from persistence (Zoeteman et al. 1980)  
 $t_{1/2} = 46512\text{--}100272$  h, based on unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)
- Sediment: dechlorination  $t_{1/2} = 1.8$  d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
- Soil:  $t_{1/2} > 50$  d (Ryan et al. 1988)  
disappearance  $t_{1/2} = 11.3$  d from testing soils (Anderson et al. 1991)  
 $t_{1/2} = 23256\text{--}50136$  h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991)  
 $t_{1/2} = 3\text{--}6$  yr in soil (Geyer et al. 2000)  
 $t_{1/2} = 48.7$  and  $11.7$  yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).
- Biota:  $t_{1/2} = 163$  h, clearance from fish (Neely 1980)  
 $t_{1/2} > 224$  d in rainbow trout (Niimi & Cho 1980);  
 $t_{1/2} = 210$  d at  $4^\circ\text{C}$ ,  $t_{1/2} = 80$  d at  $12^\circ\text{C}$ ,  $t_{1/2} = 70$  d at  $18^\circ\text{C}$  in subadult rainbow trout (Niimi & Palazzo 1985)  
 $t_{1/2} = 27$  d in worms at  $8^\circ\text{C}$  (Oliver 1987a)  
biological  $t_{1/2} = 12$  d in trout muscle,  $t_{1/2} > 173$  d and  $> 224$  d in trout,  $t_{1/2} = 12$  d in guppy (Niimi 1987);  
 $t_{1/2} = 30$  d in *picea omorika* (Reischl et al. 1989)  
elimination  $t_{1/2} = 1.44$  d and  $12.3$  d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994)  
elimination  $t_{1/2} = 1.9\text{--}7.5$  d from earthworm in soil (Belfroid et al. 1995)
- Depuration  $t_{1/2} = 42\text{--}43$  d in a 30-d dietary exposure and 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

TABLE 6.1.1.12.1

Reported aqueous solubilities and Henry's law constants of hexachlorobenzene at various temperatures

Solubility						Henry's law constant	
OECD 1981		Shiu et al. 1997		Oleszek-Kudlak et al. 2004		Ten Hulscher et al. 1992	
gen. col./elution method		generator column-GC/ECD		generator column-GC/ECD		gas stripping-GC	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{H}/(\text{Pa m}^3/\text{mol})$
15	0.00921 <sup>†</sup>	5	0.0022	15	0.007	14.8	23.6
25	0.00996 <sup>‡</sup>	15	0.0035	25	0.0096	20	41
		25	0.00544	25	0.010	20.1	30
<sup>†</sup> mean, 0.00206–0.0216 g/m <sup>3</sup>		35	0.00853	35	0.018	22.1	46.6
<sup>‡</sup> mean, 0.00119–0.0231 g/m <sup>3</sup>		45	0.014	45	0.024	24.1	52.5
				55	0.038	34.8	88.3
						50	217.2
		$\Delta H_{\text{sol}} = 33.7$ kJ/mol		$\Delta H_{\text{sol}} = 33.5$ kJ/mol		$\ln K_{\text{AW}} = A - B/(T/K)$	
						A	22.977
						B	5893.67



**FIGURE 6.1.1.12.1** Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for hexachlorobenzene.

**TABLE 6.1.1.12.2**

**Reported vapor pressures of hexachlorobenzene at various temperatures and the coefficients for the vapor pressure equations**

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log (P/\text{Pa}) = A - B/(C + T/K) & (3) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \ln (P/\text{Pa}) = A - B/(C + T/K) & (3a) \end{array}$$

1.

Stull 1947		Sears & Hopke 1949		Farmer et al. 1980		OECD 1981	
summary of lit. data		Rodebush gauge		gas saturation-GC		gas saturation/balance	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
114.1	133	measured 96–124°C		15	0.000528	10	0.0008
149.3	667	eq. 1	P/mmHg	25	0.00255	20	0.0026
166.4	1333			35	0.00853	30	0.0081
185.7	2666			A	11.397	45	0.0279
206	5333	B	4793.6	25	0.0023	50	0.081
219	7999					10	0.00028
235.5	13332			eq. 1	P/mmHg	20	0.0011
258.8	26664			A	12.94	30	0.003
283.5	53329			B	5279	40	0.013
309.4	101325					50	0.039
						eq. 1	P/mmHg
mp/°C	230					A	12.237
						B	5152.1

2.

Rordorf 1985		Liu & Dickhut 1994		Wania et al. 1994	
gas saturation		gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
41.05	0.0205	–15	$2.21 \times 10^{-6}$	–30	$2.567 \times 10^{-6}$
50.16	0.0547	–5.0	$2.38 \times 10^{-5}$	–20	$7.257 \times 10^{-6}$
60.3	0.165	10	$2.62 \times 10^{-4}$	–10	$3.229 \times 10^{-5}$

(Continued)

TABLE 6.1.1.11.2 (Continued)

Rordorf 1985		Liu & Dickhut 1994		Wania et al. 1994	
gas saturation		gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.3	0.452	25	$3.11 \times 10^{-3}$	0	$1.03 \times 10^{-4}$
80.3	1.155	40	0.121	10	$3.556 \times 10^{-4}$
90.4	2.77			20	$1.092 \times 10^{-3}$
100.25	6.29	$\Delta H_V/(\text{kJ mol}^{-1}) = 81.3$		30	$3.276 \times 10^{-3}$
eq. 3	P/Pa	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 105$		eq. 1	P/Pa
A	12.3243			A	10.83
B	4336.95			B	4044
C	-41.1905			$\Delta H_V/(\text{kJ mol}^{-1}) = 77.4$	

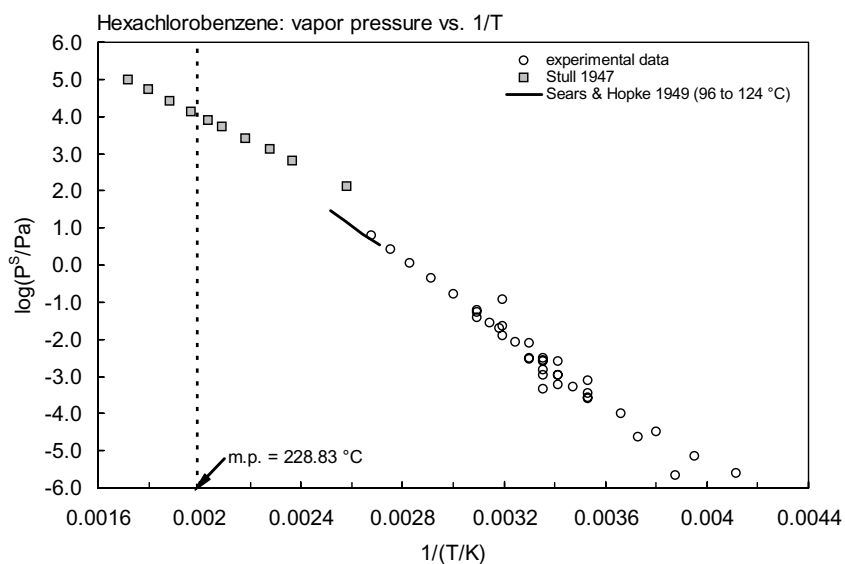


FIGURE 6.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for hexachlorobenzene.

TABLE 6.1.1.12.3

Reported octanol-water partition coefficients and octanol-air partition coefficients of hexachlorobenzene at various temperatures

log K <sub>OW</sub>				log K <sub>OA</sub>			
Oppehuizen et al. 1988		Bahadur et al. 1997		Harner & Mackay 1995		Shoeib & Harner 2002	
shake flask-GC/ECD		shake flask-GC/ECD		generator column-GC			
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>	t/°C	log K <sub>OA</sub>
13	5.68	5	5.74	25	6.9	5	8.1044
19	5.7	15	5.6	−10	8.653	10	7.887
28	5.58	25	5.46	0	8.105	15	7.7
33	4.66	35	5.3	10	6.213	20	7.5634
		45	5.17	18.5	7.185	25	7.3878
						25	7.384
ΔH/(kJ mol <sup>−1</sup> ) = −24.4		enthalpy of transfer ΔH/(kJ mol <sup>−1</sup> ) = −24.4		ΔH <sub>OA</sub> /(kJ mol <sup>−1</sup> ) = 75.2		ΔH <sub>OA</sub> /(kJ mol <sup>−1</sup> ) = 55.8	
		log K <sub>OW</sub> = A − ΔH/2.303RT		log K <sub>OA</sub> = A + B/T		log K <sub>OA</sub> = A + B/T	
		A 1.1806		A −6.3		A −2.395	
		ΔH −24400		B 3928		B 2914	

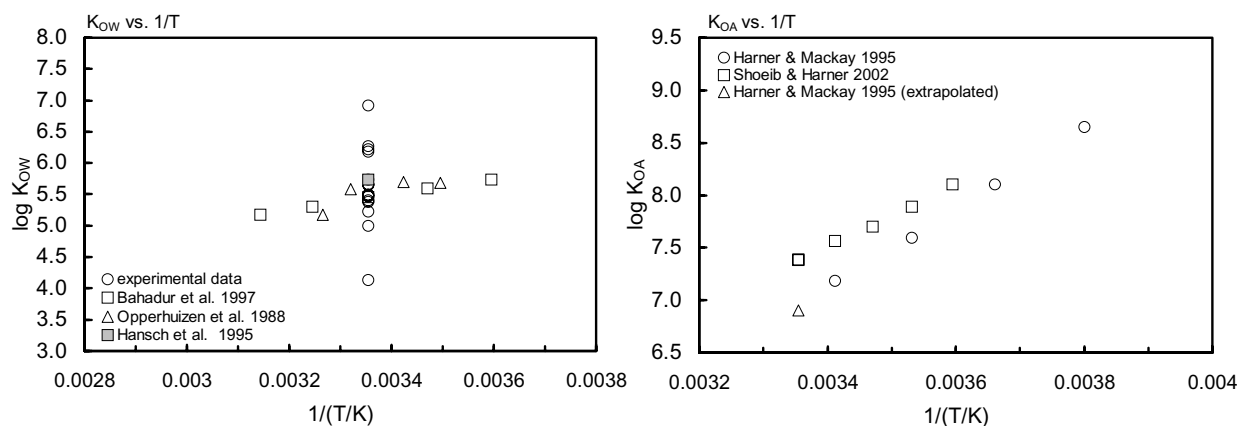
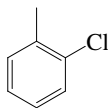


FIGURE 6.1.1.12.3 Logarithm of  $K_{\text{OW}}$  and  $K_{\text{OA}}$  versus reciprocal temperature for hexachlorobenzene.

## 6.1.2 CHLOROTOLUENES

## 6.1.2.1 2-Chlorotoluene



Common Name: 2-Chlorotoluene

Synonym: *o*-Tolylchloride, *o*-chlorotoluene, 2-chloro-1-methylbenzene

Chemical Name: 2-chlorotoluene

CAS Registry No: 95-49-8

Molecular Formula:  $C_7H_7Cl$

Molecular Weight: 126.584

Melting Point ( $^{\circ}C$ ):

-35.8 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

159.15 (Dreisbach 1955; Weast 1982-83)

159.0 (Dean 1985, 1992)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.08245, 1.07762 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955; Riddick et al. 1986)

Molar Volume ( $cm^3/mol$ ):

116.9 ( $20^{\circ}C$ , calculated-density)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

8.368 (Dreisbach 1955; Riddick et al. 1986)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section.):

372 (Isnard & Lambert 1989)

252.0 (shake flask, Fredenlund et al. 1995)

$117^* \pm 5.1$  (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

487 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/mmHg = 7.29547 - 1701.60/(T/K - 45.42)$ ; temp range  $4-75^{\circ}C$  (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

133.3\*, 666.6, 1333 (5.4, 30.6,  $43.2^{\circ}C$ , summary of lit. data, temp range  $5.4-159^{\circ}C$ , Stull 1947)

482.5 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986, Howard 1993)

$\log (P/mmHg) = 6.94763 - 1497.2/(209.0 + t/^{\circ}C)$ ; temp range  $65-220^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

482.5 (extrapolated-Antoine eq., Weast 1972-73)

$\log (P/mmHg) = (-0.2185 \times 10279.3)/(T/K) + 8.091764$ ; temp range  $5.4-159.3^{\circ}C$  (Antoine eq., Weast 1972-73)

5721\* ( $72.654^{\circ}C$ , temp range  $72.654-158.323^{\circ}C$ , Cervenkova & Boublik 1982)

473 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.09563 - 1507.930/(t/^{\circ}C + 209.846)$ ; temp range  $72.5-158.3^{\circ}C$  (Antoine eq., Boublik et al. 1984)

485 (interpolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.36797 - 1735.8/(t/^{\circ}C + 230.0)$ ; temp range  $0-65^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.94763 - 1497.2/(t/^{\circ}C + 209.0)$ ; temp range:  $65-220^{\circ}C$  (Antoine eq., Dean 1985, 1992)

472.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)



$\log (P_L/\text{Pa}) = 6.07253 - 1497.2/(T/\text{K} - 64.15)$ ; temp range 338–493K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 33.2792 - 3.4099 \times 10^3/(T/\text{K}) - 8.6743 \cdot \log (T/\text{K}) + 6.8174 \times 10^{-10} \cdot (T/\text{K}) + 1.8987 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 237–656 K (Yaws 1994)

Henry's Law Constant ( $\text{Pa} \cdot \text{m}^3/\text{mol}$  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):

370\* (23°C, equilibrium cell-GC, measured range 1–23°C, Leighton & Calo 1981)

$\ln (k_H/\text{atm}) = 17.18 - 3545/(T/\text{K})$ ; temp range: 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

295 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 3.890 - 1409/(T/\text{K})$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

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

3.42 (shake flask, Leo et al. 1971, Hansch & Leo 1979, Hansch et al. 1995)

3.52 (HPLC-RT correlation, Könnemann et al. 1979)

3.40 (HPLC- $k'$  correlation, Hanai et al. 1981)

3.59 (RP-HPLC-RT correlation, Edsforth 1986)

3.52 (recommended, Sangster 1993)

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

Bioconcentration Factor,  $\log \text{BCF}$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

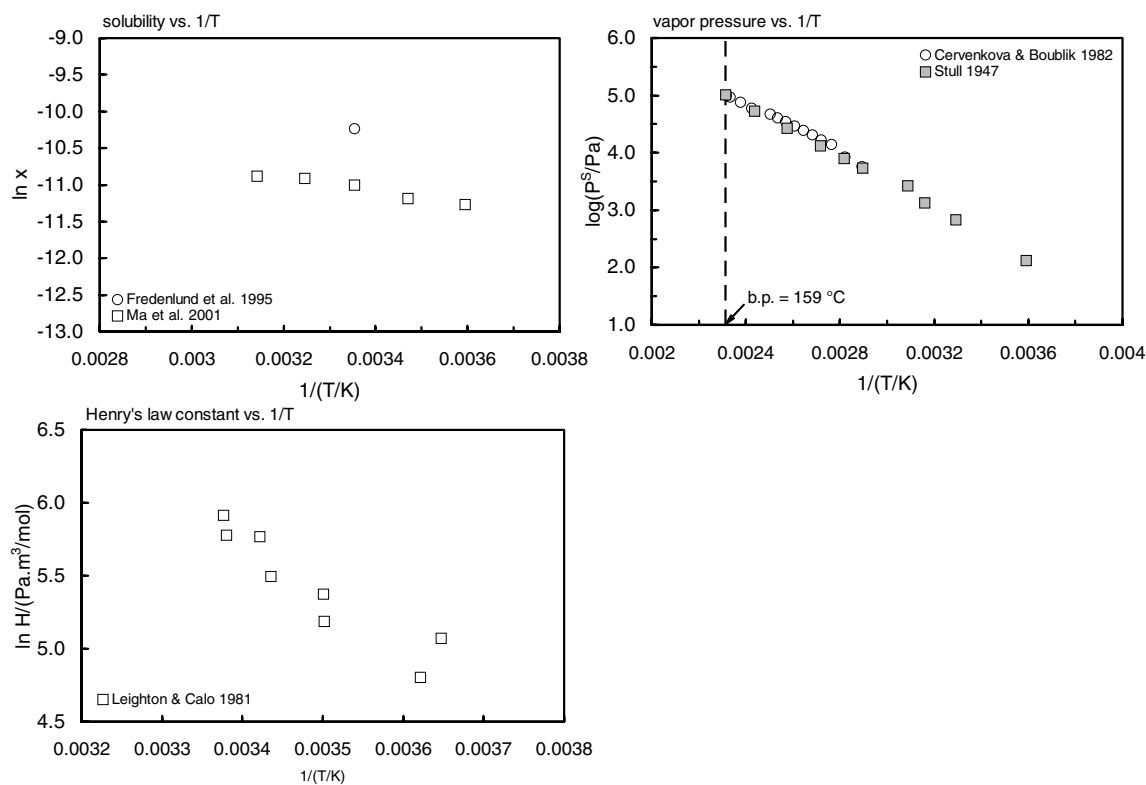
Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 6.1.2.1.1**

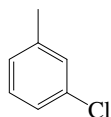
**Reported aqueous solubilities, vapor pressures and Henry's law constants of 2-chlorotoluene at various temperatures**

Aqueous solubility		Vapor pressure				Henry's law constant	
Ma et al. 2001		Stull 1947		Cernenkova & Boublik 1982		Leighton & Calo 1981	
shake flask-GC		summary of lit. data				equilibrium cell-GC	
$t/^\circ\text{C}$	$S/\text{g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$P/\text{Pa}$	$t/^\circ\text{C}$	$P/\text{Pa}$	$t/^\circ\text{C}$	$\text{Pa m}^3/\text{mol}$
5	89.4	5.4	133	72.654	5721	1	159.4
15	97.1	30.6	666.6	81.522	8325	3	112
25	117	43.2	1333	88.657	13911	12.4	178.5
35	128	56	2666	94.646	16792	12.5	216.1
45	132	72	5333	99.758	20277	17.9	243.5
		81.8	7999	105.05	24559	19.1	319.7
		94.7	13332	110.613	29367	22.7	3223
		115	26664	115.995	34778	23	369.7
		137.1	53329	121.252	40719	$\ln (H/\text{atm}) = A - B/(T/\text{K})$	
		159	101325	126.313	47579		
				139.532	60191		
		mp/°C	-	147.287	74587		
				155.689	93400		
				158.323	99991		
				bp/°C	158.849		



**FIGURE 6.1.2.1.1** Logarithm of mole fraction solubility, vapor pressure and Henry's law constant versus reciprocal temperature for 2-chlorotoluene.

## 6.1.2.2 3-Chlorotoluene



Common Name: 3-Chlorotoluene

Synonym: *m*-Tolylchloride, 3-chloro-1-methylbenzene

Chemical Name: 3-chlorotoluene

CAS Registry No: 108-41-8

Molecular Formula:  $C_7H_7Cl$

Molecular Weight: 126.584

Melting Point ( $^{\circ}C$ ):

−47.8 (Weast 1982–83; Riddick et al. 1986; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

161.8 (Dean 1985; 1992; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.0722 (Weast 1982–83)

1.0728 ( $20^{\circ}C$ , Riddick et al. 1986)

Molar Volume ( $cm^3/mol$ ):

118.1 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

43.76 (Riddick et al. 1986)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section.):

372 (Isnard & Lambert 1989)

$117^* \pm 2.1$  (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

418 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/mmHg = 7.62515 - 1887.31/(T/K - 33.40)$ ; temp range  $4-75^{\circ}C$  (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

133.3\*, 666.6, 1333 (4.8, 30.3,  $43.2^{\circ}C$ , summary of lit. data, temp range  $4.8-162.3^{\circ}C$ , Stull 1947)

488.9 (extrapolated, Antoine eq., Weast 1972–73)

$\log (P/mmHg) = (-0.2185 \times 10081.1)/(T/K) + 7.952234$ ; temp range  $4.8-162.3^{\circ}C$  (Antoine eq., Weast 1982–83)

403.0 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.09068 - 1511.858/(t/^{\circ}C + 208.119)$ ; temp range  $64.8-159.8^{\circ}C$  (Antoine eq., Boublik et al. 1984)

670.0 (Riddick et al. 1986)

$\log (P/kPa) = 6.2794 - 1637.6/(223.3 + t/^{\circ}C)$ , temp range not specified (Antoine eq., Riddick et al. 1986)

512.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P/kPa) = 6.90317 - 2028.13/[(T/K) - 11.629]$ ; temp range 277–436 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

3.28 (shake flask, Leo et al. 1971, Hansch & Leo 1979)

3.40 (HPLC- $k'$  correlation, Hanai et al. 1981)

- 3.28 (shake flask, Log P Database, Hansch & Leo 1987)  
 3.17 (calculated-UNFIC activity coefficients, Dallos et al. 1993)  
 3.28 (recommended, Sangster 1993)  
 3.28 (recommended, 1995)

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

Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

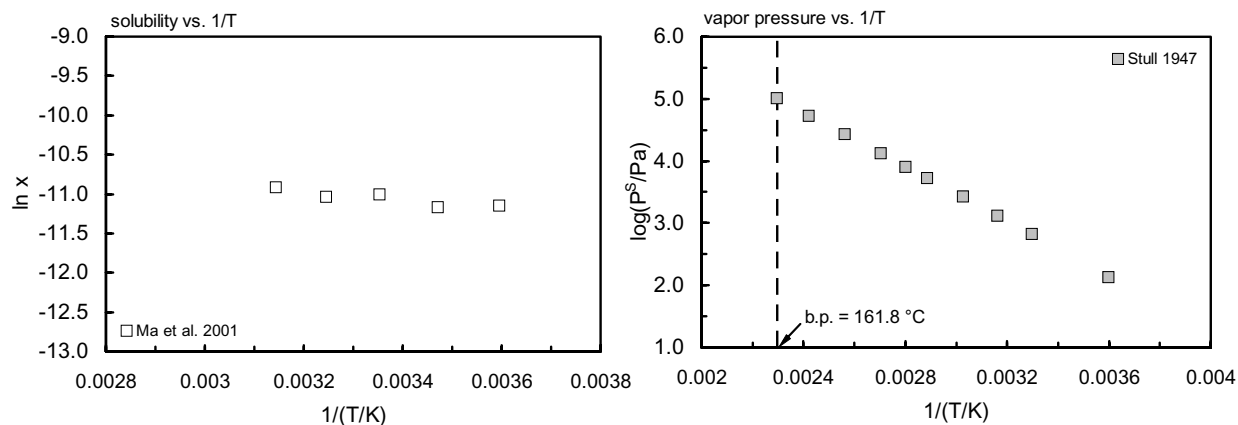
- 3.88 (activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

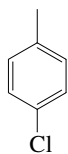
**TABLE 6.1.2.2.1**  
**Reported aqueous solubilities and vapor pressures of 3-chlorotoluene at various temperatures**

Aqueous solubility		Vapor pressure	
Ma et al. 2001		Stull 1947	
shake flask-GC		summary of literature data	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$P/\text{Pa}$
5	101	4.8	133
15	99.3	30.3	666.6
25	117	43.2	1333
35	113	57.4	2666
45	128	73	5333
		83.7	7999
		96.3	13332
		116.6	26664
		139.7	53329
		162.3	101325
		mp/ $^{\circ}\text{C}$	–



**FIGURE 6.1.2.2.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 3-chlorotoluene.

## 6.1.2.3 4-Chlorotoluene



Common Name: 4-Chlorotoluene

Synonym: *p*-Tolylchloride, 4-chloro-1-methylbenzene

Chemical Name: 4-chlorotoluene

CAS Registry No: 106-43-4

Molecular Formula:  $C_7H_7Cl$

Molecular Weight: 126.584

Melting Point ( $^{\circ}C$ ):

7.5 (Weast 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

162.4 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.0697 (Weast 1982–83; Riddick et al. 1986; Dean 1985, 1992; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

118.3 (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section.):

106.0 ( $20^{\circ}C$ , Yalkowsky 1987)

$123 \pm 6.1$  (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

422 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/mmHg = 23.07210 - 3041.02/(T/K) - 5 \cdot \log (T/K)$ ; temp range  $4-75^{\circ}C$  (vapor pressure eq. based on exptl. data, Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)

133.3\*, 666.6, 1333 ( $5.5, 31.0, 43.8^{\circ}C$ , temp range  $5.5-162.3^{\circ}C$ , summary of lit. data, Stull 1947)

471.6 (interpolated, Antoine eq., Weast 1982–83)

$\log (P/mmHg) = (-0.2185 \times 10151.7)/(T/K + 7.988366)$ ; temp range  $5.5-162.3^{\circ}C$  (Antoine eq., Weast 1982–83)

$\log (P/kPa) = 6.09068 - 1511.858/(t/^{\circ}C + 208.199)$ ; temp range  $65-160^{\circ}C$  (Antoine eq., Boublik et al. 1984)

670 ( $30.3^{\circ}C$ , Riddick et al. 1986)

$\log (P/kPa) = 6.75005 - 1887.31/(239.75 + t/^{\circ}C)$ , temp range not specified (Antoine eq., Riddick et al. 1986)

506.7 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P/kPa) = 6.90317 - 2107.52/(T/K - 5.373)$ ; temp range  $304-436 K$  (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 61.8901 - 4.3760 \times 10^3/(T/K) - 19.840 \cdot \log (T/K) + 7.991 \times 10^{-3} \cdot (T/K) + 1.0781 \times 10^{-13} \cdot (T/K)^2$ , temp range  $281-660 K$  (Yaws 1994)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

412.4 (calculated-P/C, Howard 1993)

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

- 3.33 (shake flask, Leo et al. 1971; Hansch & Leo 1979; 1985)
- 3.42 (HPLC-RT correlation, Könemann et al. 1979)
- 3.40 (HPLC- $k'$  correlation, Hanai et al. 1981)
- 3.30 (shake flask, Wang et al. 1987)
- 3.33 (recommended, Sangster 1993)
- 3.33 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :Bioconcentration Factor,  $\log BCF$ :

- 1.65–2.30 (estimated from  $\log K_{OW}$ , Lyman et al. 1990; Howard 1993)

Sorption Partition Coefficient,  $\log K_{OC}$ :

- 2.65–3.19 (estimated from  $\log K_{OW}$ , Lyman et al. 1990; Howard 1993)
- 4.10 (activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Volatilization: based on the Henry's law constant, the volatilization  $t_{1/2} \sim 3.5$  h from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 8.4$  d in the atmosphere with rate constant  $k = 1.9 \times 10^{-12}$  cm<sup>3</sup>/molecule·s at 25°C for the reaction with photochemically produced hydroxyl radicals (Atkinson 1987; quoted, Howard 1993).

Hydrolysis:

Biodegradation:

Biotransformation:

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

## Half-Lives in the Environment:

Air:  $t_{1/2} = 8.4$  d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Atkinson 1987; quoted, Howard 1993).

Surface water:  $t_{1/2} = 1.2$  d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

TABLE 6.1.2.3.1

Reported aqueous solubilities and vapor pressures of 4-chlorotoluene at various temperatures

Aqueous solubility		Vapor pressure			
Ma et al. 2001		Stull 1947		Cervenkova & Boublik 1982	
shake flask-GC		summary of lit. data			
t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	P/Pa
5	99	5.50	133	64.855	3584
15	103	31.0	666.6	75.304	5727
25	123	43.8	1333	84.258	8333
35	136	57.8	2666	91.408	11078
45	153	73.5	5333	97.416	13924
		83.2	7999	102.574	16819
		96.6	13332	107.91	20322
		117.1	26664	113.464	24580
		139.8	53329	118.857	29380
		162.3	101325	124.14	34794
				129.212	40761
		mp/°C	7.3	134.395	47661
				142.507	60218
				150.285	74704
				158.718	93384
				159.801	96011
				bp/°C	161.904

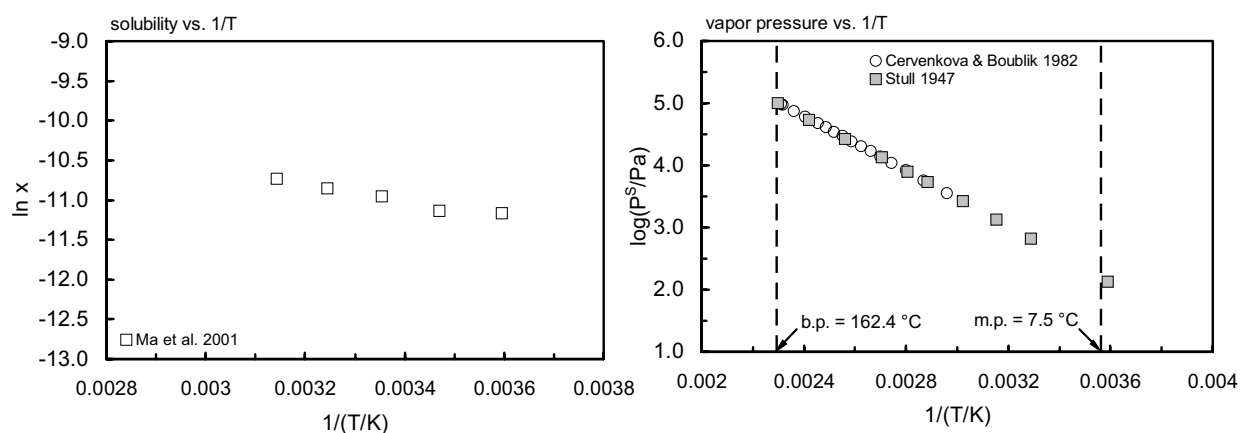
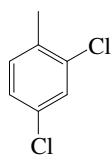


FIGURE 6.1.2.3.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 4-chlorotoluene.

## 6.1.2.4 2,4-Dichlorotoluene



Common Name: 2, 4-Dichlorotoluene

Synonym: 2, 4-dichloro-1-methylbenzene

Chemical Name: 2, 4-dichlorotoluene

CAS Registry No: 95-73-8

Molecular Formula:  $C_7H_6Cl_2$

Molecular Weight: 161.029

Melting Point ( $^{\circ}C$ ):

-13.5 (Weast 1982–83, Lide 2003)

Boiling Point ( $^{\circ}C$ ):

201 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.2498 (Weast 1982–83)

1.2476 (Riddick et al. 1986, Lide 2003)

1.246 (Dean 1985, 1992)

Molar Volume ( $cm^3/mol$ ):

128.6 (calculated-density, Stephenson & Malanowski 1987)

160.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

$26.20 \pm 2.1$  (shake flask-GC/FID, Ma et al. 2001)

18.9, 26.2, 30.7, 37 (15, 25, 35,  $45^{\circ}C$ , shake flask-GC, Ma et al. 2001)

$25.9 \pm 2.2$  (generator column-GC/FID, Ma et al. 2001)

22.3, 23.1, 25.9, 32, 36.6 (5, 15, 25, 35,  $45^{\circ}C$ , generator column-GC, Ma et al. 2001)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

55.5 (Riddick et al. 1986)

$\log(P/kPa) = 5.6199 - 1330.4/(t/^{\circ}C + 168.5)$  (Antoine eq., Riddick et al. 1986)

55.51 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.6199 - 1330.4/(T/K - 104.65)$ ; temp range 346–475 K (Antoine eq., Stephenson & Malanowski 1987)

61.06 (Daubert & Danner 1989)

$\log(P/mmHg) = 31.9325 - 3.7438 \times 10^3/(T/K) - 8.0123 \cdot \log(T/K) - 7.5077 \times 10^{-11} \cdot (T/K) + 1.250 \times 10^{-6} \cdot (T/K)^2$ , temp range 260–705 K (Yaws 1994)

Henry's Law Constant ( $Pa\ m^3/mol$  at  $25^{\circ}C$ ):

350.6 (calculated, Hine & Mookerjee 1975)

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

4.24 (HPLC-RT correlation, Könemann et al. 1979)

4.24 (recommended, Sangster 1993)

4.24 (shake flask, Hansch et al. 1995)



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

Bioconcentration Factor,  $\log BCF$ :

2.99 (estimated from  $\log K_{OW}$ , Howard 1997)

Sorption Partition Coefficient,  $\log K_{OC}$ :

3.68 (estimated from  $\log K_{OW}$ , Howard 1997)

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Volatilization:  $t_{1/2} = 4.0$  h in a model river 1-m deep with a 1 m/s current and a 3 m/s wind,  $t_{1/2} = 1$  d in the Rhine River in the Netherlands (Howard 1997)

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 11.6$  d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

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

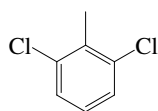
Half-Lives in the Environment:

Air:  $t_{1/2} = 11.6$  d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Surface water:  $t_{1/2} = 1.0$  d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

volatilization  $t_{1/2} = 4$  h in a model river,  $t_{1/2} = 1$  d in Rhine River in the Netherlands (Howard 1993)

## 6.1.2.5 2,6-Dichlorotoluene



Common Name: 2, 6-Dichlorotoluene

Synonym:

Chemical Name: 2, 6-dichlorotoluene

CAS Registry No: 118-69-4

Molecular Formula:  $C_7H_6Cl_2$

Molecular Weight: 161.029

Melting Point ( $^{\circ}C$ ): liquid

25.8 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

198 (Weast 1982–83, Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.254 (Dean 1992)

1.2686 (Lide 2003)

Molar Volume ( $cm^3/mol$ ):

126.9 ( $20^{\circ}C$ , calculated-density)

160.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

$23.3 \pm 0.81$  (shake flask-GC/FID, Ma et al. 2001)

16.7, 19.8, 23.3, 30.1, 33 (5, 15, 25, 35,  $45^{\circ}C$ , shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

53.19 (estimated, Lyman et al. 1990, Howard 1997)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

350.6 (Hine & Mookerjee 1975)

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

4.29 (HPLC- $k'$  correlation, Könnemann et al. 1979)

4.29 (recommended, Sangster 1983)

4.29 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

3.03 (estimated from  $\log K_{ow}$ , Howard 1997)

Sorption Partition Coefficient,  $\log K_{OC}$ :

3.71 (estimated from  $\log K_{ow}$ , Howard 1997)

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Volatilization: based on Henry's law constant, an estimated  $t_{1/2} = 4.0$  h of volatilization from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Howard 1997).

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 11.6$  d in the atmosphere for reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

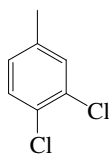
Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 11.6$  d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

## 6.1.2.6 3,4-Dichlorotoluene



Common Name: 3, 4-Dichlorotoluene

Synonym: 3, 4-dichloro-1-methylbenzene

Chemical Name:

CAS Registry No: 95-75-0

Molecular Formula:  $C_7H_6Cl_2$

Molecular Weight: 161.029

Melting Point ( $^{\circ}C$ ):

-15.2 (Weast 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

208.9 (Weast 1982–83; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.25256, 1.24751 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955; Riddick et al. 1986)

1.2564 (Weast 1982–83; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

127.9 (calculated-density, Stephenson & Malanowski 1987)

160.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

13.33, 10.13 ( $25^{\circ}C$ , bp, Dreisbach 1955; Riddick et al. 1986)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

10.544 (Dreisbach 1955)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

26 ( $30^{\circ}C$ , Dreisbach 1955; IUPAC Solubility Data Series, Horvath & Getzen 1985; Riddick et al. 1986)

Vapor Pressure (Pa at  $25^{\circ}C$  and the reported temperature dependence equations):

42 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.97925 - 1655.4/(195.0 + t/^{\circ}C)$ ; temp range  $105$ – $270^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = 6.91048 - 946.35/(246.68 + t/^{\circ}C)$ ; temp range  $-87$  to  $7^{\circ}C$  (Antoine eq., Dean 1985, 1992)

42.0 (Riddick et al. 1986)

$\log(P/kPa) = 6.10415 - 1655.44/(195.0 + t/^{\circ}C)$ , temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.10415 - 1655.4/(T/K - 78.15)$ ; temp range  $378$ – $543\ K$  (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

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

4.067 (Verhaar et al. 1992)

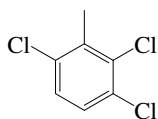
Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**6.1.2.7 2,3,6-Trichlorotoluene**

Common Name: 2, 3, 6-Trichlorotoluene

Synonym:

Chemical Name: 2, 3, 6-trichlorotoluene

CAS Registry No: 2077-46-5

Molecular Formula:  $C_7H_5Cl_3$

Molecular Weight: 195.474

Melting Point ( $^{\circ}C$ ):

45–46 (Weast 1982–83)

Boiling Point ( $^{\circ}C$ ):

229.5 (Weast 1982–83)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

180.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.629 (mp at  $45.5^{\circ}C$ )

Water Solubility ( $g/m^3$  or mg/L at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

1.08 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.6249 - 1323/(T/K - 144.15)$ ; temp range 384–509 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

152 (gas stripping-GC, Oliver 1985)

245 (calculated-bond contribution method, Meylan & Howard 1991)

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

4.80 (calculated as per Hansch & Leo 1979, Oliver 1987b)

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

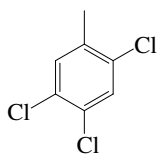
Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

Biota: elimination  $t_{1/2} < 5$  d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b)

**6.1.2.8 2,4,5-Trichlorotoluene**

Common Name: 2, 4, 5-Trichlorotoluene

Synonym: 2, 4, 5-TCT

Chemical Name: 2, 4, 5-trichlorotoluene

CAS Registry No: 6639-30-1

Molecular Formula:  $C_7H_5Cl_3$

Molecular Weight: 195.474

Melting Point ( $^{\circ}C$ ):

82.4 (Weast 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

231 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.1004 (Lide 2003)

Molar Volume ( $cm^3/mol$ ):

115.0 ( $20^{\circ}C$ , calculated-density)

180.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.273 (mp at  $82.4^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

$2.33 \pm 0.22$  (shake flask-GC/FID, Ma et al. 2001)

1.10, 1.38, 2.33, 3.33, 5.64 (5, 15, 25, 35,  $45^{\circ}C$ , shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

152 (gas stripping-GC, Oliver 1985)

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

4.82 (calculated- $\pi$  method of Hansch & Leo 1979, Oliver & Niimi 1984, 1985)

4.80 (Oliver & Niimi 1985)

4.780 (Verhaar et al. 1992)

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

Bioconcentration Factor,  $\log BCF$ :

3.68 (rainbow trout, Oliver & Niimi 1984; Oliver 1987)

3.54–3.99 with mean value of 3.88; 3.52–4.04 with mean value of 3.93 (rainbow trout, wet wt.,  $15^{\circ}C$ , steady-state BCF on 7- to 96-d laboratory study on two tanks of different water concn, Oliver & Niimi 1985)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

## Half-Lives in the Environment:

Air:

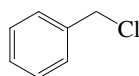
Surface water:  $t_{1/2} = 1.8$  d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} < 5$  d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b).

6.1.2.9  $\alpha$ -Chlorotoluene

Common Name:  $\alpha$ -Chlorotoluene

Synonym: chloromethylbenzene, benzyl chloride

Chemical Name:

CAS Registry No: 100-44-7

Molecular Formula:  $C_7H_7Cl$ ,  $C_6H_5CH_2Cl$

Molecular Weight: 126.584

Melting Point ( $^{\circ}C$ ):

−45 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

179 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

118.0 (calculated-density, Stephenson & Malanowski 1987)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

493 ( $20^{\circ}C$ , Riddick et al. 1986)

579 (calculated-fragment const., Wakita et al. 1986)

236 (calculated-group contribution, Kühne et al. 1995)

409 ( $20^{\circ}C$ , limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

133.3\* ( $22.0^{\circ}C$ , summary of lit. data, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11158.7/(T/K)] + 8.290189$ ; temp range  $22-179.4^{\circ}C$  (Antoine eq., Weast 1972–73)

641\* ( $47.84^{\circ}C$ , isoteniscope method, measured range  $47.84-117.08^{\circ}C$ , Ashcroft 1976)

$\log(P/mmHg) = 6.801 - 1477/(216.9 + t/^{\circ}C)$ ; temp range  $48-117^{\circ}C$  (isoteniscope method, Ashdroft 1976)

641 (Riddick et al. 1986)

$\log(P/kPa) = 5.926 - 1477/(193.7 + t/^{\circ}C)$ , temp range not specified (Antoine eq., Riddick et al. 1986)

170 (interpolated-Anotine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.7176 - 1954.13/(T/K - 38.02)$ ; temp range  $295-453$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 7.73903 - 2642.08/(T/K + 12.819)$ ; temp range  $320-390$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 12.1503 - 2.9139 \times 10^3/(T/K) - 0.3712 \cdot \log(T/K) - 5.2889 \times 10^{-3} \cdot (T/K) + 2.6296 \times 10^{-6} \cdot (T/K)^2$ , temp range  $234-686$  K (Yaws 1994)

133.05\* ( $24.05^{\circ}C$ , transpiration method, measured range  $276-309$  K, Krasnykh et al. 2002)

$\ln(P/Pa) = 281.417/R - 71588.799/R(T/K) - (72.0/R) \cdot \ln[(T/K)/298.15]$ ; temp range  $276-309$  K (transpiration method, Krasnykh et al. 2002)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

159.4, 122, 178, 216, 243.5, 320, 322, 370 (1.0, 3.0, 12.4, 12.5, 17.9, 19.1, 22.7,  $23.0^{\circ}C$ , equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)

$\ln(k_H/atm) = 17.18 - 3545/(T/K)$ ; temp range  $1.0-23.0^{\circ}C$  (equilibrium cell-concn ratio, Leighton & Calo 1981)

36.07 ( $20^{\circ}C$ , equilibrium air stripping-GC, Hovorka & Dohnal 1997)



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

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

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

$k_{O_3} < 0.04 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K with a tropospheric lifetimes  $\tau > 290 \text{ d}$  and  $\tau \sim 3 \text{ d}$  due to reactions with  $O_3$  and OH radical at room temp. (Atkinson et al. 1982)

$k_{OH} = (2.95 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a atmospheric lifetime  $\tau = 3.9 \text{ d}$  at room temp. (relative rate method, Edney et al. 1986)

$k_{OH}(\text{calc}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs}) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = 2.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

$t_{1/2} = 22\text{--}218 \text{ h}$ , based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: rate constant  $k = 1.28 \times 10^{-5} \text{ s}^{-1}$  and  $t_{1/2} = 15 \text{ h}$  at 25°C and pH 7 (Mabey & Mill 1978)

neutral rate constant  $k = 8.5 \pm 0.5 \text{ min}^{-1}$  at 25°C (Ellington et al. 1988)

$t_{1/2} = 25\text{--}290 \text{ h}$  based on overall hydrolysis rate constant (Howard et al. 1991)

Biodegradation:  $t_{1/2}(\text{aerobic}) = 168\text{--}672 \text{ h}$ , based on unacclimated aqueous screening test data;  $t_{1/2}(\text{anaerobic}) = 672\text{--}2688 \text{ h}$ , based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric lifetimes  $\tau > 290 \text{ d}$  and  $\tau \sim 3 \text{ d}$  due to reactions with  $O_3$  and OH radical, respectively, at room temp. (Atkinson et al. 1982);

calculated atmospheric lifetime  $\tau = 3.9 \text{ d}$  due to reaction with OH radical at room temp. (Edney et al. 1986)

$t_{1/2} = 22\text{--}218 \text{ h}$ , based on photooxidation half-life in air (Howard et al. 1991)

Surface water:  $t_{1/2} = 15\text{--}290 \text{ h}$ , based on estimated hydrolysis half-lives (Howard et al. 1991)

Groundwater:  $t_{1/2} = 15\text{--}290 \text{ h}$ , based on estimated hydrolysis half-lives (Howard et al. 1991)

Sediment:

Soil:  $t_{1/2} = 15\text{--}290 \text{ h}$ , based on estimated hydrolysis half-lives (Howard et al. 1991)

Biota:

**TABLE 6.1.2.9.1**

**Reported vapor pressures of *a*-chlorotoluene at various temperatures and the coefficients for the vapor pressure equations**

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

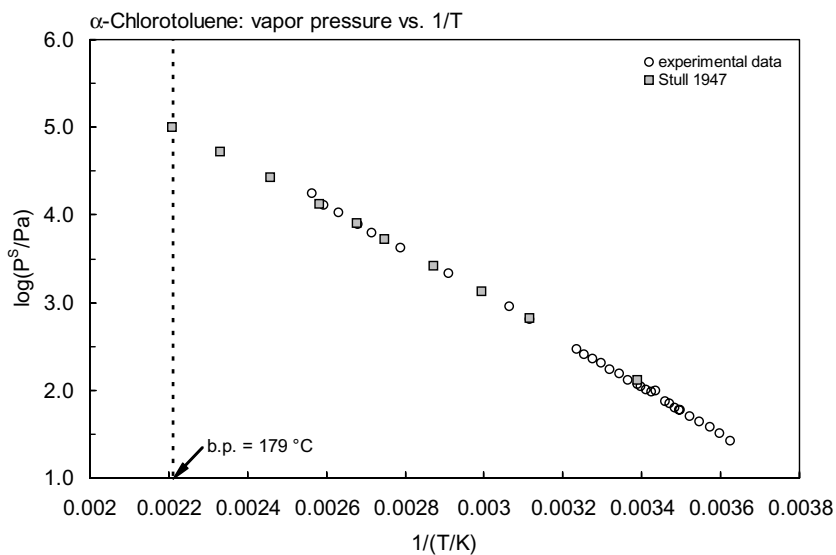
$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

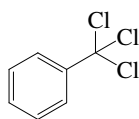
Stull 1947		Ashcroft 1976		Krasnykh et al. 2002	
summary of lit. data		isoteniscope method		transpiration method	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
22.0	133	47.84	641.3	2.85	26.95
47.8	666.6	53.37	905.3	4.85	32.31
60.8	1333	70.60	2177	6.85	38.60

(Continued)

TABLE 6.1.2.9.1 (Continued)

Stull 1947		Ashcroft 1976		Krasnykh et al. 2002	
summary of lit. data		isoteniscope method		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
75.0	2666	85.63	4246	8.85	43.78
90.7	5333	95.35	6330	10.85	51.48
100.5	7999	100.2	7905	12.85	60.14
114.2	13332	106.95	10566	12.95	60.61
134.0	26664	122.67	12883	13.95	64.27
1558	53329	117.08	17857	14.95	70.50
179.4	101325			15.95	75.36
		eq. 2	P/mmHg	17.95	98.72
mp/°C	-39	A	6.801	18.95	97.84
		B	1477	20.05	101.6
		C	193.7	21.15	111.0
				22.05	117.44
				24.05	133.06
				26.05	153.53
				28.15	175.98
				30.15	204.90
				32.15	232.87
				34.15	257.42
				36.15	295.82
				$\Delta H_V(\text{kJ mol}^{-1}) = 50.12$	
				at 25°C	

FIGURE 6.1.2.9.1 Logarithm of vapor pressure versus reciprocal temperature for  $\alpha$ -chlorotoluene.

**6.1.2.10  $\alpha, \alpha, \alpha$ -Trichlorotoluene**

Common Name:  $\alpha, \alpha, \alpha$ -Trichlorotoluene

Synonym: trichloromethylbenzene, benzotrichloride

Chemical Name:  $\alpha, \alpha, \alpha$ -Trichlorotoluene

CAS Registry No: 98-07-7

Molecular Formula:  $C_7H_5Cl_3$ ,  $C_6H_5CCl_3$

Molecular Weight: 195.474

Melting Point ( $^{\circ}C$ ):

−4.42 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

221 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.3723 ( $20^{\circ}C$ , Lide 2003)

Molar Volume ( $cm^3/mol$ ):

142.4 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

180.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

5.30 ( $5^{\circ}C$ , Riddick et al. 1986)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

133.3\* (45.8, summary of lit. data, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 8869.7/(T/K)] + 8.071972$ , temp range  $32-102.2^{\circ}C$  (Antoine eq., Weast 1972–73)

34.67 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.95923 - 2268.82/(T/K - 28.669)$ ; temp range  $318-487$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 0.4912 - 2.7285 \times 10^3/(T/K) + 4.4706 \cdot \log(T/K) - 1.058 \times 10^{-2} \cdot (T/K) + 4.7621 \times 10^{-6} \cdot (T/K)^2$ ; temp range  $268-737$  K (Yaws 1994)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

2.92 (shake flask, Leo et al. 1979, Hansch & Leo 1979, Hansch et al. 1995; quoted, Sangster 1993)

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

Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation:  $t_{1/2} = 173.7-1737$  h, based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: rate constant  $k = 6.3 \times 10^{-2} s^{-1}$  and  $t_{1/2} = 19$  s at  $25^{\circ}C$  and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 11$  s – 3 min, based on overall hydrolysis rate constants (Howard et al. 1991)

Biodegradation:  $t_{1/2}$ (aerobic) = 24–168 h, based on limited aqueous screening test data;  $t_{1/2}$  = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2}$  = 173.7–1737 h, based on photooxidation half-life in air (Howard et al. 1991)

Surface water:  $t_{1/2}$  = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Groundwater:  $t_{1/2}$  = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Sediment:

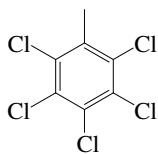
Soil:  $t_{1/2}$  = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Biota:

**TABLE 6.1.2.10.1**  
**Reported vapor pressures of  $\alpha$ ,  $\alpha$ ,  $\alpha$ -chlorotoluene at various temperatures**

Stull 1947	
summary of literature data	
$t/^{\circ}\text{C}$	$P/\text{Pa}$
45.8	133.3
73.7	666.6
87.6	1333
102.7	2666
119.8	5333
130.0	7999
144.3	13332
165.6	26664
189.2	53329
213.5	101325
mp/ $^{\circ}\text{C}$	–21.2

## 6.1.2.11 Pentachlorotoluene



Common Name: Pentachlorotoluene

Synonym:

Chemical Name: pentachlorotoluene

CAS Registry No: 877-11-1

Molecular Formula:  $C_7H_3Cl_5$

Molecular Weight: 264.364

Melting Point ( $^{\circ}C$ ):

224.8 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

301 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

222.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.011 (mp at  $224.8^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

$0.028 \pm 0.001$ ,  $0.047 \pm 0.004$  (25,  $35^{\circ}C$ , shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

6.20 (calculated as per Hansch & Leo 1979, Oliver & Niimi 1985; Oliver 1987b)

5.50 (assumed to have approx. the same  $K_{ow}$  of HCB, Oliver & Charlton 1984)

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

Bioconcentration Factor,  $\log BCF$  at  $25^{\circ}C$  or as indicated:

3.38–3.86 mean 3.83 (rainbow trout, wet wt.,  $15^{\circ}C$ , steady-state BCF, 7- to 96-d laboratory study, Oliver & Niimi 1985)

3.83; 4.36 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)

4.45; 3.83 (oligochaete worm; fish, Oliver 1987b)

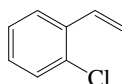
Sorption Partition Coefficient,  $\log K_{OC}$ :

5.30 (field data of sediment trap material; Oliver & Charlton 1984)

Environmental Fate Rate Constants, k or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

Biota: elimination  $t_{1/2} = 22$  and  $26$  d, observed and corrected for growth dilution, respectively, in oligochaete worms (Oliver 1987b)

**6.1.2.12 *o*-Chlorostyrene**

Common Name: *o*-Chlorostyrene

Synonym: *o*-chlorovinylbenzene, 2-chlorostyrene

Chemical Name: *o*-chlorostyrene

CAS Registry No: 2039-87-4

Molecular Formula: C<sub>8</sub>H<sub>7</sub>Cl

Molecular Weight: 138.595

Melting Point (°C):

-63.1 (Lide 2003)

Boiling Point (°C):

188.7 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm<sup>3</sup>):

1.10001, 1.09532 (20°C, 25°C, Dreisbach 1955)

Molar Volume (cm<sup>3</sup>/mol):

126.0 (20°C, calculated-density, Stephenson & Malanowski 1987)

153.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

51.03, 40.01 (25°C, bp, Dreisbach 1955)

Enthalpy of Sublimation, ΔH<sub>subl</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

127.5 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.86644 – 1542.1/(198 + t/°C); temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/kPa) = 6.11856 – 1627.284/(207.112 + t/°C); temp range 98.5–154.9°C (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)

log (P<sub>L</sub>/kPa) = 5.99134 – 1541.1/(-75.15 + T/K); temp range 363–543 K (Antoine eq., Stephenson & Malanowski 1987)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

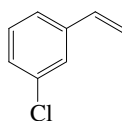
Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF or log K<sub>B</sub>:

Sorption Partition Coefficient, log K<sub>OC</sub>:

Environmental Fate Rate Constants, k, and Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

6.1.2.13 *m*-Chlorostyrene

Common Name: *m*-Chlorostyrene

Synonym: *m*-chlorovinylbenzene, 3-chlorostyrene

Chemical Name: *m*-chlorostyrene

CAS Registry No: 2039-85-2

Molecular Formula: C<sub>8</sub>H<sub>7</sub>Cl

Molecular Weight: 138.595

Melting Point (°C):

Boiling Point (°C):

Density (g/cm<sup>3</sup>):

1.1033 (20°C, Lide 2003)

Molar Volume (cm<sup>3</sup>/mol):

124.1 (20°C, calculated-density, Stephenson & Malanowski 1987)

153.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

Enthalpy of Sublimation, ΔH<sub>subl</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F:

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

Vapor Pressure (Pa 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.):

133.3\* (25.3°C, summary of literature data, Stull 1947)

148.06 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P<sub>L</sub>/kPa) = 6.83847 – 2156.77/(–16.882 + T/K); temp range 298–463 K (Antoine eq., Stephenson & Malanowski 1987)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

Octanol/Air Partition Coefficient, log K<sub>oa</sub>:

Bioconcentration Factor, log BCF or log K<sub>B</sub>:

Sorption Partition Coefficient, log K<sub>oc</sub>:

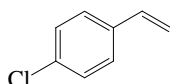
Environmental Fate Rate Constant, k, and Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

**TABLE 6.1.2.13.1****Reported vapor pressures of m-chlorostyrene at various temperatures****Stull 1947****summary of literature data**

<b>t/°C</b>	<b>P/Pa</b>
25.3	133.3
51.3	666.6
65.2	1333
80.0	2666
96.5	5333
107.2	7999
121.1	13332
142	26664
165.7	53329
190	101325



6.1.2.14 *p*-Chlorostyrene

Common Name: *p*-Chlorostyrene

Synonym: *p*-chlorovinylbenzene, 4-chlorostyrene

Chemical Name: *p*-chlorostyrene

CAS Registry No: 1073-67-2

Molecular Formula: C<sub>8</sub>H<sub>7</sub>Cl

Molecular Weight: 138.595

Melting Point (°C):

−15.9 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

192.0 (Dreisbach 1955, Lide 2003)

Density (g/cm<sup>3</sup>):

1.08682, 1.08214 (20°C, 25°C, Dreisbach 1955)

1.0868 (20°C, Lide 2003)

Molar Volume (cm<sup>3</sup>/mol):

127.5 (20°C, calculated-density, Stephenson & Malanowski 1987)

153.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

51.11, 40.07 (25°C, bp, Dreisbach 1955)

Enthalpy of Sublimation, ΔH<sub>subl</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

133.3\* (28.0°C, summary of literature data, temp range 28.0–191.0°C, Stull 1947)

6287\* (100.91°C, ebulliometry, measured range 100.91–127.27°C, Dreisbach & Shrader 1949)

116.3 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.84248 – 1545.0/(198 + t/°C); temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/kPa) = 9.18404 – 4186.871/(398.256 + t/°C); temp range 100.9–127.27°C (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)

log (P<sub>L</sub>/kPa) = 5.96738 – 1545.0/(−75.15 + T/K); temp range 363–523 K (Antoine eq., Stephenson & Malanowski 1987)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

3.66 (estimated, Kaiser 1987)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF or log K<sub>B</sub>:

Sorption Partition Coefficient, log K<sub>OC</sub>:

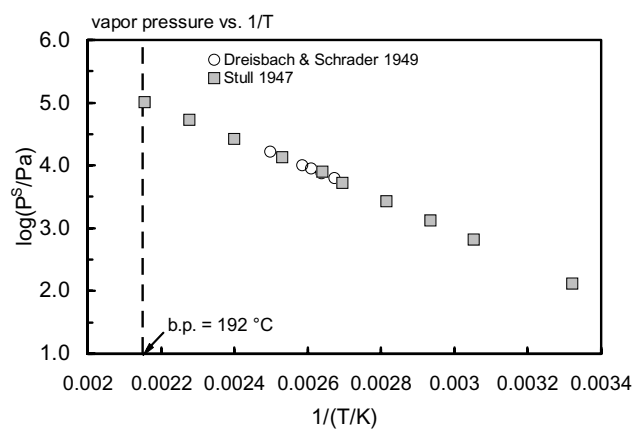
Environmental Fate Rate Constant, k, and Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

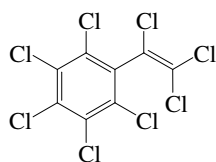
TABLE 6.1.2.14.1

Reported vapor pressures of *p*-chlorostyrene at various temperatures

Stull 1947		Dreisbach & Shrader 1949	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
28.0	133.3	100.91	6287
54.5	666.6	106.09	7605
67.5	1333	109.97	8851
82.0	2666	113.76	10114
98.0	5333	127.27	16500
105.8	7999		
122.0	13332		
143.5	26664		
166.0	53329		
191.0	101325		

FIGURE 6.1.2.14.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-chlorostyrene.

## 6.1.2.15 Octochlorostyrene



Common Name: Octochlorostyrene

Synonym:

Chemical Name: octachlorostyrene

CAS Registry No: 29082-74-4

Molecular Formula:  $C_8Cl_8$

Molecular Weight: 379.710

Melting Point ( $^{\circ}C$ ):

99 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

300.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.188 (mp at  $99^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

22.9( $20^{\circ}C$ , calculated-bond contribution method, Meylan & Howard 1991)

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

6.29 (HPLC-RT correlation, Veith et al.1979b)

6.20 (HPLC-RT correlation, Veith et al. 1979a)

Bioconcentration Factor,  $\log BCF$ :

4.52 (fathead minnow, 32-d exposure, Veith et al. 1979b)

2.91–3.91, mean 3.91 (rainbow trout,  $15^{\circ}C$ , wet wt., steady-state BCF on 7- to 96-d laboratory study; Oliver & Niimi 1985)

5.38; 6.15 (rainbow trout, calculated- $K_{ow}$ , Lake Ontario field BCF, Oliver & Niimi 1985)

4.49; 3.91 (oligochaete worms; fish, Oliver 1987b)

Sorption Partition Coefficient,  $\log K_{oc}$ :

6.10 (field data of sediment trap material, Oliver & Charlton 1984)

5.90–7.30; 6.60 (suspended sediment: range; mean, Oliver 1987a)

6.30 (algae  $> 50 \mu m$ , mean, Oliver 1987a)

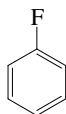
Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

Biota: elimination  $t_{1/2} = 71$  d, observed and  $t_{1/2} = 100$  d, corrected for growth dilution in worms ( $8^{\circ}C$ , Oliver 1987).

## 6.1.3 FLUOROBENZENES

## 6.1.3.1 Fluorobenzene



Common Name: Fluorobenzene

Synonym: phenyl fluoride

Chemical Name: fluorobenzene, phenyl fluoride

CAS Registry No: 462-06-6

Molecular Formula:  $C_6H_5F$

Molecular Weight: 96.102

Melting Point ( $^{\circ}C$ ):

−42.18 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

84.73 (Riddick et al. 1986; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.0225 (Horvath 1982; Lide 2003)

1.0131 ( $30^{\circ}C$ , Riddick et al. 1986)

Molar Volume ( $cm^3/mol$ ):

94.4 (Stephenson & Malanowski 1987; Wang et al. 1992)

101.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

11.305 (quoted, Riddick et al. 1986)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

1540 ( $30^{\circ}C$ , shake flask-IR, Gross et al. 1933)

1550 (shake flask-UV spectrophotometer, Andrews & Keefer 1950)

1296 (Deno & Berkheimer 1960)

922 (shake flask-GC, Jones et al. 1977/1978)

189.3\* (shake flask-GC, measured range  $5-45^{\circ}C$ , Nelson & Smit 1978)

1559 (Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

1540 ( $27.5^{\circ}C$ , recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

1530 ( $30^{\circ}C$ , Riddick et al. 1986)

1700\*, 1550 ( $19.2^{\circ}C$ ,  $29.7^{\circ}C$ , shake flask-GC/TC, measured range  $0-80^{\circ}C$ , Stephenson 1992)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

10246\* ( $24.9^{\circ}C$ , Ramsay-Young method, measured range  $-17.85$  to  $83.85^{\circ}C$ , Young 1889)

7999\* ( $19.6^{\circ}C$ , summary of literature data, temp range  $-43.4$  to  $84.7^{\circ}C$ , Stull 1947)

19920\* ( $39.4^{\circ}C$ , comparative ebulliometry, measured range  $39.4-120.5^{\circ}C$ , Scott et al. 1956)

$\log(P/mmHg) = 6.95208 - 1248.083/(221.827 + t/^{\circ}C)$ ; temp range  $34.5-120.5^{\circ}C$  (Antoine eq., comparative ebulliometry, Scott et al. 1956)

$\log(P/mmHg) = [-0.2185 \times 7980.4/(T/K)] + 7.699237$ ; temp range  $-43.4-279.3^{\circ}C$  (Antoine eq., Weast 1972-73)

10200 (interpolated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/mmHg) = 7.18703 - 1381.828/(235.563 + t/^{\circ}C)$ ; temp range  $-17.85$  to  $83.85^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log(P/kPa) = 6.31155 - 1381.646/(235.548 + t/^{\circ}C)$ ; temp range  $-17.85$  to  $83.85^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.1870 - 1381.8/(235.6 + t/^{\circ}\text{C})$ ; temp range  $-18$  to  $84^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)  
10480 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.07698 - 1248.083/(221.827 + t/^{\circ}\text{C})$ , temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.07234 - 1245.564/(-51.587 + T/\text{K})$ ; temp range 312–394 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.4113 - 1398.61/(-31.295 + T/\text{K})$ ; temp range 358–530 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14135 - 1291.116/(-45.664 + T/\text{K})$ ; temp range 373–419 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.37857 - 1478.807/(-18.847 + T/\text{K})$ ; temp range 414–501 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.59182 - 2876.741/(171.093 + T/\text{K})$ ; temp range 497–561 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -5.4849 - 1.8597 \times 10^3/(T/\text{K}) + 7.1515 \cdot \log (T/\text{K}) - 1.6467 \times 10^{-2} \cdot (T/\text{K}) + 9.2622 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 231–560 K (Yaws 1994)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at  $25^{\circ}\text{C}$ ):

632 (computer value, Yaws et al. 1991)

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

2.27 (shake flask-AS, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)

2.28 (calculated-fragment const., Rekker 1977)

2.27 (recommended, Sangster 1989, 1993)

2.26 (centrifugal partition chromatography, El Tayar et al. 1991)

2.27 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log \text{BCF}$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with  $\text{NO}_3$  radical and  $k_{O_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}(\text{calc}) = 2.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs}) = 0.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (6.31 \pm 0.84) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{OH} = 6.31 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k(\text{soln}) = 1.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{OH} = 6.90 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , independent of temperature over the range 234–303 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 1.08 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 6.1.3.1.1

Reported aqueous solubilities of fluorobenzene at various temperatures

Gross et al. 1933		Nelson & Smit 1978		Stephenson 1992	
shake flask-interferometer		shake flask-GC		shake flask-GC/TC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
30	1540	5	118.4	0	1620
		25	189.3	9.5	1660
		35	336	29.7	1700
		45	512	39.6	1530
				47.7	1730
Andrews & Keefer 1950				60.1	1900
shake flask-UV				70	1901
t/°C	S/g·m <sup>-3</sup>			80	1880
25	1550				

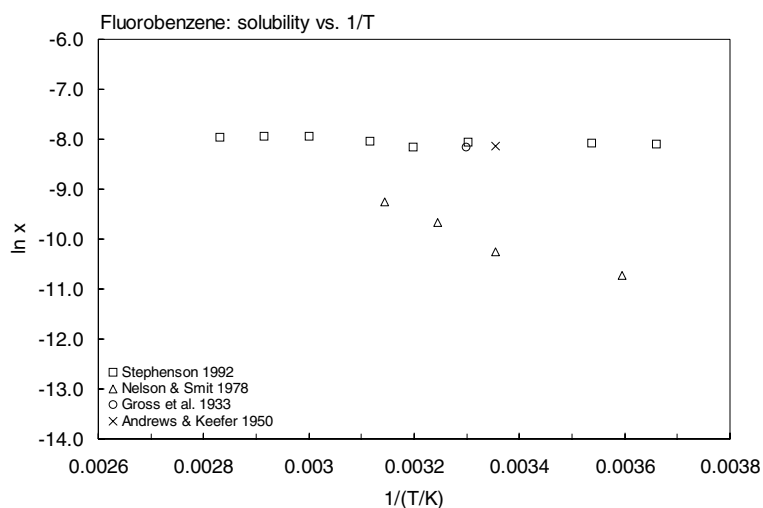
FIGURE 6.1.3.1.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for fluorobenzene.

TABLE 6.1.3.1.2

Reported vapor pressures of fluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Young 1889		Stull 1947		Scott et al. 1956	
Ramsay-Young method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-17.85	927	-43.4	133.3	39.404	19920
-5.95	1980	-22.8	666.6	44.920	25007
0.15	2806	-12.4	1333	50.480	31160
4.7	3613	-1.20	2666	56.081	38567
10.65	5000	11.5	5333	61.726	47359
16.75	6873	19.6	7999	67.412	57803
19.5	7866	30.4	13332	73.141	70109
24.9	10246	47.2	26664	78.916	84525
30.35	12999	65.7	53329	84.734	101325
36.05	16759	84.7	101325	90.590	120798
42.05	21558			96.497	143268
49.6	29317	mp/°C	-42.1	102.438	169-53
56.2	37610			108.431	198530
62.75	47889			114.462	232088
71	63995			120.538	270111
78.75	82473				
83.85	97378				

complete set of data see [ref.](#)

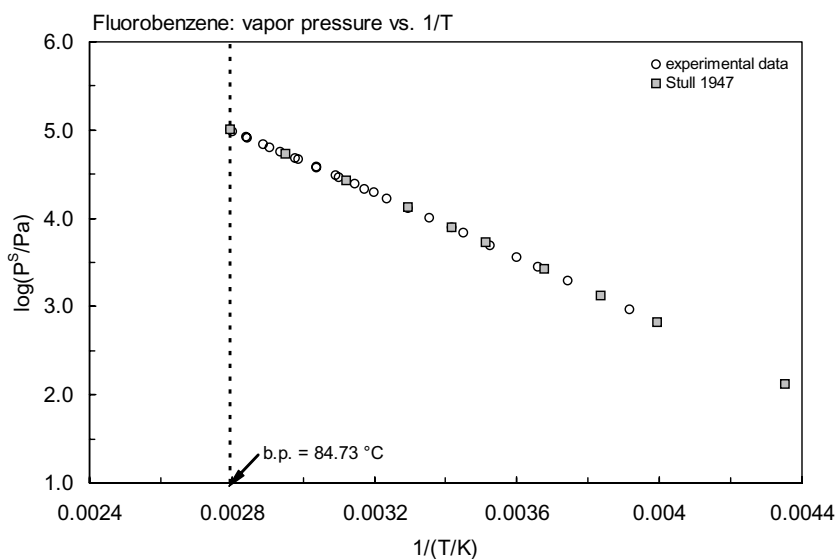
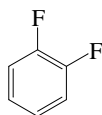


FIGURE 6.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for fluorobenzene.

## 6.1.3.2 1,2-Difluorobenzene



Common Name: 1,2-Difluorobenzene

Synonym: *o*-difluorobenzene

Chemical Name: 1,2-Difluorobenzene

CAS Registry No: 367-11-3

Molecular Formula: C<sub>6</sub>H<sub>4</sub>F<sub>2</sub>

Molecular Weight: 114.093

Melting Point (°C):

−47.1 (Lide 2003)

Boiling Point (°C):

94 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.158 (Dean 1992)

Molar Volume (cm<sup>3</sup>/mol):

99.2 (calculated-density, Stephenson & Malanowski 1987)

106.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

1141 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)

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):

9582\* (31.17°C, comparative ebulliometry, measured range 31–130°C, Scott et al. 1963)

log (P/kPa) = 6.12360 – 1297.243/(211.103 + t/°C); temp range 31.2–130°C (Antoine eq. derived from experimental data of Scott et al. 1963, Boublik et al. 1984)

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25°C):

713 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

2.59 (calculated-fragment const., Valvani & Yalkowsky 1980)

2.58 (calculated-fragment const., Yalkowsky et al. 1983)

2.56 (calculated-molar volume correlation, Wang et al. 1992)

2.43 (calculated, Müller & Klein 1992)

2.37 (recommended, Hansch et al. 1995)

2.25; 2.33 (predicted; calc-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K<sub>oa</sub>:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K<sub>oc</sub>:

Environmental Fate Rate Constants, k or Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:



TABLE 6.1.3.2.1

Reported vapor pressures of 1,2-difluorobenzene at various temperatures

Scott et al. 1963					
comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa		
31.168	9582	111.903	169053		
33.916	10884	117.980	198530	data also fitted to Cox eq.	
36.668	12335	124.099	232088	Cox eq. P/mmHg	
39.436	13950	130.256	270111	$\log (P/760)=A[1-B/(T/K)]$	
42.210	15740			$\log A = a - b(T/K) + c(T/K)^2$	
44.996	17725	mp/K	226.0148	a	0.841936
47.803	19920	bp/K	367.07	$10^{-4} \cdot b$	6.77698
53.423	25007	$\Delta H_{\text{fus}} = 11.045 \text{ kJ/mol}$		$10^{-7} \cdot c$	6.52099
59.084	31160	$\Delta H_{\text{v}} = 36.11 \text{ kJ/mol}$		B	367.072
64.787	38547	Antoine eq.			
70.530	47359	$\log P = A - B/(C + t/^{\circ}\text{C})$			
76.314	57803		P/mmHg		
82.142	70109	A	7.00003		
88.009	84525	B	1298.053		
93.921	101325	C	221.197		
99.874	120798				
105.869	143268				

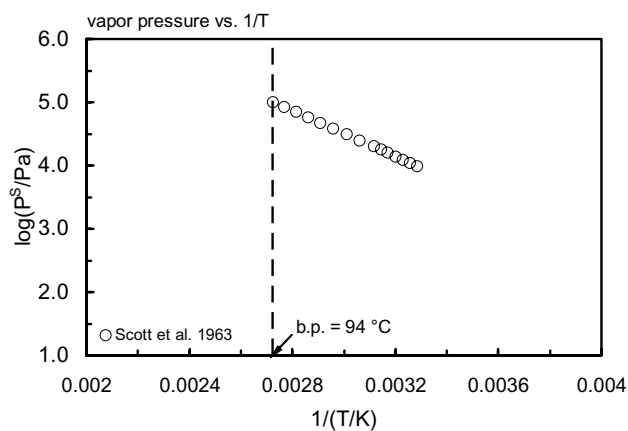
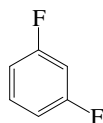


FIGURE 6.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-difluorobenzene.

**6.1.3.3 1,3-Difluorobenzene**

Common Name: 1,3-Difluorobenzene

Synonym: *m*-difluorobenzene

Chemical Name: 1,3-Difluorobenzene

CAS Registry No: 372-18-9

Molecular Formula: C<sub>6</sub>H<sub>4</sub>F<sub>2</sub>

Molecular Weight: 114.093

Melting Point (°C):

−69.12 (Lide 2003)

Boiling Point (°C):

82.6 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.1552 (18°C, Horvath 1982)

1.1572 (Lide 2003)

Molar Volume (cm<sup>3</sup>/mol):

98.6 (20°C, calculated-density, Stephenson & Malanowski 1987, Ruelle & Kesselring 1997)

106.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

1141 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

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):

19924\* (38.284°C, comparative ebulliometry, measured range 311.334–391.523 K, Osborn & Scott 1980)

Henry's Law Constant (Pa·m<sup>3</sup>/mol):

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

2.58 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

2.56 (calculated-molar volume correlation, Wang et al. 1992)

2.43 (calculated, Müller & Klein 1992)

2.26; 2.33 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K<sub>oa</sub>:

Bioconcentration Factor, log BCF:

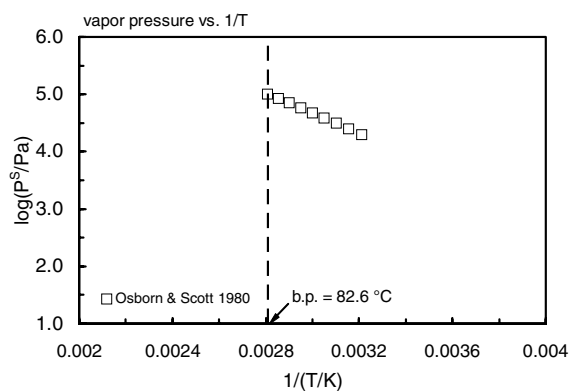
Sorption Partition Coefficient, log K<sub>oc</sub>:

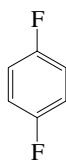
Environmental Fate Rate Constants, k or Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

**TABLE 6.1.3.3.1****Reported vapor pressures of 1,3-difluorobenzene at various temperatures**

Osborn & Scott 1980			
ebulliometry			
t/°C	P/Pa	t/°C	P/Pa
38.184	19924	88.808	120800
43.646	25014	94.641	143270
49.148	31167	100.511	169050
54.692	38553	106.425	198540
60.273	47363	112.378	232090
65.898	57806	118.373	270120
71.564	70112		
77.272	84528	data fitted to a 4-constant vapor pressure eq.	
83.02	101325		

**FIGURE 6.1.3.3.1** Logarithm of vapor pressure versus reciprocal temperature for 1,3-difluorobenzene.

**6.1.3.4 1,4-Difluorobenzene**

Common Name: 1,4-Difluorobenzene

Synonym: *p*-difluorobenzene

Chemical Name: 1,4-Difluorobenzene

CAS Registry No: 540-36-3

Molecular Formula: C<sub>6</sub>H<sub>4</sub>F<sub>2</sub>

Molecular Weight: 114.093

Melting Point (°C):

−23.55 (Lide 2003)

Boiling Point (°C):

89 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.1701 (20°C, Horvath 1982, Dean 1992; Lide 2003)

Molar Volume (cm<sup>3</sup>/mol):

97.4 (20°C, calculated-density, Stephenson & Malanowski 1987)

106.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

1222 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)

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):

9577\* (27.25°C, comparative ebulliometry, measured temp range 300.4–397.7 K, Osborn & Scott 1980)

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

776 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

2.58 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

2.43 (calculated, Müller & Klein 1992)

2.84 (calculated-molar volume, Wang et al. 1992)

2.24; 2.33 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K<sub>OC</sub>:

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

TABLE 6.1.3.4.1

Reported vapor pressures of 1,4-difluorobenzene at various temperatures

Osborn & Scott 1980			
ebulliometry			
t/°C	P/Pa	t/°C	P/Pa
28.248	9577	84.078	84528
30.95	10879	89.886	101325
33.658	12331	95.727	120800
36.376	13944	101.611	143270
39.101	15736	107.535	169050
41.837	17721	113.503	198540
44.588	19924	119.507	232090
50.109	25104	125.552	270120
55.671	31167		
61.273	38553	data fitted to a 4-constant vapor pressure eq.	
66.910	47363		
72.593	57806		
78.319	70112		

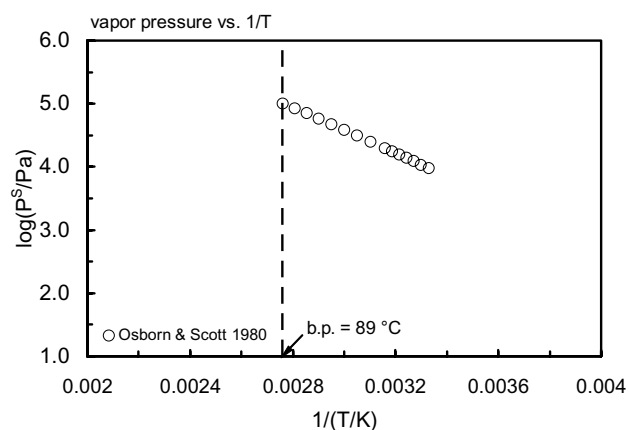
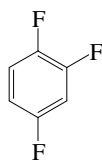


FIGURE 6.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-difluorobenzene.

## 6.1.3.5 1,2,4-Trifluorobenzene



Common Name: 1,2,4-Trifluorobenzene

Synonym:

Chemical Name: 1,2,4-trifluorobenzene

CAS Registry No: 367-23-7

Molecular Formula:  $C_6H_3F_3$

Molecular Weight: 132.083

Melting Point ( $^{\circ}C$ ):

Boiling Point ( $^{\circ}C$ ):

90 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

2.52 (HPLC-RT correlation, Garst 1984, quoted, Sangster 1993)

2.41 (recommended, Hansch et al. 1995)

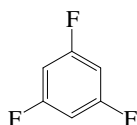
Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**6.1.3.6 1,3,5-Trifluorobenzene**

Common Name: 1,3,5-Trifluorobenzene

Synonym:

Chemical Name: 1,3,5-trifluorobenzene

CAS Registry No: 372-38-3

Molecular Formula:  $C_6H_3F_3$

Molecular Weight: 132.083

Melting Point ( $^{\circ}C$ ):

-5.5 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

75.4 (Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

103.4 (calculated-density, Stephenson & Malanowski 1987)

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

139.68\* ( $25.21^{\circ}C$ , static system-Hg manometer, measured range  $6.18$ – $50^{\circ}C$ , Findlay 1969)

$\log(P/mmHg) = 6.91873 - 1196.385/(219.01 + t/^{\circ}C)$ ; temp range  $6.18$ – $50^{\circ}C$  (Hg manometer, Findlay 1969)

$\log(P_L/kPa) = 6.04363 - 1198.385/(-54.131 + T/K)$ ; temp range  $279$ – $350$  K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{oc}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

TABLE 6.1.3.6.1

Reported vapor pressures of 1,3,5-trifluorobenzene at various temperatures

Findlay 1969					
Hg manometer					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
6.18	5385	25.24	13965	46.97	35156
6.19	5389	29.98	17331	46.97	35168
10.03	6615	29.98	17339	49.98	39.453
15.01	8530	35.15	21679	49.99	39.462
15.01	8534	35.25	21806		
19.99	10915	35.39	21846	log P = A - B/(C + t/°C)	
19.99	10911	40.05	26654		
20.49	11.202	40.11	26704	A	P/mmHg
20.53	11210	43.85	31019	B	6.91873
22.79	12468	43.94	31188	C	1196.385
25.21	13968	44.2	31463		219.019

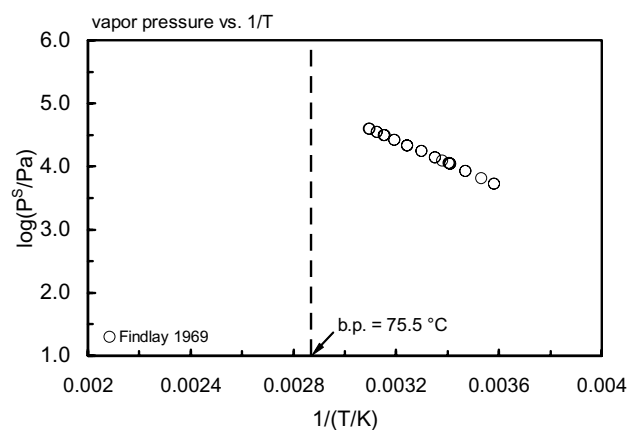
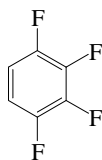


FIGURE 6.1.3.6.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trifluorobenzene.



## 6.1.3.7 1,2,3,4-Tetrafluorobenzene



Common Name: 1,2,3,4-Tetrafluorobenzene

Synonym:

Chemical Name: 1,2,3,4-tetrafluorobenzene

CAS Registry No: 551-62-2

Molecular Formula:  $C_6H_2F_4$

Molecular Weight: 150.074

Melting Point ( $^{\circ}C$ ):

−42 (Stephenson & Malanowski 1987)

Boiling Point ( $^{\circ}C$ ):

94.3 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

105.5 (calculated-density, Stephenson & Malanowski 1987)

116.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

33.0 (Ambrose et al. 1975)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

6545\* (24.82 $^{\circ}C$ , static-system-Hg manometer, Findlay 1969)

$\log(P/mmHg) = 7.19386 - 1396.067/(228.837 + t/^{\circ}C)$ ; temp range 6.05–49.87 $^{\circ}C$  (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)

6509\* (extrapolated from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.15854 - 1291.080/(-50.617 + T/K)$ ; temperature range 300.8–367.51(normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.16107 - 1292.550/(-56.453 + T/K)$ ; temperature range 300.8–391.65 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.21410 - 1341.655/(223.721 + t/^{\circ}C)$ ; temp range 24.78–84.98 $^{\circ}C$  (Antoine eq. derived from Findlay 1969 data, Boublik et al. 1984)

$\log(P/kPa) = 6.15932 - 1291.522/(216.58 + t/^{\circ}C)$ ; temp range 27.65–118.5 $^{\circ}C$  (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.31876 - 1396.067/(-44.277 + T/K)$ ; temp range 279–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.16042 - 1292.174/(-56.495 + T/K)$ ; temp range 300–392 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

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

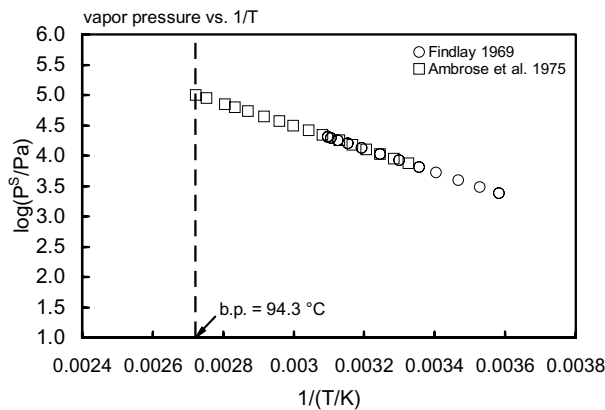
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants, k, and Half-Lives, t<sub>1/2</sub>:  
Half-Lives in the Environment:

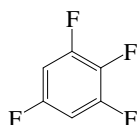
**TABLE 6.1.3.7.1**  
**Reported vapor pressures of 1,2,3,4-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations**

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Findlay 1969		Ambrose et al. 1975					
Hg manometer		ebulliometry					
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
6.05	2385	44.01	15919	27.65	7437	90.123	88.788
6.06	2377	46.91	18024	31.417	8945	94.228	100917
10.36	3041	46.91	18024	35.073	10646	95.082	103593
15.21	3970	48.82	19620	38.868	12.688	99.87	119685
20.64	5277	48.83	19621	42.74	15095	104.196	135850
24.82	6545	49.84	20380	46.466	17757		
24.82	6547	49.87	20.428	51.321	21794	Antoine eq. for temp.	
29.98	8433			55.476	25823	range 300–367 K	
29.99	8433	eq. 2	P/mmHg	60.207	31137	eq. 3	P/kPa
35.05	10722	A	7.19386	64.859	37177	A	6.15854
35.06	10722	B	1396.067	69.749	44535	B	129.08
40.07	13438	C	228.984	75.125	53942	C	–56.617
40.07	13439			79.797	63.331		
43.99	15904			83.34	71.305		



**FIGURE 6.1.3.7.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,4-tetrafluorobenzene.

## 6.1.3.8 1,2,3,5-Tetrafluorobenzene



Common Name: 1,2,3,5-Tetrafluorobenzene

Synonym:

Chemical Name: 1,2,3,5-tetrafluorobenzene

CAS Registry No: 2367-82-0

Molecular Formula:  $C_6H_2F_4$

Molecular Weight: 150.074

Melting Point ( $^{\circ}C$ ):

−46.25 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

84.4 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

107.7 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

116.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

32.1 (Ambrose et al. 1975)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section:

9770\* ( $24.81^{\circ}C$ , static method-Hg manometer, measured range  $6.08$ – $50^{\circ}C$ , Findlay 1969)

$\log(P/mmHg) = 7.07758 - 1290.984/(222.855 + t/^{\circ}C)$ ; temp range  $6.08$ – $49.83^{\circ}C$  (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)

9801\* (interpolated from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.15414 - 1255.781/(-54.898 + T/K)$ ; temperature range  $287.6$ – $357.61$  (normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.15507 - 1255.981/(-54.919 + T/K)$ ; temperature range  $287.6$ – $381.5$  K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.12070 - 1250.027/(218.829 + t/^{\circ}C)$ ; temp range  $6.08$ – $49.83^{\circ}C$  (Antoine eq. derived from Findlay 1969 data, Boublik et al. 1984)

$\log(P/kPa) = 6.1500 - 1253.079/(217.903 + t/^{\circ}C)$ ; temp range  $14.44$ – $108.37^{\circ}C$  (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.20248 - 1290.984/(-50.295 + T/K)$ ; temp range  $279$ – $323$  K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.15119 - 1253.771/(-55.168 + T/K)$ ; temp range  $287$ – $382$  K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.24644 - 1317.349/(-46.898 + T/K)$ ; temp range  $385$ – $416$  K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa\ m^3/mol$  at  $25^{\circ}C$ ):

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

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

Bioconcentration Factor, log BCF or log  $K_B$ :

Sorption Partition Coefficient, log  $K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

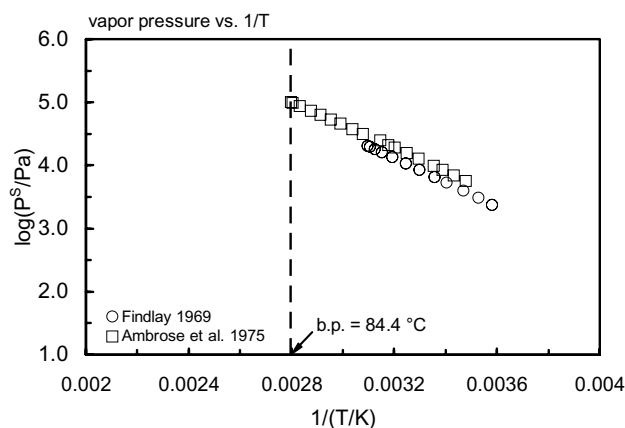
Half-Lives in the Environment:

**TABLE 6.1.3.8.1**

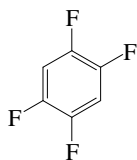
**Reported vapor pressures of 1,2,3,5-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations**

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Findlay 1969				Ambrose et al. 1975			
Hg manometer				ebulliometry			
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	T/K	P/Pa	T/K	P/Pa
6.05	2385	48.82	19620	287.593	5719	357.291	100305
6.06	2377	48.83	19621	291.414	6987	357.743	101755
10.36	3041	49.84	20380	295.169	8457	362.582	118237
15.21	3970	49.87	20428	298.091	9773	366.716	133926
20.64	5277			303.399	12598	371.603	154528
24.82	6545	eq. 2	P/mmHg	307.963	15541	376.423	177795
24.82	6547	A	7.07758	312.406	18930	381.524	203.907
29.98	8433	B	1290.984	314.635	20846		
29.99	8433	C	223.855	317.751	24802	Antoine eq. for temp range 287–356 K	
35.05	10722			324.852	31779		
35.06	10722			329.202	37666		
40.07	13438			334.506	46007	eq. 2	P/kPa
40.07	13439			338.643	53501	A	6.15414
43.99	15904			343.224	62911	B	1255.781
44.01	15919			347.715	73374	C	–54.898
46.91	18024			352.951	87269		
46.91	18024			356.719	98504		



**FIGURE 6.1.3.8.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetrafluorobenzene.

**6.1.3.9 1,2,4,5-Tetrafluorobenzene**

Common Name: 1,2,4,5-Tetrafluorobenzene

Synonym:

Chemical Name: 1,2,4,5-tetrafluorobenzene

CAS Registry No: 327-54-8

Molecular Formula:  $C_6H_2F_4$

Molecular Weight: 150.074

Melting Point ( $^{\circ}C$ ):

3.88 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

90.2 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.4255 (Lide 2003)

Molar Volume ( $cm^3/mol$ ):

105.3 ( $20^{\circ}C$ , calculated-density)

105.4 (calculated-density, Stephenson & Malanowski 1987)

116.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

32.9 (Ambrose et al. 1975)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

7556\* (interpolated from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.17340 - 1277.452/(-56.889 + T/K)$ ; temp range 293.2–363.413 (normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.17788 - 1279.904/(-56.642 + T/K)$ ; temp range 293.2–387.6 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.17439 - 1277.918/(216.289 + t/^{\circ}C)$ ; temp range  $20.05$ – $114.42^{\circ}C$  (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.17614 - 1278.93/(-56.748 + T/K)$ ; temp range 293–390 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.42009 - 1454.406/(-33.675 + T/K)$ ; temp range 390–488 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.88521 - 3090.851/(174.387 + T/K)$ ; temp range 488–543 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa  $m^3/mol$  at  $25^{\circ}C$ ):

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

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

TABLE 6.1.3.9.1

Reported vapor pressures of 1,2,4,5-tetrafluorobenzene at various temperatures:

Ambrose et al. 1975			
ebulliometry			
T/K	P/Pa	T/K	P/Pa
293.198	5855	363.049	100177
296.489	6944	363.591	101.896
300.519	8505	368.237	117566
303.459	9822	372.427	133286
308.374	12399	377.572	154790
313.302	15524	382.398	177330
315.839	17370	387.568	204254
320.056	20841		
324.073	24655	Antoine eq. for temp	
330.275	31652	range 293–363 K	
334.497	37286	$\log P = A - B/(C + T/K)$	
339.931	45699	P/kPa	
344.142	53227	A	6.1734
348.439	61895	B	1277.452
353.384	73237	C	-56.889
358.929	87873		
362.593	98750		

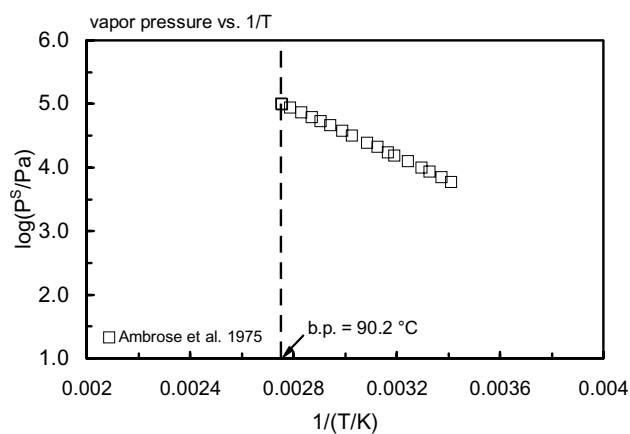
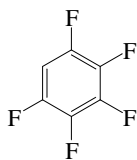


FIGURE 6.1.3.9.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4,5-tetrafluorobenzene.

**6.1.3.10 Pentafluorobenzene**

Common Name: Pentafluorobenzene

Synonym:

Chemical Name: pentafluorobenzene

CAS Registry No: 363-72-4

Molecular Formula:  $C_6HF_5$

Molecular Weight: 168.064

Melting Point ( $^{\circ}C$ ):

−47.4 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

85.74 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

111.0 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

121.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

32.38 (Ambrose 1968)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

9015\* ( $24.78^{\circ}C$ , static method, measured range  $24.78$ – $84.98^{\circ}C$ , Patrick & Prosser 1964)

$\log(P/mmHg) = 6.94904 - 1218.91/(213.313 + t/^{\circ}C)$ ; temp range  $24.98$ – $84.98^{\circ}C$ , Patrick & Prosser 1964)

26584\* ( $48.729^{\circ}C$ , ebulliometry, measured range  $49$ – $94^{\circ}C$ , Ambrose et al. 1975)

$\log(P/mmHg) = 7.03348 - 1253.043/(215.897 + t/^{\circ}C)$ ; temp range  $48.7$ – $94.3^{\circ}C$  (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/kPa) = 6.07634 - 1220.72/(213.425 + t/^{\circ}C)$ ; temp range  $24.78$ – $84.98^{\circ}C$  (Antoine eq. derived from Patrick & Prosser 1946 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.15571 - 1250.946/(-57.457 + T/K)$ ; temp range 322–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.20712 - 1282.574/(-53.619 + T/K)$ ; temp range 358–397 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.47368 - 1477.401/(-27.81 + T/K)$ ; temp range 393–479 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

2.53 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

TABLE 6.1.3.10.1

Reported vapor pressures of pentafluorobenzene 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)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Patrick & Prosser 1964		Ambrose 1968			
static method-Hg manometer		ebulliometry			
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa		
24.78	9015	48.729	26584		
29.85	11492	54.355	33360		
34.85	14540	59.041	40023		
39.85	18206	63.033	46499		
44.85	22507	66.698	53178		
49.85	27527	69.91	59642		
54.87	33877	72.828	66050		
59.92	41071	75.604	72643		
64.95	49217	78.158	79163		
69.95	59052	80.643	85953		
74.95	70191	82.998	92792		
79.95	82728	85.123	99333		
84.98	97125	85.496	100521		
		87.212	106123		
bp/ $^{\circ}\text{C}$	86.3	89.093	112557		
Antoine eq.		91.014	119417		
eq. 2	P/mmHg	92.509	124989		
A	6.94904	94.296	131878		
B	1218.91				
C	213.313	eq. 2	P/mmHg		
$\Delta H_v/(\text{kJ mol}^{-1}) =$		A	7.03488		
at $25^{\circ}\text{C}$	36.67	B	1253.043		
at bp	32.07	C	215.987		

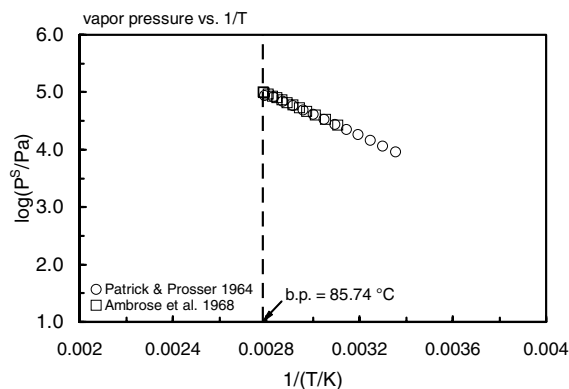
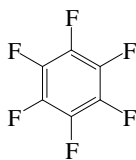


FIGURE 6.1.3.10.1 Logarithm of vapor pressure versus reciprocal temperature for pentafluorobenzene.



## 6.1.3.11 Hexafluorobenzene



Common Name: Hexafluorobenzene

Synonym: perfluorobenzene

Chemical Name: hexafluorobenzene

CAS Registry No: 392-56-3

Molecular Formula:  $C_6F_6$

Molecular Weight 180.054

Melting Point ( $^{\circ}C$ ):

5.0.3 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

80.26 (Lide 2003)

Density ( $g/cm^3$ ):

1.61866, 1.60732 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

1.6184 ( $20^{\circ}C$ , Lide 2003)

Molar Volume ( $cm^3/mol$ ):

115.8 (calculated-density, Stephenson & Malanowski 1987)

126.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

35.47 ( $25^{\circ}C$ , Findlay 1969)

35.69, 31.67 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

Enthalpy of Sublimation,  $\Delta H_{subl}$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

11.585 (Riddick et al. 1986)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

11196\* ( $24.78^{\circ}C$ , static method, measured range  $19.75$ – $84.98^{\circ}C$ , Patrick & Prosser 1964)

$\log(P/mmHg) = 7.39075 - 1432.91/(237.470 + t/^{\circ}C)$ ; temp range  $19.76$ – $84.98^{\circ}C$ , Patrick & Prosser 1964)

19957\* ( $37.303^{\circ}C$ , gas saturation/manometer, measured range  $37.303$ – $88.79^{\circ}C$ , Counsell et al. 1965)

11402\* ( $25.1^{\circ}C$ , Hg manometer, measured range  $4.74$ – $47.85^{\circ}C$ , Findlay 1969)

$\log(P/mmHg) = 6.86088 - 1152.442/(208.663 + t/^{\circ}C)$ ; temp range  $4.74$ – $47.85$  (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)

10733\* ( $24.005^{\circ}C$ , ebulliometry, measured range  $290$ – $377\ K$ , Ambrose 1981)

$\log(P/kPa) = 6.05252 - 1177.973/(210.677 + t/^{\circ}C)$ ; temp range  $19.75$ – $84.98^{\circ}C$  (Antoine eq. derived from Patrick & Prosser 1964 data, Boublik et al. 1984)

$\log(P/kPa) = 6.14363 - 1220.148/(214.610 + t/^{\circ}C)$ ; temp range  $37.3$ – $88.8^{\circ}C$  (Antoine eq. derived from Counsell et al. 1965 data, Boublik et al. 1984)

$\log(P/kPa) = 6.15013 - 1223.989/(215.084 + t/^{\circ}C)$ ; temp range  $17$ – $104^{\circ}C$  (Antoine eq. derived from Ambrose 1981 data, Boublik et al. 1984)

10733 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.14213 - 1219.41/(214.55 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_s/kPa) = 11.49514 - 3518.13/(44.44 + T/K)$ ; temp range  $215$ – $278\ K$  (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15233 - 1224.974/(-57.984 + T/\text{K})$ ; temp range 278–354 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.19544 - 1251.177/(-54.775 + T/\text{K})$ ; temp range 348–389 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -38.8085 - 1.3422 \times 10^3/(T/\text{K}) + 22.204 \cdot \log (T/\text{K}) - 3.8813 \times 10^{-221} \cdot (T/\text{K}) + 2.10 \times 10^{-5} \cdot (T/\text{K})^2$ ; temp range 278–517 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ( $\text{Pa} \cdot \text{m}^3/\text{mol}$  at  $25^\circ\text{C}$ ):

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

2.22 (shake flask, Log P Database, Hansch & Leo 1987)

2.22 (recommended, Sangster 1993)

2.54 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log \text{BCF}$  or  $\log K_{\text{B}}$ :

Sorption Partition Coefficient,  $\log K_{\text{OC}}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis: rate constant  $k = 1.7 \times 10^{-5} \text{ h}^{-1}$ ,  $1.32 \times 10^{-4} \text{ h}^{-1}$ , with  $\text{H}_2\text{O}_2$  under photolysis at  $25^\circ\text{C}$  in F-113 solution and with HO in the gas (Dilling et al. 1988).

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{\text{OH}}$  for reaction with OH radical,  $k_{\text{NO}_3}$  with  $\text{NO}_3$  radical and  $k_{\text{O}_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = 2.19 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{\text{OH}}(\text{obs}) = 2.19 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{\text{OH}}^* = (1.61 \pm 0.24) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{OH}}^* = 1.72 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

Half-Lives in the Environment:

**TABLE 6.1.3.11.1**

**Reported vapor pressures of hexafluorobenzene 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)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
<b>Patrick &amp; Prosser 1964</b>	<b>Counsell et al. 1965</b>	<b>Findlay 1969</b>	<b>Ambrose 1981</b>				
<b>static method-Hg manometer</b>	<b>gas saturation/manometer</b>	<b>Hg manometer</b>	<b>comparative ebulliometry</b>				
<b>t/^{\circ}C</b>	<b>P/Pa</b>	<b>t/^{\circ}C</b>	<b>P/Pa</b>	<b>t/^{\circ}C</b>	<b>P/Pa</b>	<b>T/K</b>	<b>P/Pa</b>
19.75	8714	37.303	19957	4.74	3849	290.029	7747
24.78	11196	43.536	26124	5.7	4065	293.503	8940
29.85	14289	49.109	32880	7.07	4426	297.155	10733
34.85	17966	53.82	39638	7.14	4429	300.564	12667
39.85	22461	57.848	46271	9.77	5118	304.801	15466
44.85	27687	61.585	53199	17.23	7646	309.383	19,045

TABLE 6.1.3.11.1 (Continued)

Patrick & Prosser 1964		Counsell et al. 1965		Findlay 1969		Ambrose 1981	
static method-Hg manometer		gas saturation/manometer		Hg manometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
49.85	33860	64.655	59496	17.23	7650	313.187	22511
54.87	41446	67.63	66152	19.68	8757	316.417	25904
59.92	50169	70.172	72295	24.28	10915	321.165	31474
64.95	59860	72.666	78764	24.4	10988	325.511	37460
69.95	71569	75.337	86190	25.1	11402	330.676	45736
74.95	84741	77.535	92707	27.08	12511	335.031	53811
80.05	100199	79.632	99284	29.92	14296	339.642	63567
84.98	117109	81.446	105264	29.92	14300	343.774	73469
		83.445	112211	29.92	14303	349.246	88.428
Antoine eq.		85.353	119111	35.92	18822	352.884	88642
eq. 2	P/mmHg	87.027	125463	41.81	24289	353.038	100.13
A	7.39075	88.79	132447	47.32	30456	353.849	102794
B	1432, 91			47.85	31064	358.125	117749
C	237.470	bp/°C	80.261			362.14	133296
		Antoine eq.		eq. 2	P/mmHg	366.773	153.186
bp/°C	80.3	eq. 2	P/mmHg	A	6.86088	371.657	176.601
$\Delta H_v$ /(kJ mol <sup>-1</sup> ) =		A	7.01741	B	1152.442	377.323	207.154
at 25°C	35.75	B	1219.410	C	208.663		
at bp	32.70	C	214.525			eq. 2	P/mmHg
		Kirchhoff eq.				A	
		eq. 4	P/mmHg			B	
		A	22.85552			C	
		B	2524.92				
		C	5.03484				

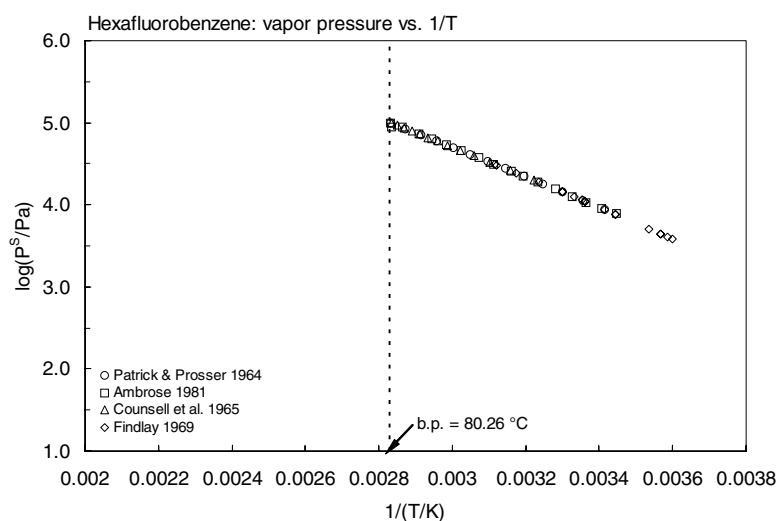
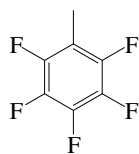


FIGURE 6.1.3.11.1 Logarithm of vapor pressure versus reciprocal temperature for hexafluorobenzene.

## 6.1.3.12 Pentafluorotoluene



Common Name: Pentafluorotoluene

Synonym: 2, 3, 4, 5, 6-pentafluorotoluene

Chemical Name: 2, 3, 4, 5, 6-pentafluorotoluene

CAS Registry No: 771-56-2

Molecular Formula:  $C_7H_3F_5$ ,  $C_6(CH_3)F_5$

Molecular Weight: 182.091

Melting Point ( $^{\circ}C$ ):

-29.78 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

117.5 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.440 (Lide 2003)

Molar Volume ( $cm^3/mol$ ):

126.5 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

143.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

35.19 (Ambrose 1968)

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

5056\* ( $39.164^{\circ}C$ , ebulliometry, measured range  $39$ – $138^{\circ}C$  or pressure range  $30$ – $1500$  mmHg, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.07209 - 1384.062/(212.731 + t/^{\circ}C)$ ; temp range  $\sim 76$ – $127^{\circ}C$  or pressure range  $200$ – $1000$  mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.09119 - 1388.288/(213.646 + t/^{\circ}C)$ ; temp range  $39$ – $138^{\circ}C$  or pressure range  $30$ – $1500$  mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 13.68523 - 2813.814/(T/K) - 1.2691 \times 10^{-2} \cdot (T/K) + 0.8888 \cdot 10^{-5} \cdot (T/K)^2$ ; temp range  $39$ – $138^{\circ}C$  (Cragoe eq., ebulliometry, Ambrose 1968)

$\log(P_L/\text{kPa}) = 6.19445 - 1382.934/(-60.494 + T/K)$ ; temp range  $312$ – $416$  K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.21241 - 1394.345/(-59.194 + T/K)$ ; temp range  $348$ – $401$  K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa  $m^3/mol$  at  $25^{\circ}C$ ):

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

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

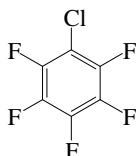
Half-Lives in the Environment:

TABLE 6.1.3.12.1

Reported vapor pressures of pentafluorotoluene 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)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot (T/K)^2$	(5)		
<b>Ambrose 1968</b>			
<b>ebulliometry</b>			
$t/^{\circ}\text{C}$	P/Pa		
39.164	5056	Antoine eq.	
50.578	8787	eq. 2	P/mmHg
58.357	12354	A	7.09119
62.734	14885	B	1396.198
66.375	17308	C	214.112
72.174	21831	for full range 30–1000 mmHg	
76.551	25854	or temp range 39–138°C	
81.824	31492		
85.651	36176	eq. 2	P/mmHg
92.625	46172	A	7.07209
97.287	54019	B	1384.062
102.370	63757	C	212.731
107.382	66700	for range 200–1000 mmHg	
112.608	87655	or temp range ~76–127°C	
116.158	97433		
117.884	102509	Cragoe eq.	
118.979	105812	eq. 5	P/mmHg
123.337	119831	A	13.68523
127.924	136155	B	2813.814
133.176	156948	C	$1.2691 \times 10^{-2}$
138.226	179191	D	$0.8888 \times 10^{-5}$
bp/ $^{\circ}\text{C}$	117.493		
$\Delta H_v = 35.18 \text{ kJ mol}^{-1}$			

## 6.1.3.13 Chloropentafluorobenzene



Common Name: Chloropentafluorobenzene

Synonym:

Chemical Name: chloropentafluorobenzene

CAS Registry No: 344-07-0

Molecular Formula:  $C_6ClF_5$

Molecular Weight: 202.509

Melting Point ( $^{\circ}C$ ):

Boiling Point ( $^{\circ}C$ ):

117.96 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

129.2 (calculated-density, Stephenson & Malanowski 1987)

141.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

35.15 (Ambrose 1968)

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

4186\* ( $35.576^{\circ}C$ , ebulliometry, measured range  $36$ – $144^{\circ}C$  or pressure range  $30$ – $1500$  mmHg, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.06976 - 1389.841/(213.833 + t/^{\circ}C)$ ; temp range  $\sim 80$ – $127^{\circ}C$  or pressure range  $100$ – $1000$  mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.06747 - 1388.288/(213.646 + t/^{\circ}C)$ ; temp range  $36$ – $144^{\circ}C$  or pressure range  $30$ – $1500$  mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 14.36999 - 2894.645/(T/K) - 1.4603 \times 10^{-2} \cdot (T/K) + 1.0612 \cdot 10^{-5} \cdot (T/K)^2$ ; temp range  $36$ – $144^{\circ}C$  (Cragoe eq., ebulliometry, Ambrose 1968)

$\log(P_L/\text{kPa}) = 6.19201 - 1388.701/(-59.393 + T/K)$ ; temp range  $348$ – $402$  K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.18873 - 1386.456/(-59.659 + T/K)$ , temp range  $307$ – $417$  K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa\ m^3/mol$  at  $25^{\circ}C$ ):

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

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 6.1.3.13.1**

**Reported vapor pressures of chloropentafluorotoluene 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)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot (T/K)^2$	(5)		

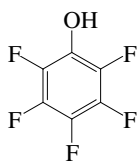
**Ambrose 1968**

**ebulliometry**

$t/^{\circ}C$	P/Pa		
35.576	4186	Antoine eq.	
44.790	6614	eq. 2	P/mmHg
55.927	11028	A	7.06747
61.852	14216	B	1388.288
65.865	16811	C	213.646
70.085	19929	full range 30–1000 mmHg	
75.343	24459	or temp range 35.6–144°C	
81.691	31024		
86.763	37244	eq. 2	P/mmHg
92.135	44900	A	7.06976
97.254	53331	B	1389.841
102.357	62963	C	213.833
107.155	73251	for range 200–1000 mmHg	
112.764	86927	or temp range ~80–128°C	
116.436	96926		
117.448	99832	Cragoe eq.	
118.893	104118	eq. 5	P/mmHg
125.580	118997	A	14.36999
127.992	134517	B	2894.645
133.467	155905	C	$1.4603 \times 10^{-2}$
138.689	178705	D	$1.0612 \times 10^{-5}$
144.131	205189		

bp/ $^{\circ}C$  117.954

$\Delta H_v = 35.15 \text{ kJ mol}^{-1}$

**6.1.3.14 Pentafluorophenol**

Common Name: Pentafluorophenol

Synonym:

Chemical Name: pentafluorophenol

CAS Registry No: 771-61-9

Molecular Formula:  $C_6(OH)F_5$

Molecular Weight: 184.063

Melting Point ( $^{\circ}C$ ):

37.5 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

145.6 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

128.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

41.59 (Ambrose 1968)

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.754 (mp at  $37.5^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

26578\* ( $105.448^{\circ}C$ , ebulliometry, measured range  $105.5$ – $155^{\circ}C$ , Ambrose 1968)

$\log(P/mmHg) = 7.06296 - 1377.185/(183.680 + t/^{\circ}C)$ ; temp range  $105$ – $155^{\circ}C$  (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P_s/kPa) = 11.291 - 3523/(T/K)$ ; temp range  $273$ – $296$  K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.18665 - 1377.011/(-89.435 + T/K)$ ; temp range  $378$ – $428$  K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa  $m^3/mol$  at  $25^{\circ}C$ ):

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

3.23 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

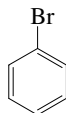
Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:



**TABLE 6.1.3.14.1****Reported vapor pressures of pentafluorophenol at various temperatures**

Ambrose 1968			
ebulliometry			
t/°C	P/Pa	t/°C	P/Pa
105.448	26578	153.041	125269
111.328	32076	154.963	132153
116.192	39393		
120.720	46087	bp/°C	145.621
124.827	52940	$\Delta H_v = 41.59 \text{ kJ mol}^{-1}$	
128.292	59367	Antoine eq.	
131.565	65904	$\log P = A - B/(C + t/^\circ\text{C})$	
134.647	72670	P/mmHg	
137.240	78804	A	7.03488
140.302	86489	B	1253.043
142.507	92412	C	215.897
145.002	99506	full range 200–1000 mmHg	
147.069	105684	or temp range 105–155°C	
149.090	112009		
151.190	118917		

**6.1.4 BROMOBENZENES AND BROMOTOLUENES****6.1.4.1 Bromobenzene**

Common Name: Bromobenzene

Synonym: phenyl bromide

Chemical Name: bromobenzene

CAS Registry No: 108-86-1

Molecular Formula:  $C_6H_5Br$ 

Molecular Weight: 157.008

Melting Point ( $^{\circ}C$ ):

-30.72 (Dean 1985; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

156.06 (Dreisbach &amp; Martin 1949; Dreisbach 1955; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):1.4950, 1.48824 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.4950 (Weast 1982-83; Lide 2003)

1.4952 (Dean 1985)

Molar Volume ( $cm^3/mol$ ):105.0 ( $20^{\circ}C$ , calculated-density, Chiou 1985)

119.3 (Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

10.63 (Dreisbach 1955)

10.70 (Riddick et al. 1986)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

446 ( $30^{\circ}C$ , shake flask-IR, Gross & Saylor 1931)

410 (shake flask-UV, Andrews &amp; Keefer 1950)

462 (shake flask-interferometry, Donahue &amp; Bartell 1952)

328 (Deno &amp; Berkheimer 1960)

458.5 ( $35^{\circ}C$ , shake flask-UV spectrophotometry, Hine et al. 1963)457\* (shake flask-spectrophotometry, measured range  $10-35^{\circ}C$ , Vesala 1973)

446 (shake flask-UV, Vesala 1974)

148\* (shake flask-GC, measured range  $5-45.5^{\circ}C$ , Nelson & Smit 1978)

360 (shake flask-UV, Yalkowsky et al. 1979)

274\* (summary of literature data, temp range  $25-40^{\circ}C$ , Horvath 1982)

411 (generator column-HPLC/UV, Wasik et al. 1983)

330 (headspace-GC, McNally &amp; Grob 1984)

445\* (recommended, temp range  $10-40^{\circ}C$ , IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(g/kg) = 1.8293 - 1.35675 \times 10^{-2} \cdot (T/K) + 2.99322 \times 10^{-5} \cdot (T/K)^2$ ; temp range 288-308 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

384\* ( $20^{\circ}C$ , limiting activity coeff. by equilibrium air stripping-GC, temp range  $10-50^{\circ}C$ , Hovorka & Dohnal 1997)

384\* (estimated- RP-HPLC- $k'$  correlation, measured range  $5-35^{\circ}C$ , Finizio & Di Guardo 2001)

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):

- 666.6\* (29.8°C, static method-pressure gauge, Kahlbaum 1898)  
 666.6\* (27.8°C, summary of literature data, Stull 1947)  
 $\log(P/\text{mmHg}) = 7.25422 - 1688.4/(230 + t/^\circ\text{C})$  (Antoine eq., Dreisbach & Martin 1949)  
 6287\* (71.86°C, ebulliometry, measured range 71.86–158.06°C, Dreisbach & Shrader 1949)  
 3066\* (56.07°C, temp range 56.07–154.24°C, Dreyer et al. 1954)  
 558 (calculated by formula, Dreisbach 1955)  
 $\log(P/\text{mmHg}) = 6.91444 - 1474.06/(209.4 + t/^\circ\text{C})$ ; temp range 60–190°C (Antoine eq. for liquid state, Dreisbach 1955)  
 997 (35°C, gas saturation-gravitational or UV, Hine et al. 1963)  
 697 (ebulliometry, extrapolated-Antoine eq., measured range 49–131°C, Hammaker & Kerlinger 1969)  
 $\log(P/\text{mmHg}) = 7.7807 - 2105.4/(T/\text{K})$ ; temp range 49–131°C (ebulliometry, Hammaker & Kerlinger 1969)  
 570 (extrapolated-Antoine eq., Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 10157.7/(T/\text{K})] + 8.07500$ ; temp range –26 to –15°C (Antoine eq., Weast 1972–73)  
 552 (extrapolated-Antoine eq., Boublik et al. 1973)  
 $\log(P/\text{mmHg}) = 5.86064 - 1438.817/(205.441 + t/^\circ\text{C})$ ; temp range 56.07–154°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 553, 555 (extrapolated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 5.99238 - 1443.265/(205.94 + t/^\circ\text{C})$ ; temp range 56.07–154°C (Antoine eq. from reported exptl. data of Dreyer et al. 1954/55, Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 5.98225 - 1433.858/(204.562 + t/^\circ\text{C})$ ; (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)  
 $\log(P/\text{mmHg}) = 6.86064 - 1438.817/(205.441 + t/^\circ\text{C})$ ; temp range 56–154°C (Antoine eq., Dean 1985, 1992)  
 557.6 (Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 6.37912 - 1688.4/(230 + t/^\circ\text{C})$ , temp range not specified (Antoine eq., Riddick et al. 1986)  
 $\log(P_L/\text{kPa}) = 6.03934 - 1474.03/(-63.75 + T/\text{K})$ ; temp range 333–463 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.40524 - 1776.58/(-25.639 + T/\text{K})$ ; temp range 429–633 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log(P/\text{mmHg}) = -9.4583 - 2.5177 \times 10^3/(T/\text{K}) + 9.2584 \cdot \log(T/\text{K}) - 1.9386 \times 10^{-2} \cdot (T/\text{K}) + 9.6324 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 242–670 K (vapor pressure eq., Yaw et al. 1994)  
 $\log(P/\text{kPa}) = 5.99238 - 1443.265/(T/\text{K})$  (database of CDATA 1991, Hovorka & Dohnal 1997)

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

- 211 (1/K<sub>AW</sub> or C<sub>w</sub>/C<sub>A</sub>, Hine & Mookerjee 1975;)  
 247 (gas stripping-GC, Mackay & Shiu 1981, 1990)  
 210 (recommended, Mackay & Shiu 1981)  
 211 (computer value, Yaws et al. 1991)  
 256, 332, 579 (30.0, 35, 44.8°C, EPICS-GC, Hansen et al. 1993)  
 $\ln[H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -5341/(T/\text{K}) + 16.0$ ; temp range 30–45°C (EPICS measurements, Hansen et al. 1993)  
 92.0, 167, 280, 430, 610 (10, 20, 30, 40, 50°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 139 (20°C, selected from literature of experimentally measured data, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 6.375 - 2233/(T/\text{K})$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K<sub>OW</sub> (at 25°C or as indicated):

- 2.99 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)  
 3.03 (calculated-fragment const.; Rekker 1977)  
 3.16 (HPLC-k' correlation, McDuffie 1981)  
 2.98 (generator column-HPLC, Wasik et al. 1983)  
 3.02 (HPLC-RT correlation, D'Amboise & Hanai 1982)  
 3.01 (shake flask-GC, Watarai et al. 1982)  
 3.02 (HPLC-RT correlation, Eadsforth & Moser 1983)

- 3.01 (HPLC-RT correlation, Garst & Wilson 1984)
- 3.15 (HPLC correlation, Eadsforth 1986)
- 2.99 (recommended, Sangster 1989, 1993)
- 2.75, 2.94 (shake flask-UV/VIS spec. 25, 60°C; Kramer & Henze 1990)
- 2.99 (recommended, Hansch et al. 1995)
- 3.29, 3.25, 3.14, 3.12 (5, 15, 25, 35°C, estimated- RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

Bioconcentration Factor, log BCF:

- 3.18 (activated sludge, Freitag et al. 1984)
- 2.28 (algae, Freitag et al. 1984)
- 1.68 (fish, Freitag et al. 1984)
- 1.68, 2.28, 3.18 (fish, algae, activated sludge, Halfon & Reggiani 1986)
- 1.70 (Freitag et al. 1985)
- 1.899, 1.928 (calculated- $K_{OW}$ , calculated- MCI  $\chi$ , Lu et al. 1999)

Sorption Partition Coefficient, log  $K_{OC}$ :

- 2.18 (soil, selected lit., Kenaga & Goring 1980)
- 2.18 (calculated-S. Kenaga 1980)
- 2.80 (calculated-MCI  $\chi$ , Koch 1983)
- 2.56 (calculated-MCI. Sabjic 1984)
- 2.65 (calculated-MCI, Bahnick & Doucette 1988)
- 2.65 (HPLC-RT correlation, cyanopropy column, Hodson & Williams 1988)
- 3.37 (activated carbon, Blum et al. 1994)
- 2.49 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

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

$k_{OH}^* = 7.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp., measured range 245–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{OH}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs}) = 0.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (9.15 \pm 0.97) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 234–438 K ((flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{OH} = 7.70 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , independent of temperature over the range 234–362 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 0.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: relative rate from activated sludge approximately of 34.8%  $CO_2$  (Freitag et al. 1984).

Biotransformation:

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

Half-Lives in the Environment:

TABLE 6.1.4.1.1  
Reported aqueous solubilities of bromobenzene at various temperatures

$S(\text{wt}\%) = 1.09002 \times 10^{-2} + 4.43314 \times 10^{-4} \cdot (t/^{\circ}\text{C}) + 1.20007 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 - 1.33342 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3$  (1)

$S(\text{g/kg}) = 1.8293 - 1.35675 \times 10^{-2} \cdot (T/\text{K}) + 2.99322 \times 10^{-5} \cdot (T/\text{K})^2$  (2)

1.

Vesala 1973		Nelson & Smit 1978		Horvath 1982		Horvath & Getzen 1985	
shake flask-UV		shake flask-GC		summary of literature data		IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
10	389.57	5	1168	25	274	10	387
15.2	406.05	25	148	30	314	15	405
19.6	411.07	39	244	40	393	20	424
25.0	457.19	45.5	314			25	445
30.0	464.56			eq. 1	S/wt%	30	467
35.0	489.19					35	491
						40	516
						eq. 2	S/(g/kg)

2.

Hovorka & Dohnal 1997		Finizio & Di Guardo 2001	
γ <sup>∞</sup> by air stripping-GC		RP-HPLC-k' correlation	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
10	354.6	5	278
20	384.3	15	274.5
30	427.6	25	384
40	499.0	35	368
50	598.7		

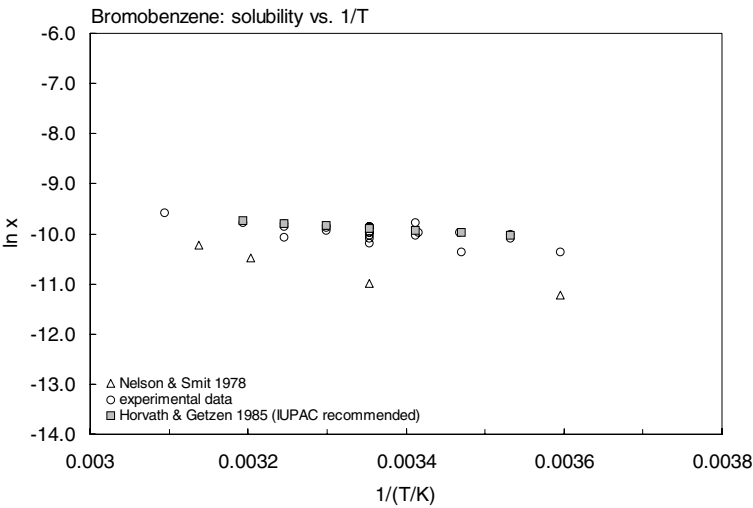


FIGURE 6.1.4.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for bromobenzene.

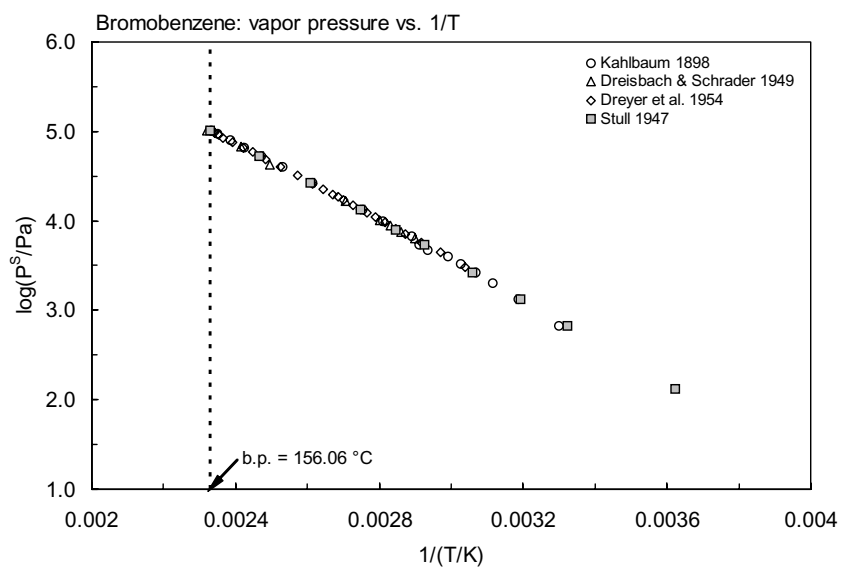
TABLE 6.1.4.1.2

Reported vapor pressures of bromobenzene at various temperatures and the coefficients for the vapor pressure equations

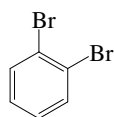
$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Dreyer et al. 1954	
static method*		summary of lit. data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
29.8	666.6	2.9	133.3	71.86	6287	56.07	3066
40.6	1333.2	27.8	666.6	76.39	7605	63.52	4400
47.7	1999.8	40	1333	80.08	8851	69.7	5706
52.8	2666.4	53.8	2666	83.99	10114	74.88	7119
57.3	3333	68.6	5333	96.32	16500	78.25	8213
61.2	3999.7	78.1	7999	127.47	42066	81.9	9546
67.7	4666	90.8	13332	140.69	67661	85.55	10986
70.4	5333	110.1	26664	158.06	101325	88.53	12332
73.0	6666.1	132.3	53329			90.82	13426
82.8	9999.2	156.2	101325	bp/°C	156.06	93.49	14839
90.0	13332			mp/°C	−30.82	97.09	16932
109.5	26664	mp/°C	−30.7			99.41	18465
122.0	39997			eq. 2	P/mmHg	101.26	19705
131.6	53329			A	7.25422	105	22425
139.4	66661			B	1688.4	109.5	26118
145.9	79993			C	230	115.59	31877
152.5	93326					122.79	39970
155.5	101325					129.61	49156
						135.48	58275
						139.94	66128
						144.73	75527
						149.51	85433
						151.95	91046
						154.24	96685
						bp/°C	156.083

\*complete list see [ref.](#)

\*complete list see [ref.](#)



## 6.1.4.2 1,2-Dibromobenzene



Common Name: 1,2-Dibromobenzene

Synonym: *o*-dibromobenzene

Chemical Name: 1,2-Dibromobenzene

CAS Registry No: 583-53-9

Molecular Formula:  $C_6H_4Br_2$

Molecular Weight: 235.904

Melting Point ( $^{\circ}C$ ):

7.1 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

225 (Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.98429, 1.9767 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.9843 ( $20^{\circ}C$ , Weast 1982–83; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

120.2 (calculated-density, Stephenson & Malanowski 1987)

142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

59.31, 42.594 ( $25^{\circ}C$ , bp, Dreisbach 1961)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

7.279 (Dreisbach 1955)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

74.55 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

74.8 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

$\log(P/mmHg) = 7.44451 - 2050.3/(230 + t/^{\circ}C)$  (Antoine eq., Dreisbach & Martin 1949)

25.7 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.10265 - 1825.77/(207.0 + t/^{\circ}C)$ ; temp range  $115$ – $295^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

26.0 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.50128 - 2093.1/(t/^{\circ}C + 230)$ ; temp range  $28$ – $117^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.10265 - 1825.77/(t/^{\circ}C + 207)$ ; temp range  $117$ – $300^{\circ}C$  (Antoine eq., Dean 1985, 1992)

22.80 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.22755 - 1825.77/(T/K - 66.15)$ ; temp range  $388$ – $588\ K$  (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

3.64 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)

3.68 (HPLC-RT correlation, Garst & Wilson 1984)

3.64 (recommended, Sangster 1993)

3.64 (recommended, Hansch et al. 1995)



Bioconcentration Factor, log BCF:

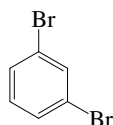
2.70; 3.50 (*Pimephales promelas*; *Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log  $K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 6.1.4.3 1,3-Dibromobenzene



Common Name: 1,3-Dibromobenzene

Synonym: *m*-dibromobenzene

Chemical Name: 1,3-Dibromobenzene

CAS Registry No: 108-36-1

Molecular Formula:  $C_6H_4Br_2$

Molecular Weight: 235.904

Melting Point ( $^{\circ}C$ ):

−7.0 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

218 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.9523 ( $20^{\circ}C$ , Weast 1982–83; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

120.8 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

67.4 ( $30^{\circ}C$ , shake flask-UV, Hine et al. 1963)

98.45 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

64.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

57.06 ( $35^{\circ}C$ , gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)

22.78 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 5.971 - 1603.4/(T/K - 87.55)$ ; temp range 417–500 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

157, 61.05 (calculated- $\Delta S_v$ , mp and bp, Antoine eq., Yalkowsky & Mishra 1990, Mishra & Yalkowsky 1991)

$\log(P/mmHg) = 59.2974 - 4.6960 \times 10^3/(T/K) - 18.444 \cdot \log(T/K) + 6.7598 \times 10^{-3} \cdot (T/K) - 2.5567 \times 10^{-13} \cdot (T/K)^2$ ; temp range 226–761 K (vapor pressure eq., Yaw et al. 1994)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

3.75 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)

3.79 (shake flask-GC, Watarai et al. 1982)

3.78 (Oliver & Niimi 1984)

3.74 (HPLC- $k'$  correlation, Haky & Yeung 1984)

3.75 (recommended, Sangster 1993)

3.75 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

2.78 (mean value, rainbow trout, Oliver & Niimi 1984)

2.82 (rainbow trout, Oliver 1987)

2.82 (*Oncorhynchus mykiss*, under flow-through conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis: pseudo-first order reaction rate constant for direct photolysis  $k = 0.009 \text{ min}^{-1}$  with  $t_{1/2} = 76.8 \text{ min.}$  in dilute aqueous solution (Peijnenburg et al. 1992).

Half-Lives in the Environment:

Air:

Surface water: pseudo-first order reaction rate constant for direct photolysis  $k = 0.009 \text{ min}^{-1}$  with  $t_{1/2} = 76.8 \text{ min.}$  in dilute aqueous solution (Peijnenburg et al. 1992).

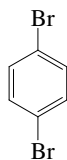
Groundwater:

Sediment:

Soil:

Biota:  $t_{1/2} = 3 \text{ d}$  (guppy, Niimi 1987)

## 6.1.4.4 1,4-Dibromobenzene



Common Name: 1,4-Dibromobenzene

Synonym: *p*-dibromobenzene

Chemical Name: 1,4-Dibromobenzene

CAS Registry No: 106-37-6

Molecular Formula: C<sub>6</sub>H<sub>4</sub>Br<sub>2</sub>

Molecular Weight: 235.904

Melting Point (°C):

87.43 (Lide 2003)

Boiling Point (°C):

218.5 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.5742 (20°C, Weast 1982–83)

Molar Volume (cm<sup>3</sup>/mol):

121 (calculated-density, Lande & Banerjee 1981)

142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

4.837 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.244 (mp at 87.43°C)

Water Solubility (g/m<sup>3</sup> 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.):

20.0 (shake flask-UV, Andrews & Keefer 1950)

26.42 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)

20.08 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

20.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

17.0\* (shake flask-HPLC, measured range 10–35°C, Kuramochi et al. 2004)

ln [S/(mol/L)] = −3151.3.7/(T/K) + 1.06; temp range 10–35°C (shake flask-HPLC, Kuramochi 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):

133.3\* (61°C, summary of literature data, Stull 1947)

log (P/mmHg) = 7.44830 − 2057.2/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

9.33\* (25.8°C, manometer, temp range 25.8–80.5°C, Walsh & Smith 1961)

log (P/mmHg) = 11.592 − 3826.2/(T/K); temp range 25.8–80.5°C (manometer, Walsh & Smith 1961)

17.87 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)

log (P/mmHg) = [−0.2185 × 13047.8/(T/K)] + 8.769771; temp range 61–218.6°C (Antoine eq., Weast 1972–73)

3.96\* (18.13°C, capacitance manometer; De Kruif et al. 1981)

7.65 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

log P/kPa = 10.717 − 3826.2/(T/K); temp range 298–354 K (Antoine eq., solid, Stephenson & Malanowski 1987)

log P/kPa = 6.5732 − 2047.2/(T/K − 43.15); temp range 373–493 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

35.95, 53.18 (calculated-bp, Antoine eq., Yalkowsky & Mishra 1990)

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25°C):

106 (derived from γ<sub>w</sub>, infinite dilution activity coefficient, Kuramochi et al. 2004)

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

3.75	(shake flask, Hansch & Leo 1979)
4.07	(calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)
4.13	(calculated-fragment const., Yalkowsky et al. 1983)
3.79	(shake flask-GC, Watarai et al. 1982)
3.89	(Gobas et al. 1989)
3.79	(recommended, Sangster 1993)
3.79	(recommended, Hansch et al. 1995)
3.62	(GC-RT correlation, Kuramochi et al. 2004)

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

5.21	(calculated- $S_{oct}$ and vapor pressure, Abraham et al. 2001)
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Bioconcentration Factor, log BCF:

3.15	(guppy, lipid-weight based, Gobas et al. 1989)
1.96	( <i>Poecilia reticulata</i> , under flow-through conditions, Devillers et al. 1996)
2.70; 3.40	( <i>Poecilia reticulata</i> ; <i>Pimephales promelas</i> , under static and semi-static conditions, Devillers et al. 1996)
3.15	(Gobas et al. 1989)

Sorption Partition Coefficient, log  $K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Bioconcentration, Uptake ( $k_1$ ) and Elimination ( $k_2$ ) Rate Constants:  
 log  $k_1 = 2.11 \text{ d}^{-1}$ ; log  $k_2 = 0.15 \text{ d}^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

**TABLE 6.1.4.4.1**

**Reported aqueous solubilities and vapor pressures of 1,4-dibromobenzene 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/mmHg) = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log (P/Pa) = A – B/(C + T/K)		(3)					
log (P/mmHg) = A – B/(T/K) – C·log (T/K)		(4)					
Aqueous solubility		Vapor pressure					
Kuramochi et al.2004		Stull 1947		Walsh & Smith 1961		de Kruif et al. 1981	
shake flask-GC		summary of literature data		manometry		diaphragm gauge	
t/°C	S/(g m <sup>-3</sup> )	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	9.91	61.0	133.3	25.8	9.33	1.54	0.617
25	17.0	79.3	666.6	26.8	9.33	3.93	0.829
35	24.6	87.7	1333	27.5	10.67	3.95	0.832
		103.6	2666	31.9	14.67	7.62	1.253
mp/°C	84.55	120.8	5333	38.1	26.66	10.54	1.736
		131.6	7999	42.6	38.66	14.02	2.544
ΔH <sub>sol</sub> /(kJ mol <sup>-1</sup> ) = 26.2		146.5	13332	42.6	40.0	18.13	3.960
ΔH <sub>fusl</sub> /(kJ mol <sup>-1</sup> ) = 18.6		168.5	26664	44.6	48.0		
		192.5	53329	50.2	73.33		
		218.6	101325	51.2	83.99	eq. 1	P/Pa

(Continued)

TABLE 6.1.4.4.1 (Continued)

Aqueous solubility		Vapor pressure					
Kuramochi et al.2004		Stull 1947		Walsh & Smith 1961		de Kruif et al. 1981	
shake flask-GC		summary of literature data		manometry		diaphragm gauge	
t/°C	S/(g m <sup>-3</sup> )	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
$\ln S = -3151.3/(T/K) + 1.06$				56.4	129.3	A	13.86395
S in mol/L		mp/°C	87.5	57.2	136.0	B	3864.8
				57.3	141.3		
				64.3	238.7		
				71.8	420.0		
				80.5	791.9		
				mp/°C	87.24		
				eq. 1	P/mmHg		
				A	11.592		
				B	3826.2		
				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 73.26$			

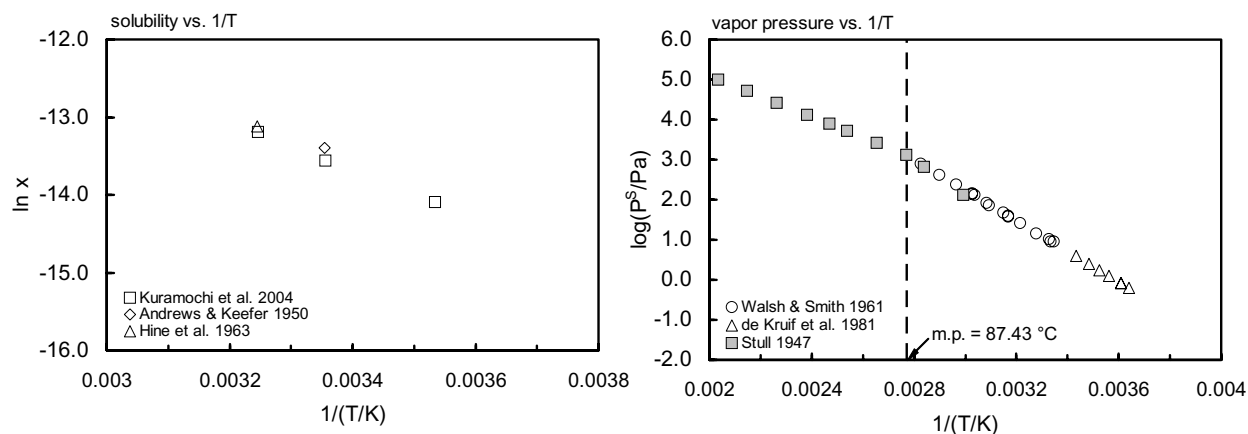
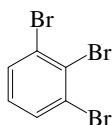


FIGURE 6.1.4.4.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,4-dibromobenzene.

**6.1.4.5 1,2,3-Tribromobenzene**

Common Name: 1,2,3-Tribromobenzene

Synonym:

Chemical Name: 1,2,3-tribromobenzene

CAS Registry No: 608-21-9

Molecular Formula:  $C_6H_3Br_3$

Molecular Weight: 314.800

Melting Point ( $^{\circ}C$ ):

87.8 (Weast 1982–83)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

2.658 (Weast 1982–83, Horvath 1982)

Molar Volume ( $cm^3/mol$ ):

137.7 (Ruelle & Kesselring 1997)

118 (calculated-density, Wang et al. 1992)

165.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.242 (mp at  $87.8^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

2.94 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

4.98; 4.25 (quoted exptl value; calculated-molar volume, Wang et al. 1992)

4.57; 4.42 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

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

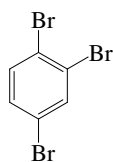
Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

Biota:  $t_{1/2} = 3\ d$  in guppy (for tribromobenzenes, Niimi 1986).

**6.1.4.6 1,2,4-Tribromobenzene**

Common Name: 1,2,4-Tribromobenzene

Synonym:

Chemical Name: 1,2,4-tribromobenzene

CAS Registry No: 615-54-3

Molecular Formula:  $C_6H_3Br_3$

Molecular Weight: 314.800

Melting Point ( $^{\circ}C$ ):

44.5 (Weast 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

275 (Weast 1982–83; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

137.7 (Ruelle & Kesselring 1997)

165.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.644 (mp at  $44.5^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

9.96 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

10.1 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)

3.67, 7.21, 11.0 (10, 25,  $35^{\circ}C$ , generator column-HPLC, Kuramochi et al. 2004)

$\ln [S/(mol/L)] = -3836.9/(T/K) + 2.19$ ; temp range  $10$ – $35^{\circ}C$  (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

31.9 (derived from  $\gamma_w$ , infinite dilution activity coefficient, Kuramochi et al. 2004)

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

4.51 (shake flask-GC, Watarai et al. 1982)

4.54 (Oliver & Niimi 1984)

4.32 (GC-RT correlation, Kuramochi et al. 2004)

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

Bioconcentration Factor,  $\log BCF$ :

3.63 (rainbow trout, Oliver 1984, Oliver & Niimi 1984, Oliver 1987)

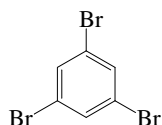
Sorption Partition Coefficient,  $\log K_{oc}$ :

Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

Biota:  $t_{1/2} = 3$  d in guppy (for tribromobenzenes, Niimi 1987)



**6.1.4.7 1,3,5-Tribromobenzene**

Common Name: 1,3,5-Tribromobenzene

Synonym:

Chemical Name: 1,3,5-tribromobenzene

CAS Registry No: 626-39-1

Molecular Formula:  $C_6H_3Br_3$

Molecular Weight: 314.800

Melting Point ( $^{\circ}C$ ):

122.8 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

271 (Weast 1982–83; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

137.7 (Ruelle & Kesselring 1997)

165.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.11 (mp at  $122.8^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

200 (shake flask-residue volume method, Booth & Everson 1948)

0.04 (Stephen & Stephen 1963)

0.787 (shake flask-UV, Yalkowsky et al. 1979)

0.789 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

5.187 (GC-RT correlation, Watanabe & Tatsukawa 1989)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

4.51 (shake flask-GC, Watarai et al. 1982)

5.07 (calculated-fragment const., Yalkowsky et al. 1983)

4.60, 4.63 (HPLC-RT correlation, Garst 1984)

5.26 (HPLC-RT correlation, Gobas et al. 1989)

5.18 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

4.51 (recommended, Sangster 1993)

4.51 (selected, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

3.70 (rainbow trout, Oliver & Niimi 1984, Oliver 1987)

3.26–4.08 mean 3.97; 3.53–4.20 mean 4.08 (rainbow trout, wet wt. basis,  $15^{\circ}C$ , steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

4.42 (guppy, lipid-weight based, Gobas et al. 1989)

3.23; 3.70, 3.97, 4.08 (*Poecilia reticulata*; *Oncorhynchus mykiss*, quoted values, Devillers et al. 1996)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis: pseudo-first order reaction rate constant in dilute aqueous solution  $k = 0.005 \text{ min}^{-1}$  with  $t_{1/2} = 140.5 \text{ min}$ . (Peijeneburg et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

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

$\log k_1 = 2.85 \text{ d}^{-1}$ ;  $\log k_2 = -0.38 \text{ d}^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Air:

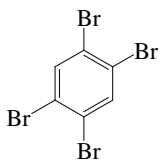
Surface water: pseudo-first order reaction rate constant for direct photolysis in dilute aqueous solution  $k = 0.005 \text{ min}^{-1}$  with  $t_{1/2} = 140.5 \text{ min}$ . (Peijeneburg et al. 1992).

Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} = 3 \text{ d}$  (guppy, for tribromobenzenes, Niimi 1987)

**6.1.4.8 1,2,4,5-Tetrabromobenzene**

Common Name: 1,2,4,5-Tetrabromobenzene

Synonym:

Chemical Name: 1,2,4,5-tetrabromobenzene

CAS Registry No: 636-28-2

Molecular Formula:  $C_6H_2Br_4$

Molecular Weight: 393.696

Melting Point ( $^{\circ}C$ ):

182 (Weast 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

3.072 (Weast 1982–83)

Molar Volume ( $cm^3/mol$ ):

128.2 (calculated-density, Wang et al. 1992)

153.8 (Ruelle & Kesselring 1997)

189.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0288 (mp at  $182^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

0.0433 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

0.0434 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)

0.044 (shake flask-GC, Kim & Saleh 1990)

0.0182, 0.0435, 0.0778 (10, 25,  $35^{\circ}C$ , generator column-HPLC, Kuramochi et al. 2004)

$\ln [S/(mol/L)] = -4967.5/(T/K) + 0.681$ ; temp range  $10$ – $35^{\circ}C$  (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

0.157 (GC-RT correlation, Watanabe & Tatsukawa 1989)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

376 (derived from  $\gamma_w$ , infinite dilution activity coefficient, Kuramochi et al. 2004)

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

5.13 (shake flask-GC, Watarai et al. 1982)

5.25 (HPLC-RT correlation, Garst 1984)

5.56 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.13 (recommended, Sangster 1993)

5.13 (recommended, Hansch et al. 1995)

5.00 (GC-RT correlation, Kuramochi et al. 2004)

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

Bioconcentration Factor,  $\log BCF$ :

3.80 (rainbow trout, Banerjee et al. 1980)

2.94–3.68 mean 3.57; 3.40–3.91 mean 3.81 (rainbow trout, wet wt. basis,  $15^{\circ}C$ , steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

3.80 (Nendza 1993; quoted, Lu et al. 1999)

3.57 (*Oncorhynchus mykiss*, flow through conditions, Devillers et al. 1996)

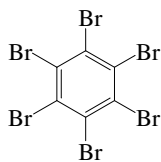
Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

Biota:  $t_{1/2} = 4$  d in guppy (for tetrabromobenzenes, Niimi 1987)

## 6.1.4.9 Hexabromobenzene



Common Name: Hexabromobenzene

Synonym:

Chemical Name: hexabromobenzene

CAS Registry No: 87-82-1

Molecular Formula:  $C_6Br_6$

Molecular Weight: 551.488

Melting Point ( $^{\circ}C$ ):

327 (Weast 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

186 (Ruelle & Kesselring 1997)

235.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

85 (Tittlemier et al. 2002)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0011 (mp at  $327^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and the reported temperature dependence equations):

0.00016 ( $22^{\circ}C$ , generator column-GC, Opperhuizen 1986)

0.0030 (generator column-GC/ECD, Tittlemier et al. 2002)

0.0000472, 0.00011, 0.000232 (10, 25,  $35^{\circ}C$ , generator column-HPLC, Kuramochi et al. 2004)

$\ln [S/(mol/L)] = -5484.7/(T/K) - 3.85$ ; temp range  $10$ – $35^{\circ}C$  (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at  $25^{\circ}C$  and the reported temperature dependence equations):

$3.133 \times 10^{-4}$  (estimated, Lyman et al. 1982)

$3.845 \times 10^{-4}$  (GC-RT correlation, Watanabe & Tatsukawa 1989)

$7.50 \times 10^{-4}$  (supercooled liquid  $P_L$ , GC-RT correlation, Tittlemier et al. 2002)

$\log (P_L/Pa) = -4454/(T/K) + 11.82$  (Claiius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

0.284 (calculated, Meylan & Howard 1991)

0.14 (calculated- $P_L/C_L$ , Tittlemier et al. 2002)

10.8 (derived from  $\gamma_w$ , infinite dilution activity coefficient, Kuramochi et al. 2004)

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

6.15, 6.07 (HPLC-RT correlation, Garst 1984)

7.80 (HPLC-RT correlation, Opperhuizen 1986)

> 6.0 (estimated, Gobas et al. 1987)

7.06 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.07 (recommended, Sangster 1993)

6.07 (Hansch et al. 1995)

6.07 (GC-RT correlation, Kuramochi et al. 2004)

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

Bioconcentration Factor,  $\log BCF$ :

2.95–3.08 mean 3.04 (rainbow trout, wet wt., 15°C, steady-state BCF on 21- to 96-d laboratory study, Oliver & Niimi 1985)

1.0 (Kawasaki 1980)

5.0 (Nendza 1993)

4.892, 4.681 (calculated-MCI, calculated- $K_{OW}$ , Lu et al. 1999)

Sorption Partition Coefficient,  $\log K_{OC}$ :

4.45, 4.68 (estimated-solubility, Lyman et al. 1982; quoted,  $K_{OW}$ , Howard 1997)

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Volatilization: estimated volatilization  $t_{1/2} = 3.3$  d from a model river is 3.3 d,  $t_{1/2} = 114$  months from a model pond with adsorptive processes (Howard 1997)

Photolysis: not expected to occur (Howard 1997)

Oxidation: not expected to occur (Howard 1997)

Hydrolysis: not expected to occur (Howard 1997)

Half-Lives in the Environment:

Air:

Surface water: estimated volatilization  $t_{1/2} = 3.3$  d from a model river,  $t_{1/2} = 114$  months from a model pond with adsorptive processes (Howard 1997)

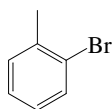
Groundwater:

Sediment:

Soil:

Biota:

## 6.1.4.10 2-Bromotoluene



Common Name: 2-Bromotoluene

Synonym: *o*-bromotoluene, 1-bromo-2-methylbenzene

Chemical Name: 2-bromotoluene

CAS Registry No: 95-46-5

Molecular Formula:  $C_7H_7Br$

Molecular Weight: 171.035

Melting Point ( $^{\circ}C$ ):

– 27.8 (Weast 1982–82; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

181.7 (Dreisbach 1959; Weast 1982–83; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.42322, 1.41774 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959)

1.4232 (Weast 1982–83; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

120.2 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

49.264, 38.995 ( $25^{\circ}C$ , bp, Dreisbach 1955)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

2.423 (Dreisbach 1955)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

51.3 (estimated, Howard 1997)

1007; 105 (quoted, calculated-molar volume and mp, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

186 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/mmHg = 7.50879 - 1913.46/(T/K - 38.34)$ ; temp range  $4-75^{\circ}C$  (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

133.3\* (24.4, summary of lit. data, Stull 1947)

181 (calculated by formula., Dreisbach 1955)

$\log (P/mmHg) = 6.90847 - 1549.39/(C + t/^{\circ}C)$ ; temp range  $80-245^{\circ}C$ , (Antoine eq. for liquid state, Dreisbach 1955)

$\log (P/mmHg) = [-0.2185 \times 11365.0/(T/K)] + 8.396578$ ; temp range  $24.4-181.8^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log (P_L/kPa) = 6.03337 - 1549.39/(T/K - 70.15)$ ; temp range  $353-518\ K$  (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

242 (estimated-group contribution method, Meylan & Howard 1991)

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

2.92 (Hansch & Leo 1979, Hansch et al. 1995)

3.61 (HPLC- $k'$  correlation, Hanai et al. 1981)

3.43 (estimated, Howard 1997)

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

Bioconcentration Factor, log BCF or log  $K_B$ :

2.38 (estimated- $K_{OW}$ , Howard 1997)

Sorption Partition Coefficient, log  $K_{OC}$ :

2.96 (estimated, Howard 1997)

Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Volatilization:  $t_{1/2} = 1.7$  h from a model river 1-m deep and  $t_{1/2} = 14.9$  d from a pond (Howard 1997).

Photolysis:

Oxidation: atmospheric  $t_{1/2} \sim 6.2$  d for reaction with hydroxyl radicals in air (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric  $t_{1/2} \sim 6.2$  d for reaction with OH radicals in air (Howard 1997).

Surface water: volatilization  $t_{1/2} = 1.7$  h from a model river 1-m deep flowing 1 m/s with a wind speed of 5 m/s and  $t_{1/2} = 14.9$  d from a model pond with adsorption from water column (Howard 1997).

**TABLE 6.1.4.10.1**  
**Reported vapor pressures of 2-bromotoluene at various temperatures**

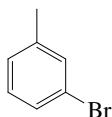
Stull 1947

summary of literature data

$t/^{\circ}\text{C}$	$P/\text{Pa}$
24.4	133.3
49.7	666.6
62.3	1333
76.0	2666
91.0	5333
100.0	7999
112.0	13332
133.6	26664
157.3	53329
181.8	101325
mp/ $^{\circ}\text{C}$	-28



## 6.1.4.11 3-Bromotoluene



Common Name: 3-Bromotoluene

Synonym: *m*-bromotoluene

Chemical Name: 3-bromotoluene

CAS Registry No: 591-17-3

Molecular Formula:  $C_7H_7Br$

Molecular Weight: 171.035

Melting Point ( $^{\circ}C$ ):

−39.8 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

183.7 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.4099 (Lide 2003)

Molar Volume ( $cm^3/mol$ ):

121.3 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

51.3 (estimated, Howard 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

133.3\* ( $14.8^{\circ}C$ , summary of lit. data, Stull 1947)

$\log P/mmHg = 7.75409 - 2049.14/(T/K - 31.44)$ ; temp range  $4-75^{\circ}C$  (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

$\log (P/mmHg) = [-0.2185 \times 10537.1/(T/K)] + 7.886560$ ; temp range  $14.8-183.7^{\circ}C$  (Antoine eq., Weast 1972-73)

145 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.86228 - 2085.49/(T/K - 27.333)$ ; temp range: 287-457 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

445 (estimated-P/C, Howard 1997)

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

3.43 (estimated, Howard 1997)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

2.38 (estimated- $K_{ow}$ , Howard 1997)

Sorption Partition Coefficient,  $\log K_{OC}$ :

2.96 (estimated, Howard 1997)

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Volatilization:  $t_{1/2} = 1.5$  h and 14.9 d from a model river 1-m deep and  $t_{1/2} = 14.9$  d from a pond (Howard 1997).

Photolysis:

Oxidation: atmospheric  $t_{1/2} \sim 3$  d for reaction with hydroxyl radical in air (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

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

## Half-Lives in the Environment:

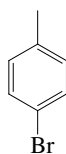
Air: atmospheric  $t_{1/2} \sim 3$  d half-life for reaction with hydroxyl radical in air (Howard 1997).

Surface water: volatilization  $t_{1/2} = 1.5$  h from a model river 1 m deep flowing 1 m/s with a wind speed of 5 m/s) and  $t_{1/2} = 14.9$  d in a model pond with adsorption, from water column (Howard 1997).

**TABLE 6.1.4.11.1****Reported vapor pressures of 3-bromotoluene at various temperatures****Stull 1947****summary of literature data**

<b>t/°C</b>	<b>P/Pa</b>
14.8	133.3
50.8	666.6
64.0	1333
78.1	2666
93.9	5333
104.1	7999
117.8	13332
138.0	26664
160.0	53329
183.7	101325
mp/°C	-39.8

## 6.1.4.12 4-Bromotoluene



Common Name: 4-Bromotoluene

Synonym: *p*-bromotoluene, 4-bromo-1-methylbenzene

Chemical Name: *p*-bromotoluene

CAS Registry No: 106-38-7

Molecular Formula: C<sub>7</sub>H<sub>7</sub>Br

Molecular Weight: 171.042

Melting Point (°C):

28.5 (Lide 2003)

Boiling Point (°C):

184.3 (Lide 2003)

Density (g/cm<sup>3</sup> at 25°C):

1.39953 (Dreisbach 1955)

Molar Volume (cm<sup>3</sup>/mol):

122.5 (Ruelle & Kesselring 1997)

141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

49.74, 39.98 (25°C, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

14.82 (Dreisbach 1955)

3.5684 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

110 (Hine & Mookerjee 1975)

110; 81.9 (quoted; calculated-molar volume and mp, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

133.3\* (10.3°C, summary of lit. data, Stull 1947)

153.2 (calculated by formula., Dreisbach 1955)

log (P/mmHg) = 7.00762 – 1612.35/(206.36 + t/°C); temp range 85–250°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/mmHg) = 7.00762 – 1612.35/(t/°C + 206.36); temp range 85–280°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.13252 – 1612.35/(T/K – 66.79); temp range 358–523 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 12.8209 – 2.6568 × 10<sup>3</sup>/(T/K) – 1.4314·log (T/K) – 8.9677 × 10<sup>-4</sup>·(T/K) + 3.9733 × 10<sup>-7</sup>·(T/K)<sup>2</sup>, temp range 300–699 K (Yaws 1994)

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25°C):

23.82 (calculated-P/C, Howard 1997)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

3.42 (quoted, Howard 1997)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

2.54 (calculated- $K_{OW}$ , Howard 1997)

Sorption Partition Coefficient,  $\log K_{OC}$ :

3.10–3.27 (estimated, Howard 1997)

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation:  $t_{1/2} \sim 9.4$  d for reaction with OH radical in the atmosphere (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric  $t_{1/2} \sim 9.4$  d for reaction with OH radical (Howard 1997).

Surface water: volatilization  $t_{1/2} = 4.3$  h from a model river 1 m deep and  $t_{1/2} = 14.9$  d from an environmental pond (Howard 1997).

**TABLE 6.1.4.12.1**

**Reported vapor pressures of 4-bromotoluene at various temperatures**

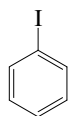
**Stull 1947**

**summary of literature data**

<b>t/°C</b>	<b>P/Pa</b>
10.3	133.3
47.5	666.6
61.1	1333
75.2	2666
91.8	5333
102.3	7999
116.4	13332
137.4	26664
160.2	53329
184.5	101325
mp/°C	28.5

### 6.1.5 IODOBENZENES

#### 6.1.5.1 Iodobenzene



Common Name: Iodobenzene

Synonym: phenyl iodide

Chemical Name: iodobenzene

CAS Registry No: 591-50-4

Molecular Formula:  $C_6H_5I$

Molecular Weight: 204.008

Melting Point ( $^{\circ}C$ ):

−31.3 (Weast 1982–83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

188.4 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.8308 (Weast 1982–83; Lide 2003)

1.8308, 1.8229( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

Molar Volume ( $cm^3/mol$ ):

111.4 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987; Wang et al. 1992)

129.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

40.794 (Riddick et al. 1986)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

340 ( $30^{\circ}C$ , Gross et al. 1933)

180 (shake flask-UV spectrophotometry, Andrews & Keefer 1950)

228\* ( $25.1^{\circ}C$ , shake flask-spectrophotometry, measured range  $10$ – $35^{\circ}C$ , Vesala 1973)

229 (shake flask-UV spectrophotometry, Vesala 1974)

158 (Deno & Berkheimer 1960)

95\* (shake flask-GC, measured range  $5$ – $45.5^{\circ}C$ , Nelson & Smit 1978)

267.6\* (summary of literature data, temp range  $25$ – $50^{\circ}C$ , Horvath 1982)

201 (Miller et al. 1985)

226\* (recommended, temp range  $10$ – $45^{\circ}C$ , IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(g/kg) = 0.59293 - 4.8616 \times 10^{-3} \cdot (T/K) + 1.21754 \times 10^{-5} \cdot (T/K)^2$ ; temp range  $283$ – $318$  K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

213\* ( $29.3^{\circ}C$ , Ramsay-Young method, measured range  $29.3$ – $100.35^{\circ}C$ , Young 1889)

133.3\*, 666.6 ( $24.1$ ,  $50.6^{\circ}C$ , summary of lit. data, temp range  $24.1$ – $188.6^{\circ}C$ , Stull 1947)

134.5 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.89506 - 1562.87/(201.0 + t/^{\circ}C)$ ; temp range:  $85$ – $270^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

132.0 (Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.01187 - 1640.124/(208.765 + t/^{\circ}C)$ ; temp range  $29.3$ – $188.2^{\circ}C$  (Antoine eq. from reported exptl. data of Young 1889, Boublik et al. 1973)

134 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.15935 - 1656.226/(210.496 + t/^{\circ}\text{C})$ ; temp range 29.3–188.2°C (Antoine eq. from reported exptl. data of Young 1889, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.0119 - 1640.1/(208.8 + t/^{\circ}\text{C})$ ; temp range 20–188°C (Antoine eq., Dean 1985, 1992)

134.5 (Riddick et al. 1986)

133 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.01996 - 1562.87/(-72.15 + T/\text{K})$ ; temp range 358–543 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.46493 - 1867.69/(-20.202 + T/\text{K})$ ; temp range 462–679 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.36129 - 1765.99/(-54.15 + T/\text{K})$ ; temp range 273–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 32.7342 - 3.5824 \times 10^3/(T/\text{K}) - 8.4197 \cdot \log (T/\text{K}) + 2.0073 \times 10^{-10} \cdot (T/\text{K}) + 1.591 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 242–721 K (Yaws 1994)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at 25°C):

130 (recommended, Mackay & Shiu 1981)

134 (computer value, Yaws et al. 1991)

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

3.25, 3.32 (quoted, calculated-fragment const., Rekker 1977)

3.25 (Hansch & Leo 1979)

3.28 (generator column-HPLC, Wasik et al. 1983)

3.28 (generator column-HPLC, Tewari et al. 1982)

3.23 (HPLC/MS correlation, Burkhard et al. 1985)

3.37 (HPLC-RT correlation, Eadsforth 1986)

3.25 (recommended, Sangster 1989)

3.25 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log \text{BCF}$ :

Sorption Partition Coefficient,  $\log K_{\text{OC}}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{\text{OH}}$  for reaction with OH radical,  $k_{\text{NO}_3}$  with  $\text{NO}_3$  radical and  $k_{\text{O}_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs}) = 0.93 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = (1.32 \pm 0.19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{OH}} = 1.32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k(\text{soln}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}} = 1.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , independent of temperature over the range 263–393 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 6.1.5.1.1  
Reported aqueous solubilities of iodobenzene at various temperatures

$S(\text{wt}\%) = -2.78956 \times 10^{-3} + 1.95862 \times 10^{-3} \cdot (t/^{\circ}\text{C}) - 4.53984 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 5.73315 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3$  (1)

$S/(\text{g/kg}) = 0.59293 - 4.816 \times 10^{-3} \cdot (T/\text{K}) + 1.21754 \times 10^{-5} \cdot (T/\text{K})^2$  (2)

Vesala 1973		Nelson & Smit 1978		Horvath 1982		Horvath & Getzen 1985	
shake flask-UV		shake flask-GC		summary of literature data		IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
10	195.29	5	54.9	25	267.6	10	193
15.2	196.56	25	95.0	30	305.9	15	203
19.6	216.42	39	143.8	40	396.1	20	214
25.0	228.45	45.5	207.2	50	533.1	25	226
30.0	236.20					30	238
35.0	251.09			eq. 1	S/wt%	35	251
						40	264
						45	279
						eq. 2	S/(g/kg)

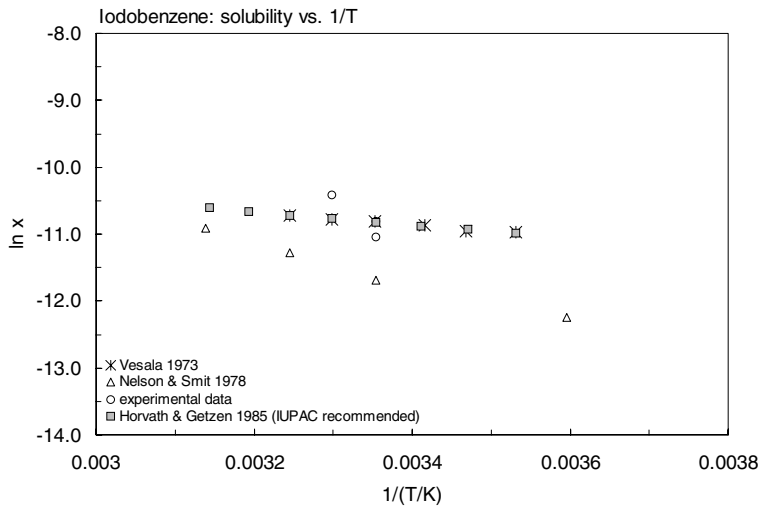


FIGURE 6.1.5.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for iodobenzene.

TABLE 6.1.5.1.2

Reported vapor pressures of iodobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Young 1889		Stull 1947	
Ramsay-Young method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
29.3	213	24.1	133.3
33	240	50.6	666.6
40.1	367	64	1333
46.3	513	78.3	2666
52.5	753	94.4	5333
57	933	105	7999
61.45	1187	118.3	13332
67.8	1627	139.8	26664
70.9	1927	163.9	53329
78.4	2700	188.6	101325
81.9	3166		
85.5	3673	mp/°C	-28.5
87.45	4026		
88.75	4266		
91.55	4820		
91.6	4820		
94.75	5466		
100.35	6919		

complete set of data see [ref.](#)

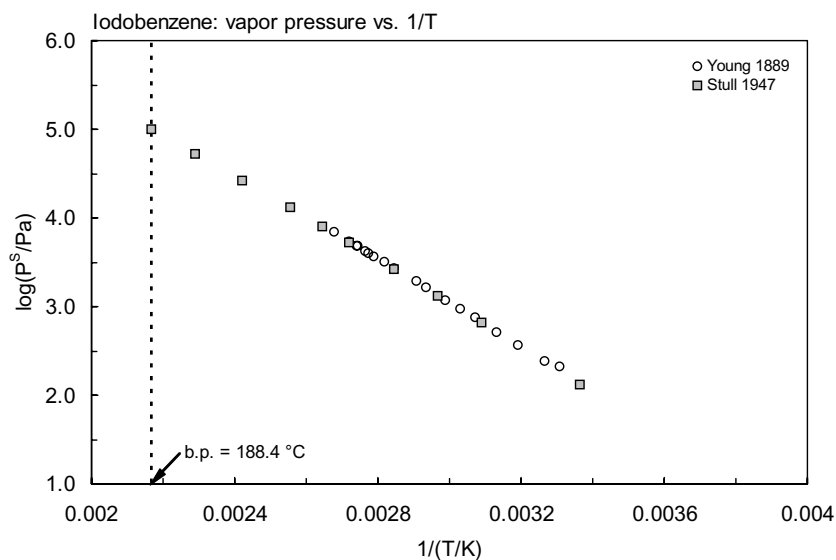
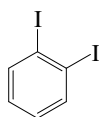


FIGURE 6.1.5.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodobenzene.



## 6.1.5.2 1,2-Diiodobenzene



Common Name: 1,2-Diiodobenzene

Synonym: *o*-diiodobenzene

Chemical Name: 1,2-Diiodobenzene

CAS Registry No: 615-42-9

Molecular Formula:  $C_6H_4I_2$

Molecular Weight: 329.051

Melting Point ( $^{\circ}C$ ):

27 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

287 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

2.54 ( $20^{\circ}C$ , Weast 1982–83, Horvath 1982; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

162.6 (calculated-Le Bas method at normal boiling point)

134.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.956 (mp at  $27^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

14.9 (shake flask-UV, Andrews & Keefer 1950)

19.0 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant (Pa· $m^3/mol$  at  $25^{\circ}C$ ):

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

4.65 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)

4.64 (calculated-fragment const., Yalkowsky et al. 1983)

4.65; 4.35 (quoted; calculated-molar volume correlation, Wang et al. 1992)

4.39 (calculated, Müller & Klein 1992)

4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)

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

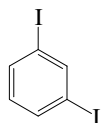
Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{oc}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 6.1.5.3 1,3-Diiodobenzene



Common Name: 1,3-Diiodobenzene

Synonym: *m*-diiodobenzene

Chemical Name: 1,3-Diiodobenzene

CAS Registry No: 626-00-6

Molecular Formula:  $C_6H_4I_2$

Molecular Weight: 329.905

Melting Point ( $^{\circ}C$ ):

40.4 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

285 (Weast 1982–83, Horvath 1982; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

2.47 (Weast 1982–83, Horvath 1982)

Molar Volume ( $cm^3/mol$ ):

162.6 (calculated-Le Bas method at normal boiling point)

134.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

3.8064 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.706 (mp at  $40.4^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

9.67 (shake flask-UV, Andrews & Keefer 1950)

8.88 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

4.39 (calculated, Müller & Klein 1992)

4.70 (calculated-molar volume correlation, Wang et al. 1992)

5.25; 4.56 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

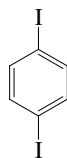
Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{oc}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**6.1.5.4 1,4-Diiodobenzene**

Common Name: 1,4-Diiodobenzene

Synonym: *p*-diiodobenzene

Chemical Name: 1,4-Diiodobenzene

CAS Registry No: 624-38-4

Molecular Formula:  $C_6H_4I_2$

Molecular Weight: 329.905

Melting Point ( $^{\circ}C$ ):

131.5 (Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

285 (sublimation, Weast 1982–83, Horvath 1982; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

162.6 (calculated-Le Bas method at normal boiling point)

134.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

5.3342 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0902 (mp at  $131.5^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

4.62 (shake flask-UV, Andrews & Keefer 1950)

1.855 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

1.545 (extrapolated Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.29504 - 33311.326/(T/K)$ ; temp range 372–401 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.8859 - 2747.88/(T/K)$ ; temp range 402–560 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983; quoted, Wang et al. 1992)

4.39 (calculated, Müller & Klein 1992)

4.11 (shake flask, recommended, Hansch et al. 1995)

4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)

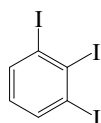
Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**6.1.5.5 1,2,3-Triiodobenzene**

Common Name: 1,2,3-Triiodobenzene

Synonym:

Chemical Name: 1,2,3-Triiodobenzene

CAS Registry No: 608-29-7

Molecular Formula:  $C_6H_3I_3$

Molecular Weight: 455.801

Melting Point ( $^{\circ}C$ ):

166 (Weast 1982–83, Horvath 1982)

Boiling Point ( $^{\circ}C$ ):

sublimation (Weast 1982–83, Horvath 1982)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

141 (Wang et al. 1992)

195.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.041 (mp at  $166^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.301 (shake flask-UV, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

5.86 (quoted, Wang et al. 1992)

6.17; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

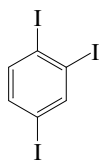
Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**6.1.5.6 1,2,4-Triiodobenzene**

Common Name: 1,2,4-Triiodobenzene

Synonym:

Chemical Name: 1,2,4-Triiodobenzene

CAS Registry No: 615-68-9

Molecular Formula:  $C_6H_3I_3$

Molecular Weight: 455.801

Melting Point ( $^{\circ}C$ ):

91.5 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

sublimation (Weast 1982–83, Horvath 1982; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

195.9 (calculated-Le Bas method at normal boiling point)

145 (Wang et al. 1992)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.223 (mp at  $91.5^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.538 (shake flask-UV, Yalowsky & Valvani 1980)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

5.85 (quoted, Wang et al. 1992)

6.58; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

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

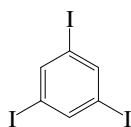
Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{oc}$ :

Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 6.1.5.7 1,3,5-Triiodobenzene



Common Name: 1,3,5-Triiodobenzene

Synonym:

Chemical Name: 1,3,5-Triiodobenzene

CAS Registry No: 626-44-8

Molecular Formula:  $C_6H_3I_3$

Molecular Weight: 455.801

Melting Point ( $^{\circ}C$ ):

184.2 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

sublimation (Weast 1982–83, Horvath 1982; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

131 (Wang et al. 1992)

195.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.0274 (mp at  $184.2^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.0706 (shake flask-UV, Yalowsky & Valvani 1980)

0.0644 (quoted, Wang et al. 1992)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa\cdot m^3/mol$  at  $25^{\circ}C$ ):

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

5.85 (quoted, Wang et al. 1992)

6.90; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

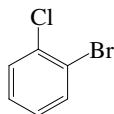
Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**6.1.6 MIXED HALOGENATED BENZENES****6.1.6.1 2-Bromochlorobenzene**

Common Name: 2-Bromochlorobenzene

Synonym: 2-bromo-1-chlorobenzene

Chemical Name:

CAS Registry No: 108-37-2

Molecular Formula:  $C_6H_4BrCl$

Molecular Weight: 191.453

Melting Point ( $^{\circ}C$ ):

-12.3 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

204 (Weast 1982–83; Horvath 1982; Lide 2003)

Density ( $g/cm^3$ ):

1.6387 (25 $^{\circ}C$ , Weast 1982–83; Horvath 1982)

Molar Volume ( $cm^3/mol$ ):

117 (calculated-density, Lande & Banerjee 1981; Wang et al. 1992)

116.8 (Ruelle & Kesselring 1997)

140.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or mg/L at 25 $^{\circ}C$ ):

124 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)

124 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25 $^{\circ}C$ ):

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25 $^{\circ}C$ ):

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

3.83 (calculated-fragment const., Yalkowsky et al. 1979)

3.86 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983)

3.44 (calculated, Müller & Klein 1992)

3.83; 3.63 (quoted; calculated-molar volume correlation, Wang et al. 1992)

3.83, 3.54; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)

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

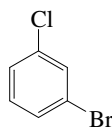
Bioconcentration Factor, log BCF or log  $K_B$ :

Sorption Partition Coefficient, log  $K_{OC}$ :

Environmental Fate Rate Constants, k, and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 6.1.6.2 3-Bromochlorobenzene



Common Name: 3-Bromochlorobenzene

Synonym: *m*-bromochlorobenzene, 3-bromo-1-chlorobenzene, 1-bromo-3-chlorobenzene

Chemical Name: 3-bromochlorobenzene

CAS Registry No: 108-37-2

Molecular Formula: C<sub>6</sub>H<sub>4</sub>BrCl

Molecular Weight: 191.453

Melting Point (°C):

–21.5 (Dreisbach & Martin 1949, Weast 1982–83; Horvath 1982; Lide 2003)

21 (Stephenson & Malanowski 1987)

Boiling Point (°C):

196 (Weast 1982–83; Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm<sup>3</sup>):

1.62745, 1.62065 (20°C, 25°C, Dreisbach & Martin 1949)

1.602 (20°C, Weast 1982–83; Horvath 1982)

1.5771 (20°C, Lide 2003)

Molar Volume (cm<sup>3</sup>/mol):

117.4 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

140.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):

118 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)

118 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

log (P/mmHg) = 7.37230 – 1912.7/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

99.2 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P<sub>L</sub>/kPa) = 6.4972 – 1912.7/(T/K – 43.15); temp range 252–469 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25°C):

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

3.83 (calculated-fragment const., Yalkowsky et al. 1979)

3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

3.74 (HPLC-k' correlation, Hanai et al. 1981)

3.72 (calculated, Müller & Klein 1992)

3.61 (calculated-molar volume correlation, Wang et al. 1992)

3.54; 3.36 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:



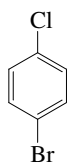
Bioconcentration Factor, log BCF or log  $K_B$ :

Sorption Partition Coefficient, log  $K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 6.1.6.3 4-Bromochlorobenzene



Common Name: 4-Bromochlorobenzene

Synonym: 4-bromo-1-chlorobenzene, 1-bromo-4-chlorobenzene

Chemical Name: 4-bromochlorobenzene

CAS Registry No: 106-39-8

Molecular Formula:  $C_6H_4BrCl$

Molecular Weight: 191.453

Melting Point ( $^{\circ}C$ ):

68 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

196 (Weast 1982–83; Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$ ):

1.576 (71 $^{\circ}C$ , Weast 1982–83; Horvath 1982)

Molar Volume ( $cm^3/mol$ ):

121.5 (calculated-density, Stephenson & Malanowski 1987)

140.2 (calculated-Le Bas method at normal boiling point)

126.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.376 (mp at 68 $^{\circ}C$ )

Water Solubility ( $g/m^3$  or mg/L at 25 $^{\circ}C$ ):

44.9; 37.3 (shake flask-UV; calculated- $K_{ow}$ , Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983; quoted, Lande & Banerjee 1981; Horvath 1982; Müller & Klein 1992)

44.9; 37.3 (quoted; calculated- $K_{ow}$ , Valvani & Yalkowsky 1980)

44.2 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

45; 11.31 (quoted; calculated-molar volume correlation, Wang et al. 1992)

44.9; 50.4 (quoted; calculated-group contribution method; Kühne et al. 1995)

44.9; 51.5 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25 $^{\circ}C$  and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section.):

133.3\* (32.0 $^{\circ}C$ , summary of literature data, temp range 32.0–196.9 $^{\circ}C$ , Stull 1947)

33.3\* (24.2 $^{\circ}C$ , manometry, measured range 21.4–64.4 $^{\circ}C$ , Walsh & Smith 1961)

34.45 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 16671.8/(T/K)] + 11.629$ ; temp range 23–63 $^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 11451.1/(T/K)] + 8.222763$ ; temp range 32–196 $^{\circ}C$  (Antoine eq., Weast 1972–73)

32.12 (calculated-bp, Mackay et al. 1982)

37.72 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.478 - 3548.4/(T/K)$ ; temp range 294–337 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.71377 - 2074.22/(T/K - 35.248)$ ; temp range 333–470 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at 25 $^{\circ}C$ ):

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

- 3.86 (calculated-fragment const., Yalkowsky et al. 1979)
- 3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983; quoted, Malihot & Peters 1988)
- 3.72 (calculated, Müller & Klein 1992)
- 3.83; 4.29 (quoted; calculated-molar volume correlation, Wang et al. 1992)
- 3.83, 3.73; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

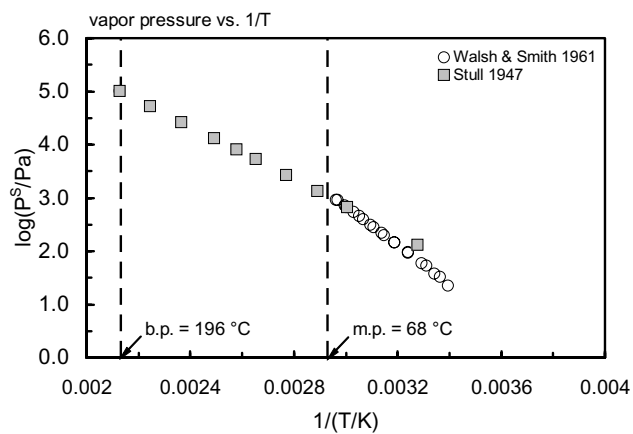
Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

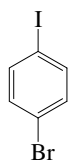
Half-Lives in the Environment:

**TABLE 6.1.6.3.1**  
**Reported vapor pressures of 4-bromochlorobenzene at various temperatures**

Stull 1947		Walsh & Smith 1961	
summary of literature data		manometry	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
32.0	133.3	21.4	22.7
59.5	666.6	24.2	33.3
72.7	1333	26.1	37.3
87.8	2666	29.0	53.3
103.8	5333	30.7	58.7
114.8	7999	35.4	96.0
128.0	13332	35.6	93.3
149.5	26664	40.5	144.0
172.6	53329	40.6	144.0
196.9	101325	44.5	200.0
		45.6	221.3
		48.9	284
		49.9	313.3
		53.0	401.3
		54.7	457.3
		57.1	545.3
		59.9	673.3
		60.7	710.6
		64.0	902.6
		64.4	911.9



**FIGURE 6.1.6.3.1** Logarithm of vapor pressure versus reciprocal temperature for 4-bromochlorobenzene.

**6.1.6.4 4-Bromoiodobenzene**

Common Name: 4-Bromoiodobenzene

Synonym: 4-bromo-1-iodobenzene

Chemical Name:

CAS Registry No: 589-87-7

Molecular Formula:  $C_6H_4BrI$

Molecular Weight: 282.904

Melting Point ( $^{\circ}C$ ):

92 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

252 (Weast 1982–83; Horvath 1982; Lide 2003)

Density ( $g/cm^3$ ):

2.235 (Weast 1982–83; Horvath 1982; Lide 2003)

Molar Volume ( $cm^3/mol$ ):

152.6 (calculated-Le Bas method at normal boiling point)

128.1 (Rulle & Kesselring 1997)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

19.13 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.22 (mp at  $92^{\circ}C$ )

Water Solubility ( $g/m^3$  or mg/L at  $25^{\circ}C$ ):

7.8 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980, Valvani & Yalkowsky 1980)

7.94 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

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

4.36 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)

4.62; 4.10 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

4.13 (calculated, Müller & Klein 1992)

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

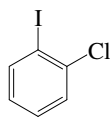
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{oc}$ :

Environmental Fate Rate Constants, k, and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 6.1.6.5 2-Chloriodobenzene



Common Name: 2-Chloriodobenzene

Synonym: 2-chloro-1-iodobenzene

Chemical Name:

CAS Registry No: 615-41-8

Molecular Formula:  $\text{ClC}_6\text{H}_4\text{I}$

Molecular Weight: 238.453

Melting Point ( $^{\circ}\text{C}$ ):

0.7 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}\text{C}$ ):

234.5 (Weast 1982–83; Horvath 1982; Lide 2003)

Density ( $\text{g}/\text{cm}^3$ ):

1.9515 (Weast 1982–83; Horvath 1982)

1.9255 ( $20^{\circ}\text{C}$ , Lide 2003)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

150.2 (calculated-Le Bas method at normal boiling point)

134.6 (Rulle & Kesselring 1997)

Enthalpy of Vaporization,  $\Delta H_v$  ( $\text{kJ}/\text{mol}$ ):

Enthalpy of Fusion,  $\Delta H_{\text{fus}}$  ( $\text{kJ}/\text{mol}$ ):

Entropy of Fusion,  $\Delta S_{\text{fus}}$  ( $\text{J}/\text{mol K}$ ):

Fugacity Ratio at  $25^{\circ}\text{C}$ , F: 1.0

Water Solubility ( $\text{g}/\text{m}^3$  or  $\text{mg}/\text{L}$  at  $25^{\circ}\text{C}$ ):

68.8 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

68.68 (quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at  $25^{\circ}\text{C}$ ):

Henry's Law Constant ( $\text{Pa}\cdot\text{m}^3/\text{mol}$  at  $25^{\circ}\text{C}$ ):

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

4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)

3.98 (calculated, Müller & Klein 1992)

2.54; 3.89 (quoted; calculated-molar volume correlation, Wang et al. 1992)

4.05, 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

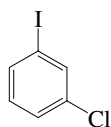
Octanol/Air Partition Coefficient,  $\log K_{\text{OA}}$ :

Bioconcentration Factor,  $\log \text{BCF}$  or  $\log K_{\text{B}}$ :

Sorption Partition Coefficient,  $\log K_{\text{OC}}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**6.1.6.6 3-Chloriodobenzene**

Common Name: 3-Chloriodobenzene

Synonym: 3-chloro-1-iodobenzene

Chemical Name:

CAS Registry No: 625-99-0

Molecular Formula:  $\text{ClC}_6\text{H}_4\text{I}$

Molecular Weight: 238.453

Melting Point ( $^{\circ}\text{C}$ ):

Boiling Point ( $^{\circ}\text{C}$ ):

230 (Weast 1982–83; Lide 2003)

Density ( $\text{g}/\text{cm}^3$ ):

1.9515 ( $25^{\circ}\text{C}$ , Weast 1982–83)

1.9255 ( $20^{\circ}\text{C}$ , Horvath 1982)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

150.2 (calculated-Le Bas method at normal boiling point)

124.9 (Rulle & Kesselring 1997)

Enthalpy of Vaporization,  $\Delta H_v$  ( $\text{kJ}/\text{mol}$ ):

Enthalpy of Fusion,  $\Delta H_{\text{fus}}$  ( $\text{kJ}/\text{mol}$ ):

Entropy of Fusion,  $\Delta S_{\text{fus}}$  ( $\text{J}/\text{mol K}$ ):

Fugacity Ratio at  $25^{\circ}\text{C}$ , F: 1.0

Water Solubility ( $\text{g}/\text{m}^3$  or  $\text{mg}/\text{L}$  at  $25^{\circ}\text{C}$ ):

68.8 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

67.4 (quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure ( $\text{Pa}$  at  $25^{\circ}\text{C}$ ):

Henry's Law Constant ( $\text{Pa}\cdot\text{m}^3/\text{mol}$  at  $25^{\circ}\text{C}$ ):

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

4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)

4.05, 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

3.98 (calculated, Müller & Klein 1992)

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

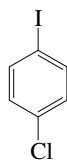
Bioconcentration Factor,  $\log \text{BCF}$  or  $\log K_{\text{B}}$ :

Sorption Partition Coefficient,  $\log K_{\text{OC}}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 6.1.6.7 4-Chloriodobenzene



Common Name: 4-Chloriodobenzene

Synonym: 4-chloro-1-iodobenzene

Chemical Name:

CAS Registry No: 637-87-6

Molecular Formula:  $\text{ClC}_6\text{H}_4\text{I}$

Molecular Weight: 238.453

Melting Point ( $^{\circ}\text{C}$ ):

57 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ( $^{\circ}\text{C}$ ):

227 (Weast 1982–83; Horvath 1982; Lide 2003)

Density ( $\text{g}/\text{cm}^3$ ):

1.886 ( $57^{\circ}\text{C}$ , Weast 1982–83; Horvath 1982)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

122 (calculated-density, Lande & Banerjee 1981)

126.4 (Stephenson & Malanowski 19987; Rulle & Kesselring 1997)

127 (Wang et al. 1992)

150.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{\text{fus}}$  ( $\text{kJ}/\text{mol}$ ):

Entropy of Fusion,  $\Delta S_{\text{fus}}$  ( $\text{J}/\text{mol K}$ ):

Fugacity Ratio at  $25^{\circ}\text{C}$  (assuming  $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$ , F: 0.4825)

Water Solubility ( $\text{g}/\text{m}^3$  or  $\text{mg}/\text{L}$  at  $25^{\circ}\text{C}$ ):

22.5 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

31.11 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at  $25^{\circ}\text{C}$  and reported temperature dependence equations):

16.26 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 8.944 - 3200/(T/\text{K})$ ; temp range 303–323 K (Antoine eq.-I, solid state, Stephenson & Malanowski 1987)

$\log(P_l/\text{kPa}) = 5.63678 - 1465.651/(T/\text{K} - 102.487)$ ; temp range 333–500 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ( $\text{Pa}\cdot\text{m}^3/\text{mol}$  at  $25^{\circ}\text{C}$ ): $k'$

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

4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky)

4.06 (HPLC- $k'$  correlation, Hanai et al. 1981)

3.98 (calculated, Müller & Klein 1992)

4.47 (calculated-molar volume correlation, Wang et al. 1992)

4.34; 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

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

Bioconcentration Factor,  $\log \text{BCF}$  or  $\log K_{\text{B}}$ :

Sorption Partition Coefficient,  $\log K_{\text{OC}}$ :

Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:



## 6.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 6.2.1

Summary of physical properties of chlorobenzenes and other halogenated mononuclear aromatics

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V <sub>M</sub> cm³/mol	
								from ρ <sup>(a)</sup>	Le Bas
<b>Chlorobenzenes:</b>									
Chlorobenzene	108-90-7	C <sub>6</sub> H <sub>5</sub> Cl	112.557	−45.31	131.72	1	1.1058	101.79	116.9
1,2-Dichloro-	95-50-1	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.002	−17.0	180	1	1.3059	112.57	137.9
1,3-Dichloro-	541-73-1	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.002	−24.8	173	1	1.2884	114.10	137.8
1,4-Dichloro-	106-46-7	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.002	53.09	174	0.530	1.2457	118.01	137.8
1,2,3-Trichloro-	87-61-6	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	181.447	51.3	218.5	0.552		125‡	158.7
1,2,4-Trichloro-	120-82-1	C <sub>3</sub> H <sub>3</sub> Cl <sub>3</sub>	181.447	16.92	213.5	1	1.4542	124.77	158.7
1,3,5-Trichloro-	108-70-3	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	181.447	62.8	208	0.426		125‡	158.7
1,2,3,4-Tetrachloro-	634-66-2	C <sub>6</sub> H <sub>2</sub> Cl <sub>4</sub>	215.892	47.5	254	0.602		142‡	179.6
1,2,3,5-Tetrachloro-	634-90-2	C <sub>6</sub> H <sub>2</sub> Cl <sub>4</sub>	215.892	54.5	246	0.514		142‡	179.6
1,2,4,5-Tetrachloro-	95-94-3	C <sub>6</sub> H <sub>2</sub> Cl <sub>4</sub>	215.892	139.5	244.5	0.0753		142‡	179.6
Pentachlorobenzene	608-93-5	C <sub>6</sub> HCl <sub>5</sub>	250.337	86	277	0.252		166‡	200.5
Hexachlorobenzene	118-74-1	C <sub>6</sub> Cl <sub>6</sub>	284.782	228.83	325	0.0100		186‡	221.4
<b>Chlorotoluenes:</b>									
2-Chlorotoluene	95-49-8	C <sub>7</sub> H <sub>7</sub> Cl	126.584	−35.8	159.0	1	1.0825	116.94	139.1
3-Chlorotoluene	108-41-8	C <sub>7</sub> H <sub>7</sub> Cl	126.584	−47.8	161.8	1	1.0722	118.06	139.1
4-Chlorotoluene	106-43-4	C <sub>7</sub> H <sub>7</sub> Cl	126.584	7.5	162.4	1	1.0697	118.34	139.1
2,4-Dichlorotoluene	95-73-8	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub>	161.029	−13.5	201	1	1.2476	129.07	160.0
2,6-Dichlorotoluene	118-69-4	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub>	161.029	25.8	198	1	1.2686	126.93	160.0
3,4-Dichlorotoluene	95-75-0	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub>	161.029	−15.2	208.9	1	1.2564	128.17	160.0
2,3,6-Trichlorotoluene	2077-46-5	C <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub>	195.474	45.5	229.5	0.629			180.9
2,4,5-Trichlorotoluene	6639-30-1	C <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub>	195.474	82.4	231	0.273			180.9
α-Chlorotoluene	100-44-7	C <sub>7</sub> H <sub>7</sub> Cl	126.584	−45	179	1	1.1004	115.03	139.1
α, α, α-Trichlorotoluene	98-07-7	C <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub>	195.474	−4.42	221	1	1.3723	142.44	180.9
Pentachlorotoluene	877-11-2	C <sub>7</sub> H <sub>3</sub> Cl <sub>5</sub>	264.364	224.8	301	0.0110			222.7
o-Chlorostyrene	2039-87-4	C <sub>8</sub> H <sub>7</sub> Cl	138.595	−63.1	188.7	1	1.1000	126.00	153.9
m-Chlorostyrene	2039-85-2	C <sub>8</sub> H <sub>7</sub> Cl	138.595				1.1033	125.62	153.9
p-Chlorostyrene	1073-67-2	C <sub>8</sub> H <sub>7</sub> Cl	138.595	15.9	192	1	1.0868	127.53	153.9
Octachlorostyrene	29082-74-4	C <sub>8</sub> Cl <sub>8</sub>	379.710	99		0.188			300.2

(Continued)

TABLE 6.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V <sub>M</sub> cm³/mol	
								from ρ <sup>(a)</sup>	Le Bas
Fluorobenzenes:									
Fluorobenzene	462-06-6	C <sub>6</sub> H <sub>5</sub> F	96.102	-42.18	84.73	1	1.0225	93.99	101.0
1,2-Difluorobenzene	367-11-3	C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	114.093	-47.1	94	1	1.158	98.53	106.0
1,3-Difluorobenzene	372-18-9	C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	114.093	-69.12	82.6	1	1.1572	98.59	106.0
1,4-Difluorobenzene	540-36-3	C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	114.093	-23.55	89	1	1.1701	97.51	106.0
1,2,4-Trifluorobenzene	367-23-7	C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>	132.083		90	1			111.0
1,3,5-Trifluorobenzene	372-38-3	C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>	132.083	-5.5	75.5	1		103.4†	111.0
1,2,3,4-Tetrafluorobenzene	551-62-2	C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	150.074		94.3	1		105.5†	116.0
1,2,3,5-Tetrafluorobenzene	2367-82-0	C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	150.074	-46.25	84.4	1		107.7†	116.0
1,2,4,5-Tetrafluorobenzene	327-54-8	C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	150.074	3.88	90.2	1	1.4255	105.28	116.0
Pentafluorobenzene	363-72-4	C <sub>6</sub> HF <sub>5</sub>	168.064	-47.4	85.74	1		111.0†	121.0
Hexafluorobenzene	392-56-3	C <sub>6</sub> F <sub>6</sub>	180.054	5.03	80.26	1	1.6184	111.25	126.0
Pentafluorotoluene	771-56-2	C <sub>7</sub> H <sub>3</sub> F <sub>5</sub>	182.091	-29.78	117.5	1	1.440	126.45	143.2
Chloropentafluorobenzene	344-07-0	C <sub>6</sub> ClF <sub>5</sub>	202.509		117.96				141.9
Pentafluorophenol	771-61-9	C <sub>6</sub> HF <sub>5</sub> O	184.063	37.5	145.6	0.754			128.4
Bromobenzenes and bromotoluenes:									
Bromobenzene	108-86-1	C <sub>6</sub> H <sub>5</sub> Br	157.008	-30.72	156.06	1	1.4950	105.02	119.3
1,2-Dibromobenzene	583-53-9	C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	235.904	7.1	225	1	1.9843	118.89	142.6
1,3-Dibromobenzene	108-36-1	C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	235.904	-7.0	218	1	1.9523	120.83	142.6
1,4-Dibromobenzene	106-37-6	C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>	235.904	87.43	218.5	0.244	1.5742	149.86	142.6
1,2,3-Tribromobenzene	608-21-9	C <sub>6</sub> H <sub>3</sub> Br <sub>3</sub>	314.800	87.8		0.242	2.6580	118.43	165.9
1,2,4-Tribromobenzene	615-54-3	C <sub>6</sub> H <sub>3</sub> Br <sub>3</sub>	314.800	44.5	275	0.644			165.9
1,3,5-Tribromobenzene	626-39-1	C <sub>6</sub> H <sub>3</sub> Br <sub>3</sub>	314.800	122.8	271	0.110			165.9
1,2,4,5-Tetrabromobenzene	636-28-2	C <sub>6</sub> H <sub>2</sub> Br <sub>4</sub>	393.696	182		0.0288	3.0720	128.16	189.2
Hexabromobenzene	87-82-1	C <sub>6</sub> Br <sub>6</sub>	551.488	327		0.0011			235.8
2-Bromotoluene	95-46-5	C <sub>7</sub> H <sub>7</sub> Br	171.035	-27.8	181.7	1	1.4232	120.18	141.5
3-Bromotoluene	591-17-3	C <sub>7</sub> H <sub>7</sub> Br	171.035	-39.8	183.7	1	1.4099	121.31	141.5
4-Bromotoluene	106-38-7	C <sub>7</sub> H <sub>7</sub> Br	171.035	28.5	184.3	1			141.5
Iodobenzenes:									
Iodobenzene	591-50-4	C <sub>6</sub> H <sub>5</sub> I	204.008	-31.3	188.4	1	1.8308	111.43	129.3
1,2-Diiodobenzene	615-42-9	C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	329.905	27	287	0.956	2.5400	129.88	162.6
1,3-Diiodobenzene	626-00-6	C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	329.905	40.4	285	0.706			162.6
1,4-Diiodobenzene	624-38-4	C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>	329.905	131.5	285	0.0902			162.6

1,2,3-Triiodobenzene	608-29-7	C <sub>6</sub> H <sub>3</sub> I <sub>3</sub>	455.801	166	sublim	0.0410		141§	195.9
1,2,4-Triiodobenzene	615-68-9	C <sub>6</sub> H <sub>3</sub> I <sub>3</sub>	455.801	91.5	sublim	0.223		145§	195.9
1,3,5-Triiodobenzene	626-44-8	C <sub>6</sub> H <sub>3</sub> I <sub>3</sub>	455.801	184.2	sublim	0.0274		131§	195.9
<b>Mixed halogenated benzenes:</b>									
2-Bromochlorobenzene	694-80-4	C <sub>6</sub> H <sub>4</sub> BrCl	191.453	-12.3	204	1		117§	140.2
3-Bromochlorobenzene	108-37-2	C <sub>6</sub> H <sub>4</sub> BrCl	191.453	-21.5	196	1	1.5771	121.40	140.2
4-Bromochlorobenzene	106-39-8	C <sub>6</sub> H <sub>4</sub> BrCl	191.453	68	196	0.379		121.5†	140.2
4-Bromiodobenzene	589-87-7	C <sub>6</sub> H <sub>4</sub> BrI	282.904	92	252	0.220	2.2350	126.58	152.6
2-Chloriodobenzene	615-41-8	ClC <sub>6</sub> H <sub>4</sub> I	238.453	0.7	234.5	1	1.9255	123.84	150.2
3-Chloriodobenzene	625-99-0	ClC <sub>6</sub> H <sub>4</sub> I	238.453		230	1	1.9255	123.84	150.2
4-Chloriodobenzene	637-87-6	ClC <sub>6</sub> H <sub>4</sub> I	238.453	57	227	0.485		127§	150.2

\* Assuming  $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$

(a) † Chiou 1985 (liquid molar volume), ‡ Stephenson & Malanowski 1987, §Wang et al. 1992, and calculated as MW/p at 20°C for this work

**TABLE 6.2.2**

**Summary of selected physical-chemical properties of chlorobenzenes and other halogenated mononuclear aromatics at 25°C**

Compound	Selected properties						Henry's law constant H/(Pa·m <sup>3</sup> /mol) calculated P/C
	Vapor pressure		Solubility			log K <sub>OW</sub>	
	P <sup>S</sup> /Pa	P <sub>L</sub> /Pa	S/(g/m <sup>3</sup> )	C <sup>S</sup> /(mol/m <sup>3</sup> )	C <sub>L</sub> /(mol/m <sup>3</sup> )		
<b>Chlorobenzenes:</b>							
Chlorobenzene	1580	1580	484	4.3000	4.2300	2.80	367
1,2-Dichloro-	170	170	140	0.9523	0.9523	3.40	178
1,3-Dichloro-	260	260	120	0.8163	0.8163	3.40	318
1,4-Dichloro-	130	245	80	0.544	1.0268	3.40	242
1,2,3-Trichloro-	28	50.72	21	0.1157	0.2100	4.10	242
1,2,4-Trichloro-	40	40	40	0.2204	0.2204	4.10	277
1,3,5-Trichloro-	25	78.05	5.3	0.0292	0.0686	4.10	856
1,2,3,4-Tetrachloro-	4.0	6.64	7.8	0.0361	0.0600	4.50	111
1,2,3,5-Tetrachloro-	9.8	19.01	3.6	0.0167	0.0324	4.50	588
1,2,4,5-Tetrachloro-	0.72	9.56	1.27	0.00588	0.0781	4.50	122
Pentachlorobenzene	0.22	0.8730	0.65	0.00260	0.0103	5.00	85
Hexachlorobenzene	0.0023	0.23	0.005	0.0000176	0.00176	5.50	131

TABLE 6.2.3

Suggested half-life classes of chlorobenzenes and other halogenated mononuclear aromatics in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Chlorobenzene	4	6	7	8
1,2-Dichloro-	5	6	7	8
1,3-Dichloro-	5	6	7	8
1,4-Dichloro-	5	6	7	8
1,2,3-Trichloro-	5	6	7	8
1,2,4-Trichloro-	5	6	7	8
1,3,5-Trichloro-	5	6	7	8
1,2,3,4-Tetrachloro-	6	7	7	8
1,2,3,5-Tetrachloro-	6	7	7	8
1,2,4,5-Tetrachloro-	6	7	7	8
Pentachlorobenzene	7	8	8	8
Hexachlorobenzene	8	9	9	9
Fluorobenzene	4	5	6	7
Bromobenzene	4	6	7	8
Iodobenzene	4	6	7	8

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	1,700 (~2 months)	1,000–3,000
7	5,500 (~8 months)	3,000–10,000
8	17,000 (~2 years)	10,000–30,000
9	55,000 (~6 years)	>30,000

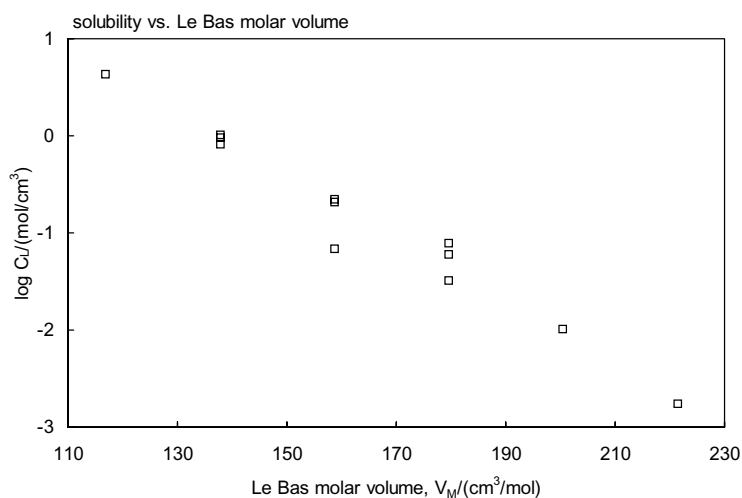
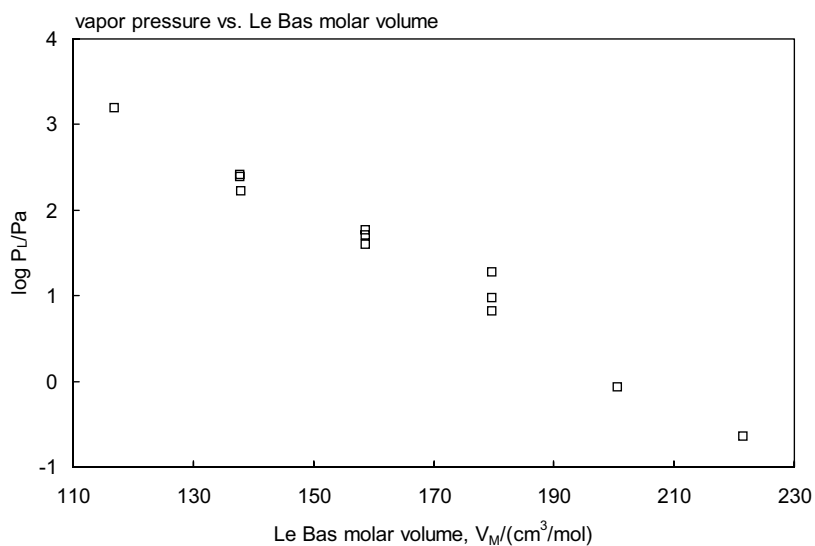
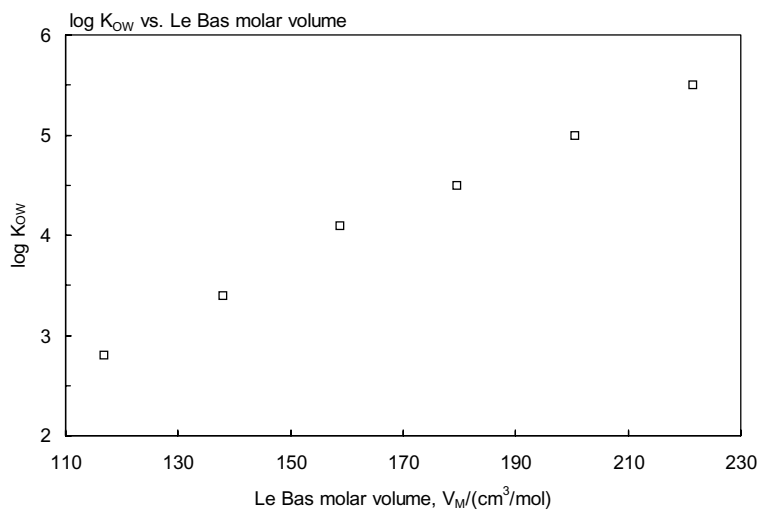


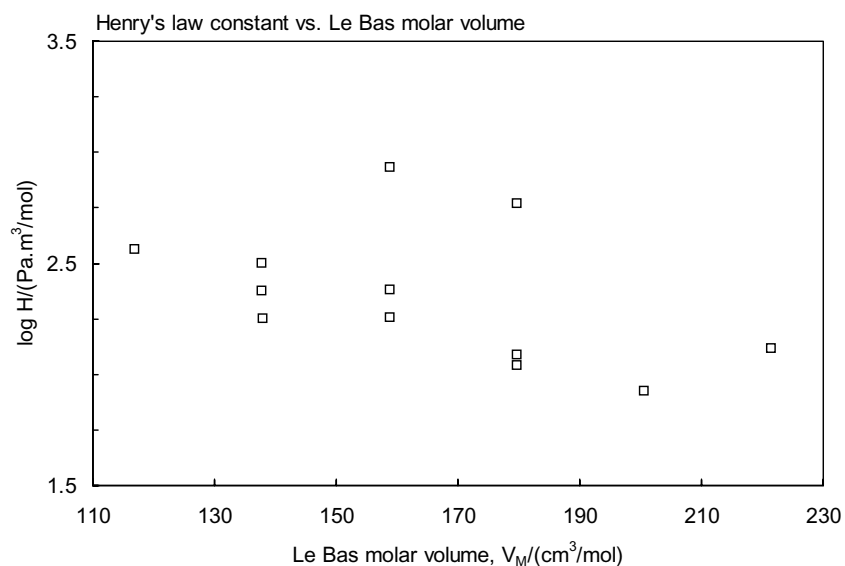
FIGURE 6.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.



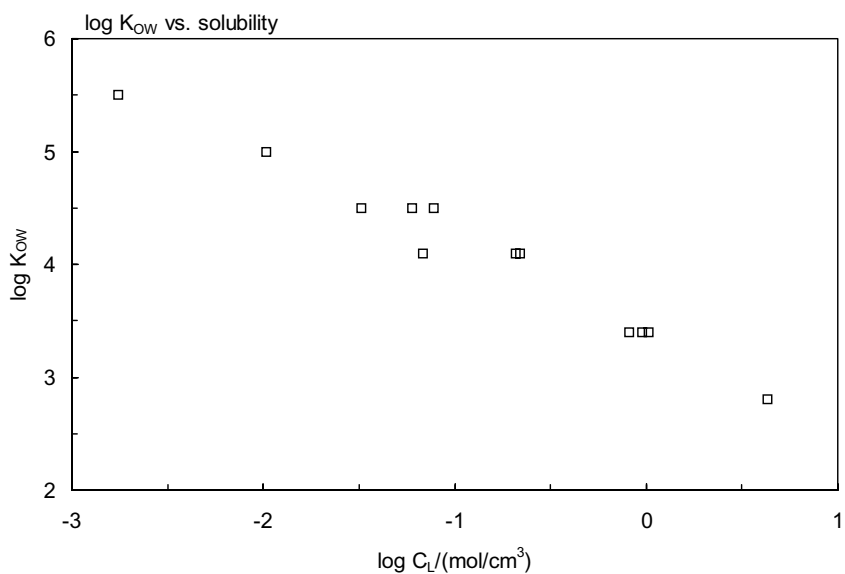
**FIGURE 6.2.2** Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.



**FIGURE 6.2.3** Octanol-water partition coefficient versus Le Bas molar volume for chlorobenzenes.



**FIGURE 6.2.4** Henry's law constant versus Le Bas molar volume for chlorobenzenes.



**FIGURE 6.2.5** Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) chlorobenzenes.

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