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# 5 Halogenated Aliphatic Hydrocarbons

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	Dichlorodifluoromethane (See also Section 5.1.4. Mixed halogenated hydrocarbons)	
	Trichlorofluoromethane (See also Section 5.1.4. Mixed halogenated hydrocarbons)	
	Fluoroethane	
	1,1-Difluoroethane	
	1,2-Difluoroethane	
	1,1,1-Trifluoroethane	
	1,1,2-Trifluoroethane	
	1,1,2,2-Tetrafluoroethane	
	1,1,1,2-Tetrafluoroethane	
	Pentafluoroethane	
	Hexafluoroethane	
	1-Chloro-2-fluoroethane	
	1-Chloro-1,1-difluoroethane	
	1-Chloro-1,1,2-trifluoroethane	
	1-Chloro-1,2,2,2-tetrafluoroethane	
	1-Chloropentafluoroethane	

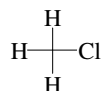
1,1-Dichloro-1-fluoroethane  
1,2-Dichloro-1,1-difluoroethane  
1,1-Dichlorotrifluoroethane  
1,2-Dichloro-1,1,2,2-tetrafluoroethane  
1,1-Dichloro-1,2,2,2-tetrafluoroethane  
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2-Fluoropropane  
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1,1,1,3,3-Pentafluoropropane  
1,1,1,2,2-Pentafluoropropane  
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1,1,1,3,3,3-Hexafluoropropane  
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Trichlorotrifluoropropane  
1-Chloro-2,2,2-trifluoropropane  
Perfluorobutane  
Perfluorocyclobutane  
Perfluoropentane  
Perfluorocyclopentane  
Perfluoro-2-methylcyclopentane  
Perfluoro-3-methylcyclopentane  
Perfluorocyclohexane  
Perfluorohexane  
Fluoroethene  
1,1-Difluoroethene  
Tetrafluoroethene  
Chlorotrifluoroethene  
1,2-Dichloro-1,2-difluoroethene  
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## 5.1 LIST OF CHEMICALS AND DATA COMPILATIONS

### 5.1.1 CHLOROALKANES AND CHLOROALKENES

#### 5.1.1.1 Chloromethane (Methyl chloride)



Common Name: Chloromethane

Synonym: methyl chloride, monochloromethane

Chemical Name: chloromethane

CAS Registry No: 74-87-3

Molecular Formula: CH<sub>3</sub>Cl

Molecular Weight: 50.488

Melting Point (°C):

−97.7 (Lide 2003)

Boiling Point (°C):

−24.09 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.9159 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

0.9214, 0.9111 (20°C, 25°C, Riddick et al. 1986)

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

55.0 (calculated-density, Wang et al. 1992)

50.6, 48.8, 54.3, 50.4 (exptl., Tyn and Calus method, Schroeder method, Le Bas method, Reid et al. 1987)

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

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

19.06, 21.45 (at 25°C, at normal boiling point, Dreisbach 1961)

18.92, 21.40 (25°C, bp, Riddick et al. 1986)

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

6.43 (Riddick et al. 1986)

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

7400 (30°C at 1 atm, McGovern 1943)

5346 (gravitational method, Glew & Moelwyn-Hughes 1953)

6450 (20°C, Dean 1973)

7250 (20°C under 101.3 kPa pressure of CH<sub>3</sub>Cl, McConnell et al. 1975; Pearson & McConnell 1975)

6270, 5380 (20, 25°C literature average at 760 mmHg, Dilling 1977)

5325\* (summary of literature data, temp range 5–80°C, Horvath 1982)

4800 (Dean 1985)

6480 (30°C, quoted, Riddick et al. 1986)

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):

98048\* (248.9 K, static-manometer, measured range 191.4–248.9 K, Messerly & Aston 1940)

101325\* (−24.0°C, summary of literature data, temp range −99.58 to 24.0°C, Stull 1947)

559860 (interpolated from graph, temp range −50 to 60°C, McGovern 1943)

100800 (Glew & Moelwyn-Hughes 1953)

574500 (calculated-Antoine eq., Dreisbach 1959; 1961)

log (P/mmHg) = 6.99445 − 902.451/(243.63 + t/°C); temp range −80 to 3°C (Antoine eq. for liquid state, Dreisbach 1959; 1961)



$\log (P/\text{mmHg}) = 6.99445 - 902.451/(243.60 + t/^{\circ}\text{C})$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

1081\* (29.43°C, concentration ratio, measured range 29.43–40.59°C, Swain & Thornton 1962)

539300 (20–25°C, calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 5375.3/(T/K)] + 7.546207$ ; temp range –99 to 137.5°C (Antoine eq., Weast 1972–73)

567900, 576300 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/\text{mmHg}) = 6.98762 - 899.739/(242.921 + t/^{\circ}\text{C})$ ; temp range –69.2 to –23°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log (P/\text{mmHg}) = 6.09349 - 948.582/(249.336 + t/^{\circ}\text{C})$ ; temp range –75.2 to 5°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

574600 (selected lit., Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.16533 - 920.86/(245.58 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P/\text{mmHg}) = 7.09349 - 948.58/(249.34 + t/^{\circ}\text{C})$ ; temp range –77 to –5°C (Antoine eq., Dean 1985, 1992)

572800 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.11935 - 902.451/(-29.55 + T/K)$ ; temp range 180–266 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04835 - 869.887/(-33.773 + T/K)$ ; temp range 247–310 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.94638 - 1448.913/(47.966 + T/K)$ ; temp range 308–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.94022 - 1447.601/(48.385 + T/K)$ ; temp range 368–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 25.7264 - 1.7503 \times 10^3/(T/K) - 6.7151 \cdot \log (T/K) - 1.2956 \times 10^{-9} \cdot (T/K) + 4.4341 \times 10^{-6} \cdot (T/K)^2$ ; temp range 175–416 K (vapor pressure eq., Yaws 1994)

498820 (293.15 K, selected summary of literature data, temp range 175.44–293.15 K, Xiang 2002)

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):

953\*, 957 (distribution ratio, measured range 4–80°C; calculated-P/C, Glew & Moelwyn-Hughes 1953)

$\log \{H/(\text{mmHg} \cdot \text{L/mol})\} = 71.005 - 21.656 \cdot \log (T/K) - 4043.9/(T/K)$ ; temp range 277.24–353.23 K (Glew & Moelwyn-Hughes 1953)

1010 (calculated as  $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

744, 892 (exptl. as per McConnell et al. 1975, calculated-P/C, Neely 1976)

739 (20°C, Pearson & McConnell 1975)

942 (calculated- $C_A/C_W$ , Dilling 1977)

875 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

$\log (k_H/\text{atm}) = 6.93 - 1248.11/(T/K)$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)

951, 950 (calculated-P/C, recommended, Mackay & Shiu 1981)

894\* (EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)

$\ln [H/(\text{atm m}^3/\text{mol})] = 9.358 - 4215/(T/K)$ , temp range: 10.3–34.6°C (EPICS measurements, Gossett 1987)

669 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

867 (computed value, Yaws et al. 1991)

363, 834 (0, 22°C, distilled water, headspace-GC, Elliot & Rowland 1993)

386 (0°C, gas stripping-GC, Moore et al. 1995)

392, 465, 533 (0, 3.0, 6.0°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

$\ln K_{AW} = 9.17 - 2982/(T/K)$ , seawater of salinity of 30.4‰, temp range: 0–6°C (Moore et al. 1995)

668 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

743 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{AW} = 3.899 - 1292/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

0.91 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

0.91 (shake flask, Log P Database, Hansch & Leo 1987)

0.89, 0.936 (calculated-MO, calculated- $\pi$  substituent const., Bodor et al. 1989)

0.91 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

1.39 (calculated-measured  $\gamma^\infty$  in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

0.505 (microorganism-water, calculated from  $K_{OW}$ , Mabey et al. 1982)

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

0.633 (calculated- $K_{OW}$ , Mabey et al. 1982)

0.778 (selected, Jury et al. 1990)

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

Volatilization: half-life of 27–28 min for initial concentration of 1 mg/L in an open container stirred at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation  $t_{1/2}(\text{exptl.}) = 27.6$  min,  $t_{1/2}(\text{calc}) = 0.599$  min, 14.9 min from water (Dilling 1977)

$t_{1/2} \sim 2.4$  h from water (estimated, Thomas 1982);

$t_{1/2} \sim 120$  d from soil (estimated, Jury et al. 1990).

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 and/or Arrhenius expression see reference:

$k_{OH} = 4.7 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , bimolecular rate constant (Yung et al. 1975)

$k_{OH} = 8.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, bimolecular rate constant with a lifetime  $\tau = 0.37$  yr in the troposphere (Cox et al. 1976)

$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 250–350 K, with a tropospheric lifetime of 1.19 yr (flash photolysis-resonance fluorescence, Davis et al. 1976)

$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K with lifetime  $\tau = 1.19$  yr, measured range 250–350 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altshuller 1980)

$k_{OH} = (3.6 \pm 0.8) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH}^* = (4.4 \pm 0.5) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298.4 K, measured range 298–423 K and the calculated  $t_{1/2} \sim 0.2$  yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)

$k_{OH} = 24.7 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at 297 K (flash photolysis-resonance absorption, Paraskevopoulos et al. 1981)

$k_{OH} = 5.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 231 d, loss of 0.4% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH}^* = 3.95 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 293 K, measured range 247–483 K (discharge-flow resonance fluorescence, Jeong & Kaufman, 1982)

$k_{OH}(\text{calc}) = 2.4 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at 300 K (Lyman 1982)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $0.05 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)

$k_{OH}^* = 4.36 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}^* = 4.9 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K, measured range 295–800 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

$k_{NO_3} = 9.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Atkinson 1991)

Hydrolysis:  $k = 6.8 \times 10^{-5} \text{ h}^{-1}$  with hydrolytic  $t_{1/2} = 417$  d at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979; Mabey et al. 1982);

hydrolysis  $k = 2.3710^{-8} \text{ h}^{-1}$  with  $t_{1/2} 0.93$  yr (Mabey & Mill 1978)

$t_{1/2} = 7000$  h, based on neutral and base catalyzed hydrolysis rate constants at 25°C extrapolated from data obtained at higher temperatures (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 168\text{--}672$  h, based on unacclimated aerobic aqueous screening test data for dichloromethane from experiments utilizing selected domestic waste water inoculum (Tabak et al. 1981; quoted, Howard et al. 1991) and activated sludge inoculum (Klecka 1982; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688$  h, based on estimated aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

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

## Half-Lives in the Environment:

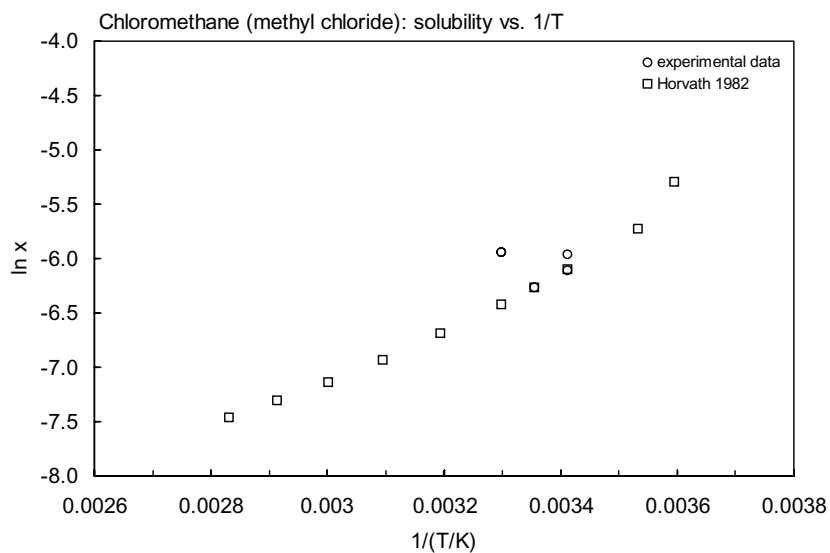
Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (Darnall et al. 1976);  
 tropospheric lifetime of 1.19 yr due to reaction with OH radical (Davis et al. 1976);  
 estimated residence time to be about 2 yr for the reaction with OH radical in troposphere (Singh et al. 1979);  
 lifetime  $\tau = 1.19$  yr for reaction with OH radical (Altshuller 1980)  
 residence time of 231 d, loss of 0.4% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)  
 estimated residence time in troposphere to be 1 yr (Lyman 1982);  
 $t_{1/2} = 1472\text{--}14717$  h, based on photooxidation half-life in air from measured rate constants for reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);  
 estimated tropospheric lifetimes of 1.3 yr, and 1.54 yr by rigorous calculation (Nimitz & Skaggs 1992).  
 lifetime for reaction with OH radicals,  $\tau = 11.7$  yr for Polar region,  $\tau = 2.2$  yr for Middle region and  $\tau = 0.8$  yr for Tropical region in the Northern hemisphere;  $\tau = 0.9$  yr for Tropical,  $\tau = 3.6$  yr for Middle and  $\tau = 12.3$  yr for Polar region in the Southern hemisphere;  $\tau = 1.4$  yr in the Global atmosphere, based on data from 1981–1996 (Khalil & Rasmussen 1999a)  
 Surface water:  $t_{1/2} = 168\text{--}672$  h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).  
 Ground water:  $t_{1/2} = 336\text{--}1344$  h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).  
 Sediment:  
 Soil:  $t_{1/2} > 50$  d (Ryan et al. 1988); estimated  $t_{1/2} = 120$  d for volatilization from soil (Jury et al. 1990);  
 $t_{1/2} = 168\text{--}672$  h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).  
 Biota:  $t_{1/2} > 50$  d, subject to plant uptake from soil via volatilization (Ryan et al. 1988).

TABLE 5.1.1.1.1

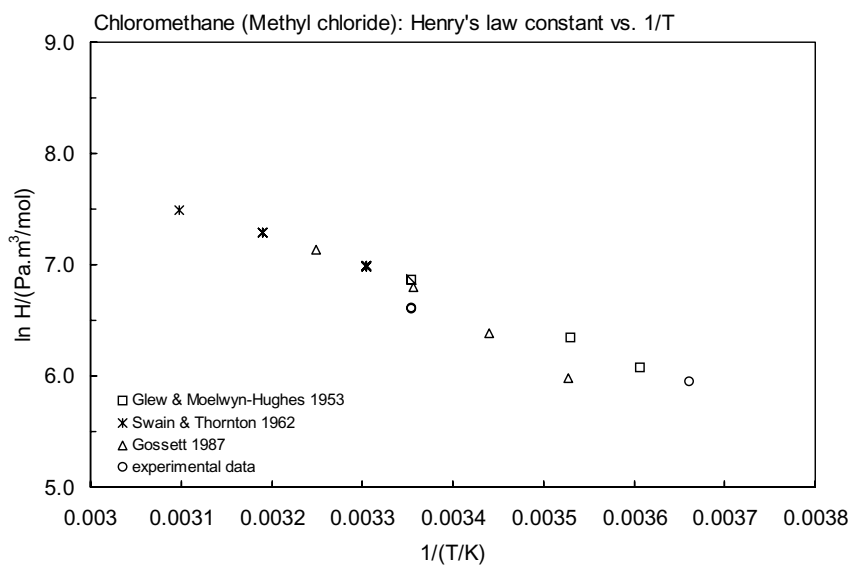
**Reported aqueous solubilities and Henry's law constants of chloromethane (methyl chloride) at various temperatures**

$$S/(\text{wt}\%) = 1.4019 - 6.3562 \times 10^{-2} \cdot (t/^{\circ}\text{C}) + 1.71977 \times 10^{-3} \cdot (t/^{\circ}\text{C})^2 - 2.8262 \times 10^{-5} \cdot (t/^{\circ}\text{C})^3 + 2.5268 \times 10^{-7} \cdot (t/^{\circ}\text{C})^4 - 9.3470 \times 10^{-10} \cdot (t/^{\circ}\text{C})^5 \quad (1)$$

Aqueous solubility		Henry's law constant					
Horvath 1982		Glew & Moelwyn-Hughes 1953		Swain & Thornton 1962		Gossett 1987	
summary of literature data		concentration ratio		concentration ratio		EPICS-GC	
t/°C	S/g·m <sup>-3</sup>	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)
5	14019	4.09	437	29.44	1081	10.3	396.2
10	9113	10.17	568	29.44	1085	17.5	591.7
20	6274	15.06	681	29.44	1073	24.8	893.7
25	5325	20.03	816	29.43	1080	34.6	1256.4
30	4579	25.01	957	29.43	1084		
40	3490	39.91	1475	40.34	1465	ln H = A - B/(T/K) H/(atm m <sup>3</sup> /mol)	
50	2742	49.78	1860	40.35	1459		
60	2228	59.99	2260	40.35	1460	A	8.637
70	1891	70.06	2746	40.59	1791	B	4128
80	1609	80.08	3173				
		25.0	956				
eq.1	S/wt%	log H = A - B·log (T/K) - C/(T/K) P/(mmHg·L/mol)					
		A	59.096				
		B	21.656				
		C	4043.9				



**FIGURE 5.1.1.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for chloromethane.



**FIGURE 5.1.1.2** Logarithm of Henry's law constant versus reciprocal temperature for chloromethane.

TABLE 5.1.1.1.2

Reported vapor pressures of chloromethane (methyl chloride) 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)		
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot (T/K)$	(5)		

Messerly & Aston 1940				Stull 1947	
static-manometer				summary of literature data	
T/K	P/Pa	T/K	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
191.424	3509	248.998	101521	-	
191.378	3498	248.943	98048	-99.58	666.6
194.556	4474			-92.4	1333
199.272	6338	eq. 5	P/mmHg	-84.8	2666
206.324	10320	A	31.07167	-76.0	5333
213.539	16343	B	1822.60	-70.4	7999
213.526	16328	C	9.287119	-63.0	13332
222.999	28384	C	0.00555556	-51.2	26664
230.184	41739			-38.0	53329
237.125	59004	mp/K	175.44	-24.0	101325
242.845	77224	bp/K	248.94		
246.441	90805	$\Delta H_v/(\text{kJ mol}^{-1}) = 0.945$		mp/ $^{\circ}\text{C}$	-97.7

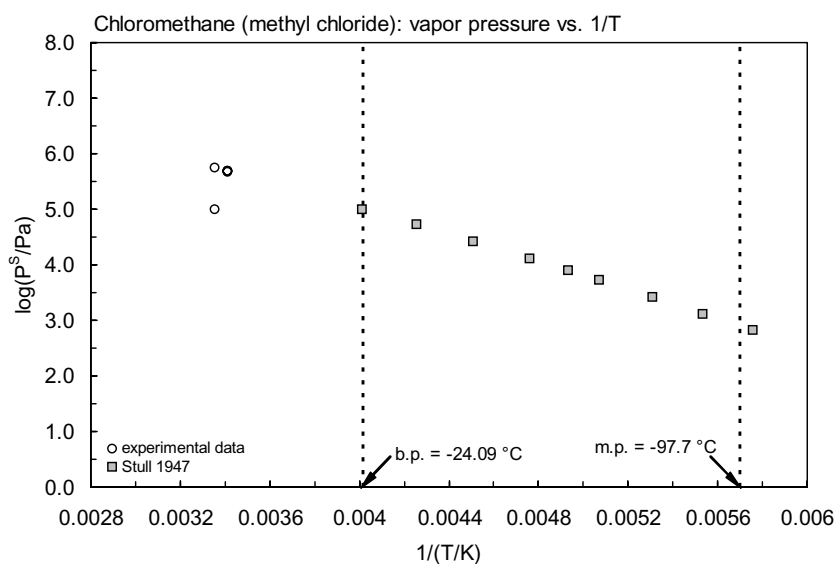
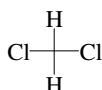


FIGURE 5.1.1.1.3 Logarithm of vapor pressure versus reciprocal temperature for chloromethane.

## 5.1.1.2 Dichloromethane



Common Name: Dichloromethane

Synonym: methylene chloride, methylene dichloride, methane dichloride, methylene bichloride

Chemical Name: dichloromethane

CAS Registry No: 75-09-2

Molecular Formula:  $\text{CH}_2\text{Cl}_2$

Molecular Weight: 84.933

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

-95.2 (Lide 2003)

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

40 (Lide 2003)

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

1.3255, 1.3163 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Dreisbach 1959; 1961)

1.3266 (Horvath 1982; Weast 1982–83)

1.3256, 1.131678 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Riddick et al. 1986)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

64.0 (calculated-density, Wang et al. 1992)

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

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

28.56, 28.98 ( $25^{\circ}\text{C}$ , bp, Riddick et al. 1986)

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

1.435 (calculated, Dreisbach 1959; 1961)

1.472 (quoted, Riddick et al. 1986)

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

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

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

20000\* ( $20^{\circ}\text{C}$ , volumetric method, Rex 1906)

19910 (Seidell 1940)

13200 ( $25^{\circ}\text{C}$ , data presented between  $0$ – $50^{\circ}\text{C}$  in graph, McGovern 1943)

34480 (shake flask-residue volume method, Booth & Everson 1948)

13200 ( $20^{\circ}\text{C}$ , McConnell et al. 1975; Pearson & McConnell 1975)

20000\* (Archer & Sterns 1977; Andelman 1978; measured range  $0$ – $30^{\circ}\text{C}$ , quoted, Horvath 1982)

22700, 19400 (1.5,  $20^{\circ}\text{C}$ , literature average, Dilling 1977)

13700 (shake flask-titration/turbidity, Coca et al. 1980)

13030\* (summary of literature data, Horvath 1982)

13000 (selected, Thomas 1982; Riddick et al. 1986; Howard 1990)

16700 (Verschuereen 1983; selected, Valsaraj 1988)

19020 (calculated-UNIFAC activity coeff., Banerjee 1985)

17200\* ( $26.8^{\circ}\text{C}$ , shake flask-GC/TC, measured range  $0$ – $35.7^{\circ}\text{C}$ , Stephenson 1992)

19260, 19830, 19500, 19500 (20, 30, 35,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\circ}$ -GC, Tse et al. 1992)

18080, 19995, 20880, 21850 (20, 30, 35,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\circ}$ -UNIFAC, Tse et al. 1992)

20080, 18800, 18880 (10, 20,  $30^{\circ}\text{C}$ , activity coeff.  $\gamma^{\circ}$ -differential pressure transducer, Wright et al. 1992)

18650 (gas stripping-GC, Li et al. 1993)

20340 ( $20^{\circ}\text{C}$ , limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

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

46510, 68170 ( $20^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , Rex 1906)

57120 (interpolated from graph, temp range  $-40$  to  $110^{\circ}\text{C}$ , McGovern 1943)

- 57480\* (Antoine eq. regression, temp range  $-70$  to  $40.7^{\circ}\text{C}$ , Stull 1947)  
 58100 (calculated-Antoine eq., Dreisbach 1959; 1961)  
 $\log(P/\text{mmHg}) = 7.07138 - 1134.6/(231.0 + t/^{\circ}\text{C})$ ; temp range  $-28$  to  $121^{\circ}\text{C}$  (Antoine eq. for liquid state, Dreisbach 1955)  
 49704\* ( $21.199^{\circ}\text{C}$ , temp range  $-9.03$  to  $39.429^{\circ}\text{C}$ , Boublik 1960; quoted, Boublik et al. 1984)  
 70530\* ( $29.993^{\circ}\text{C}$ , temp range  $29.993$ – $39.993^{\circ}\text{C}$ , Mueller & Ignatowski 1960)  
 $\log(P/\text{mmHg}) = 7.0803 - 1138.91/(231.45 + t/^{\circ}\text{C})$ ; temp range  $-28$  to  $73^{\circ}\text{C}$  (Antoine eq. for liquid state, Dreisbach 1961)  
 57390 (calculated-Antoine eq., temp range  $-70$  to  $40.7^{\circ}\text{C}$ , Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 7572.3/(T/\text{K})] + 8.18330$ ; temp range  $-70$  to  $40.7^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)  
 58275, 57270 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log(P/\text{mmHg}) = 9.72567 - 2979.516/(395.553 + t/^{\circ}\text{C})$ ; temp range  $30$ – $40^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 48200 ( $20^{\circ}\text{C}$ , McConnell et al. 1975; Pearson & McConnell 1975)  
 21065, 57062 ( $1.5$ ,  $25^{\circ}\text{C}$ , Dow Chemicals data, Dilling 1977)  
 57950, 57980 (calculated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 5.96841 - 1014.441/(216.227 + t/^{\circ}\text{C})$ ; temp range  $30$ – $40^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.18791 - 1127.232/(229.764 + t/^{\circ}\text{C})$ ; temp range  $-9.05$  to  $38.4^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 47990 (selected, Daniels et al. 1985)  
 $\log(P/\text{mmHg}) = 7.4092 - 1325.9/(252.6 + t/^{\circ}\text{C})$ ; temp range  $-40$  to  $40^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)  
 58100 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 6.07622 - 1070.07/(223.24 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 57990 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_1/\text{kPa}) = 6.18649 - 1126.53/(-43.46 + T/\text{K})$ ; temp range  $264$ – $312$  K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_1/\text{kPa}) = 6.88926 - 1545.323/(3.375 + T/\text{K})$ ; temp range  $311$ – $383$  K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log(P_1/\text{kPa}) = 5.87285 - 861.817/(-94.102 + T/\text{K})$ ; temp range  $379$ – $455$  K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log(P_1/\text{kPa}) = 5.20540 - 449.586/(-193.701 + T/\text{K})$ ; temp range  $450$ – $510$  K (Antoine eq., Stephenson & Malanowski 1987)  
 47660, 71000, 85640, 102540 ( $20$ ,  $30$ ,  $35$ ,  $40^{\circ}\text{C}$ , quoted from DIPPR, Tse et al. 1992)  
 $\log(P/\text{mmHg}) = 32.5069 - 2.5166 \times 10^3/(T/\text{K}) - 8.8015 \cdot \log(T/\text{K}) + 1.2934 \times 10^{-10} \cdot (T/\text{K}) + 3.3194 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
 temp range  $178$ – $510$  K (vapor pressure eq., Yaws 1994)  
 57844 (selected summary of literature data, temp range  $178.25$ – $338.15$  K, Xiang 2002)  
 70486 ( $30^{\circ}\text{C}$ , vapor-liquid equilibrium study, Pathare et al. 2004)

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

- 231.3 (calculated as  $1/K_{\text{AW}} \cdot C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)  
 301.0 (McConnell et al. 1975; Pearson & McConnell 1975)  
 322.3 (calculated, Neely 1976)  
 292, 271.5 (exptl., calculated- $C_{\text{A}}/C_{\text{W}}$ , Dilling 1977)  
 111.3 ( $20^{\circ}\text{C}$ , calculated- $P/C$ , Kavanaugh & Trussell 1980)  
 $\log(k_{\text{H}}/\text{atm}) = 7.92 - 1821.84/(T/\text{K})$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)  
 295 (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)  
 295\* ( $24.9^{\circ}\text{C}$  equilibrium cell-concn ratio-GC/FID, measured range  $1.9$ – $24.9^{\circ}\text{C}$  Leighton & Calo 1981)  
 $\ln(k_{\text{H}}/\text{atm}) = 17.42 - 3645/(T/\text{K})$ ; temp range  $1.9$ – $24.9^{\circ}\text{C}$  (equilibrium cell-concn ratio measurements, Leighton & Calo 1981)  
 205.7 (calculated- $P/C$ , Mabey et al. 1982)  
 303.9 (calculated- $P/C$ , Thomas 1982)  
 229.1 ( $20^{\circ}\text{C}$ , EPICS-GC, Lincoff & Gossett 1983)  
 227.9 ( $20^{\circ}\text{C}$ , EPICS-GC, Lincoff & Gossett 1984)

- 199.6 (20°C, batch air stripping-GC, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 8.200 - 4191/(T/K)$ ; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.035 - 4472/(T/K)$ ; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)  
 222.0 (EPICS-GC, Gossett 1987)  
 173.0\* (20°C, EPICS-GC/FID, measured range 9.6–34.6°C, Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.843 - 5612/(T/K)$ ; temp range: 9.6–34.6°C (EPICS measurements, Gossett 1987)  
 187.7 (20°C, EPICS, Yurteri et al. 1987)  
 323 (gas stripping-GC, Warner et al. 1987)  
 300\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm-m}^3/\text{mol})] = 8.483 - 4268/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 451.1 (calculated-QSAR, Nirmalakhandan & Speece 1988)  
 202.6 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 254.4 (calculated-P/C, Suntio et al. 1988)  
 251 (computed value, Yaws et al. 1991)  
 213, 314, 375, 456 (20, 30, 35, 40°C, infinite dilution activity coeff.  $\gamma^\circ$ -GC, Tse et al. 1992)  
 128, 209, 308 (10, 20, 30°C, activity coeff.  $\gamma^\circ$ -differential pressure transducer, Wright et al. 1992)  
 266 ( $\gamma^\circ$  from gas stripping-GC, Li et al. 1993)  
 16.72, 26.04 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 197 (20°C, inert gas stripping-GC, Hovorka & Dohnal 1997)  
 244.1 (modified EPICS method-GC, Ryu & Park 1999)  
 260; 221; 211 (EPICS-GC; quoted lit.; calculated-P/C, David et al. 2000)  
 220 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 4.561 - 1644/(T/K)$  (summary of literature 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:

- 1.25 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)  
 1.51 (Hansch & Leo 1979)  
 1.22 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)  
 1.25 (HPLC- $k'$  correlation, Tomlinson & Hafkenscheid 1986)  
 1.25 (recommended, Sangster 1989)  
 1.35\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)  
 1.25 (recommended, Hansch et al. 1995)  
 1.25 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

- 2.27 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 0.699 (calculated as per Lyman et al. 1982, Howard 1990)  
 0.778 (microorganism-water, calculated from  $K_{OW}$ , Mabey et al. 1982)  
 0.600 (calculated-MCI  $\chi$ , Koch 1983)  
 0.362 (selected, Daniels et al. 1985)

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

- 0.944 (calculated- $K_{OW}$ , Mabey et al. 1982)  
 1.440 (calculated- MCI  $\chi$ , Koch 1983; quoted, Bahnick & Doucette 1988)  
 1.000 (selected, Daniels et al. 1985)  
 1.390 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)

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

- 1.44, 1.23 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)



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

- Volatilization:  $t_{1/2}(\text{calc}) = 2.23$  min (Mackay & Wolkoff 1973; quoted, Dilling et al. 1975; Callahan et al. 1979);  
 $t_{1/2}(\text{calc}) = 20.7$  min (Mackay & Leinonen 1975; quoted, Dilling 1977; Callahan et al. 1979);  
 $t_{1/2}(\text{exptl}) = (21 \pm 3)$  min for 1 ppm in water at 25°C when stirred at 200 rpm in water (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);  
 evaporation  $t_{1/2}(\text{exptl}) = (18.3\text{--}25.2)$  min,  $t_{1/2}(\text{calc}) = 2.23$  and 20.7 min at 25°C and  $t_{1/2}(\text{exptl.}) = 34.9$  min,  $t_{1/2} = 24.5$  min at 1.5°C (Dilling 1977)  
 $t_{1/2} \sim 3.0$  h from water (estimated, Thomas 1982);  
 $t_{1/2} \sim 100$  d from soil (estimated, Jury et al. 1990).
- Photolysis: estimated photodecomposition  $t_{1/2} > 250$  h from a simulated environmental sunlight exposure ( $> 290$  nm at  $27 \pm 1^\circ\text{C}$ ) study (Dilling et al. 1976; quoted, Callahan et al. 1979);  
 photodegradation  $t_{1/2} = 30\text{--}120$  d (Darnall et al. 1976; quoted, Daniels et al. 1985);  
 photocatalyzed mineralization by the presence of  $\text{TiO}_2$  with a rate of 1.6 ppm/min per gram of catalyst (Ollis 1985).
- 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:  
 $k_{\text{OH}} = 1.24 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K corresponding to a lifetime of 0.30 yr (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)  
 $k_{\text{OH}}^* = (1.16 \pm 0.05) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K with lifetime of 0.39 yr, measured range 245–375 K (flash photolysis-resonance fluorescence, Davis et al. 1976)  
 $k_{\text{OH}} = 1.55 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (discharge flow-LMR, Howard & Evenson 1976a)  
 $k_{\text{OH}} = (14.5 \pm 2.0) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298.5 K and the calculated tropospheric half-life of  $\sim 0.05$  yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)  
 $k_{\text{OH}} = 1.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 77 d, loss of 1.3% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)  
 $k_{\text{OH}}^* = 1.53 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 292 K, measured range 251–455 K (discharge flow-resonance fluorescence, Jeong & Karfman 1982)  
 $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $0.2 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)  
 $k \leq 0.1 \text{ M}^{-1} \text{ s}^{-1}$  for reaction with  $\text{O}_3$  in water as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)  
 photooxidation  $t_{1/2} = 458\text{--}4584$  h based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)  
 $k = 4.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$  with reference to  $\text{CH}_3\text{CCl}_3$  (Buxton et al. 1988; quoted, Haag & Yao 1992)  
 $k_{\text{OH}} = 1.42 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k(\text{soln}) = 9.6 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with OH radical in aqueous solution (Wallington et al. 1988b)  
 $k_{\text{OH}}^* = 1.42 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)  
 $k_{\text{OH}}^* = 1.76 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K, measured range 298–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)  
 $k = (9 \pm 6) \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$  for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)
- Hydrolysis: a minimum hydrolysis  $t_{1/2} = 18$  months was estimated from aqueous reactivity experiments (Dilling et al. 1975; quoted, Callahan et al. 1979; Howard 1990);  
 rate constant  $k = 3.2 \times 10^{-11} \text{ s}^{-1}$  with a maximum  $t_{1/2} = 704$  yr for hydrolysis at pH 7 and 25°C was reported from the extrapolated experimental data obtained at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)  
 $t_{1/2} = 260000$  d in natural waters at pH 7 (Capel & Larson 1995)
- Biodegradation: completely biodegradable under aerobic conditions with sewage seed or activated sludge between 6 h to 7 d (Rittman & McCarty 1980; Davis et al. 1981; Tabak et al. 1981; Klecka 1982; Stover & Kincannon 1983; quoted, Howard 1990)  
 $t_{1/2}(\text{aq. aerobic}) = 168\text{--}672$  h based on unacclimated aerobic screening test data (Kawasaki 1980; Tabak et al. 1981; quoted, Howard et al. 1991);  $t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688$  h based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).  
 $t_{1/2}(\text{aerobic}) = 7$  d,  $t_{1/2}(\text{anaerobic}) = 28$  d in natural waters (Capel & Larson 1995)
- Biotransformation:  
 Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

## Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 33$  wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} = 2.4$ –24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)

lifetime of 4.4 yr in troposphere for the reaction with OH radical (Altshuller 1980)

estimated disappearance time to be 12 h to 1.0 year in simulated troposphere chamber (Dilling & Goersch 1979; quoted, Lyman 1982)

residence time of 77 d, loss of 1.3% in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

estimated residence time in troposphere to be 160–250 d (Lyman 1982);

$t_{1/2} = 458$ –4584 h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991)

Surface water: estimated  $t_{1/2} = 33$ –38 d in various locations in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

biodegradation  $t_{1/2}$ (aerobic) = 100 d,  $t_{1/2}$ (anaerobic) = 400 d, hydrolysis  $t_{1/2} = 3800$  d at pH 7 in natural waters (Capel & Larson 1995)

$t_{1/2} = 1$ –1.2 d for the first days up to 4 d and 2.71–2.80 d for a period of up to 14 d for disappearance from water calculated from a pseudo first order equation of mesocosms experiment (Merlin et al. 1992)

Ground water: estimated for the first days up to 4 d and  $t_{1/2} = 2.71$ –2.80 d for a period of up to 14 d of 10 yr in the ground water of The Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 336$ –1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

## Sediment:

Soil:  $t_{1/2} = 10$ –50 d (Ryan et al. 1988);

volatilization  $t_{1/2} \sim 100$  d from soil (Jury et al. 1990);

biodegradation  $t_{1/2}$ (aerobic) = 1.3 d (0.16 ppm, conc of dichloromethane),  $t_{1/2} = 9.4$  d (0.5 ppm),  $t_{1/2} = 191.4$  d (5 ppm), all in sandy loam soil;  $t_{1/2} = 54.8$  d in sand (0.5 ppm);  $t_{1/2} = 12.7$  d (0.5 ppm) in sandy clay loam soil;  $t_{1/2} = 7.2$  d (0.5 ppm) in clay with 50 d lag and  $t_{1/2}$ (anaerobic) = 21.5 d (5 ppm) with 70 d lag (Davis & Madsen 1991);

$t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:  $t_{1/2} = 10$ –50 d, subject to plant uptake in soil via volatilization (Ryan et al. 1988);

$t_{1/2} = 0.4$ –0.5 d to eliminate from small fish (McCarty et al. 1992).

TABLE 5.1.1.2.1

## Reported aqueous solubilities of dichloromethane at various temperatures

$$S/(\text{wt}\%) = 1.961 - 4.4883 \times 10^{-2} \cdot (t/^\circ\text{C}) + 8.6617 \times 10^{-4} \cdot (t/^\circ\text{C})^2 + 4.9463 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

1.

Rex 1906		Andelman 1978		Horvath 1982		Stephenson 1992	
volumetric method				summary of literature data		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>
0	23630	0	23100	0	19610	0	20300
10	21220	10	20800	10	15938	9.2	19200
20	20000	20	19600	20	13702	17.3	18000
30	19690	25	20000	25	13030	26.8	17200
		30	19000	30	12605	35.7	17700
				40	12350		
				50	12640		
				eq.1	S/wt%		

TABLE 5.1.1.2.1 (Continued)

2.

Tse et al. 1992		Wright et al. 1992	
activity coefficient -GC		activity coefficient	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
20	19260	10	20080
30	19830	20	18880
35	19500	30	18880
40	19500		

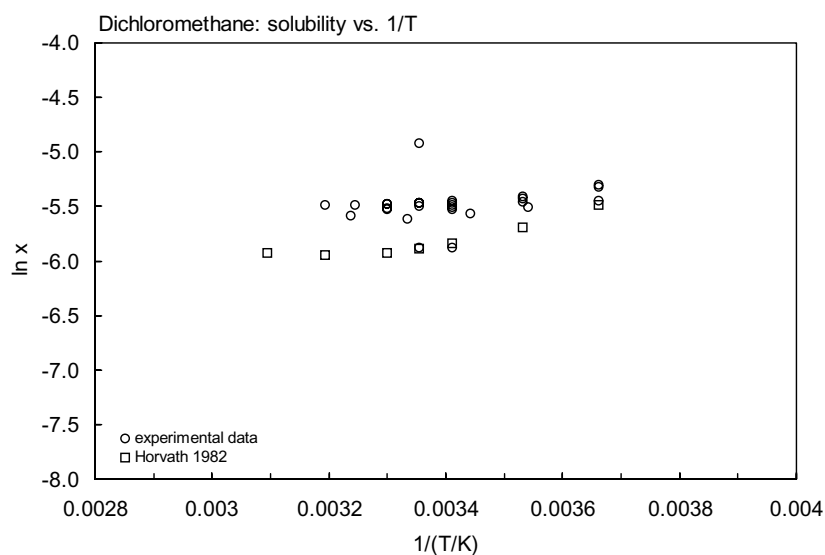
FIGURE 5.1.1.2.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.2

Reported vapor pressures of dichloromethane 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)		

Stull 1947		Mueller & Ignatowski 1960		Boublik 1960, thesis	
summary of literature data				in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-70.0	133.3	29.993	70530	-9.03	12046
-52.1	666.6	34.993	85175	-5.45	14549
-43.3	1333	38.993	98070	-1.322	17921
-33.4	2666	39.993	102117	2.228	21314
-22.3	5333			6.230	25780
-15.7	7999			9.457	29923
-6.30	13332			13.289	35493

(Continued)

TABLE 5.1.1.2.2 (Continued)

Stull 1947		Mueller & Ignatowski 1960		Boublik 1960, thesis	
summary of literature data				in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
8.0	26664			16.693	41470
24.1	53329			21.199	49704
40.7	101325			26.393	61295
				32.337	77123
mp/°C	-96.7			39.429	96484
				eq. 2	P/kPa
				A	6.18791
				B	127.232
				C	229.764
				bp	39.767

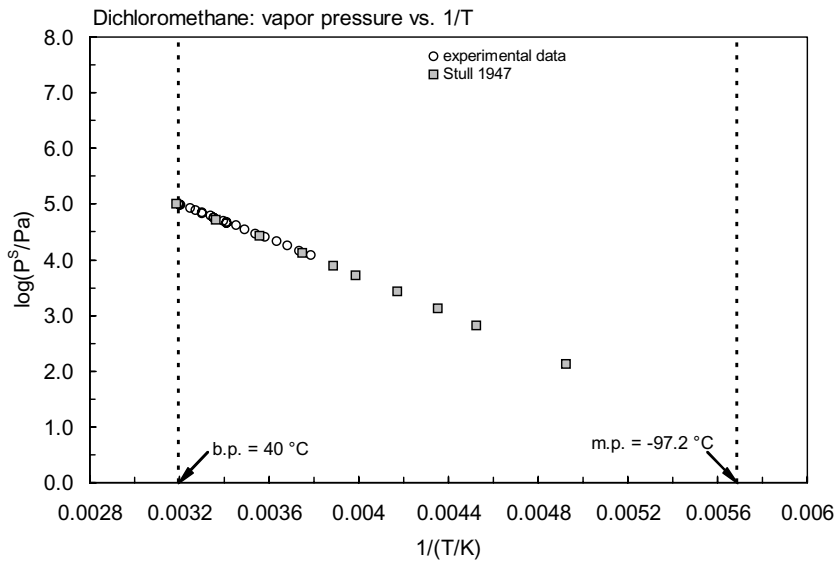


FIGURE 5.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.3  
Reported Henry’s law constants of dichloromethane 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)				
$\ln (k_H/atm) = A - B/(T/K)$	(3)						
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)				
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)						
<b>Leighton &amp; Calo 1981</b>	<b>Gossett 1987</b>	<b>Ashworth et al. 1988</b>	<b>Tse et al. 1992</b>				
<b>equilibrium cell-GC</b>	<b>EPICS-GC</b>	<b>EPICS-GC</b>	<b>activity coefficient</b>				
<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>
1.9	112	9.6	116.5	10	142	20	213
13.5	203	17.5	132.7	15	171	30	314
15.7	222	24.8	221.9	20	247	35	375
22.0	286.5	34.6	330.3	25	300	40	456
24.9	295			30	366		
25	295.3	eq. 4	H/(atm m³/mol)				
		A	6.653	eq. 4	H/(atm m³/mol)	<b>Wright et al. 1992</b>	
eq. 3	k <sub>H</sub> /atm	B	4215	A	8.483	<b>activity coefficient</b>	
A	17.42			B	4268		
B	3645					10	128
						20	209
						30	308

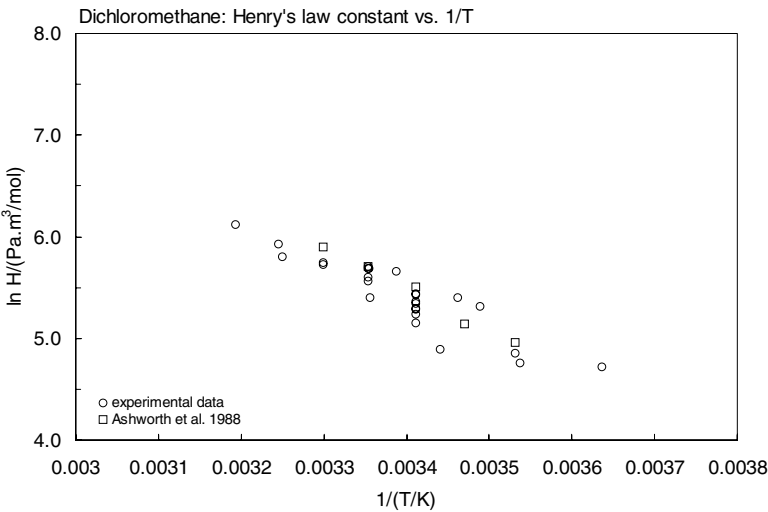
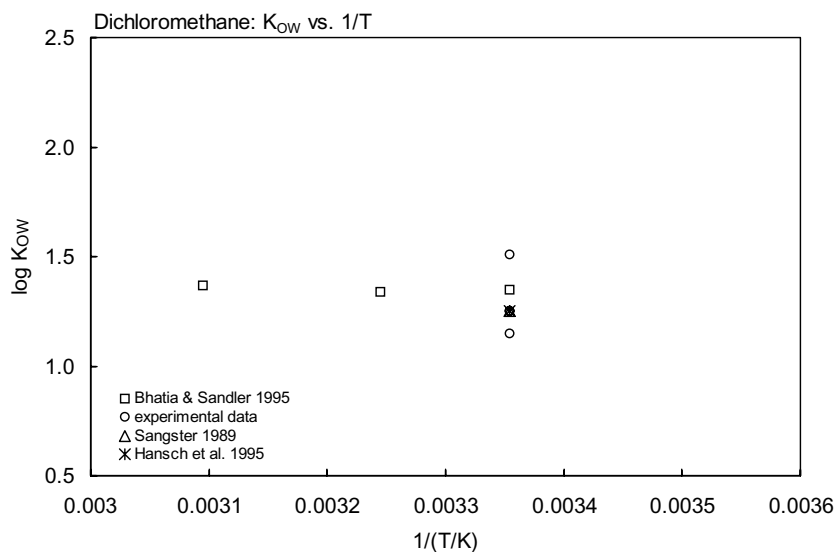


FIGURE 5.1.1.2.3 Logarithm of Henry’s law constant versus reciprocal temperature for dichloromethane.

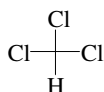
**TABLE 5.1.1.2.4**  
**Reported octanol-water partition coefficients of dichloromethane**  
**at various temperatures**

Bhatia & Sandler 1995	
relative GC-RT technique	
t/°C	log K <sub>OW</sub>
25	1.35
35	1.34
50	1.37
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$	
$\log K_{OW} = A - \Delta H/2.303RT$	
A	1.0195
$\Delta H$	-20.2



**FIGURE 5.1.1.2.4** Logarithm of K<sub>OW</sub> versus reciprocal temperature for dichloromethane.

## 5.1.1.3 Trichloromethane (Chloroform)



Common Name: Trichloromethane

Synonym: chloroform, trichloromethaneq

Chemical Name: trichloromethane

CAS Registry No: 67-66-3

Molecular Formula:  $\text{CHCl}_3$ 

Molecular Weight: 119.378

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

-63.41 (Lide 2003)

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

61.17 (Lide 2003)

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

1.4832 (Dreisbach 1961; Horvath 1982; Weast 1982-83)

1.49845, 1.48911, 1.47970 (15, 20,  $25^{\circ}\text{C}$ , Riddick et al. 1986)Molar Volume ( $\text{cm}^3/\text{mol}$ ):

80.0 (calculated-density, Mailhot 1987; Wang et al. 1992)

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

Enthalpy of Vaporization,  $\Delta H_v$  ( $\text{kJ}/\text{mol}$ ):33.35, 29.37 ( $25^{\circ}\text{C}$ , bp, Riddick et al. 1986)Enthalpy of Fusion,  $\Delta H_{\text{fus}}$  ( $\text{kJ}/\text{mol}$ )

8.80 (calculated, Dreisbach 1959)

9.54 (quoted, Riddick et al. 1986)

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  $25^{\circ}\text{C}$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

8220, 7760 ( $20^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , volumetric method, Rex 1906)8520, 7710 (15,  $30^{\circ}\text{C}$ , shake flask-interferometer, Gross & Saylor 1931)

8000 (Wright &amp; Schaffer 1932)

7361 (Seidell 1940)

7700 (Seidell 1941)

7900 (data presented from  $0$ – $50^{\circ}\text{C}$  in graph, McGovern 1943)

13320 (shake flask-residue volume method, Booth &amp; Everson 1948)

8000 ( $20^{\circ}\text{C}$ , Stephen & Stephen 1963)8150 ( $20^{\circ}\text{C}$ , Riddick & Bunger 1970)8200 ( $20^{\circ}\text{C}$ , Pearson & McConnell 1975)8000 ( $20^{\circ}\text{C}$ , Neely 1976; Verschueren 1977)10300, 7840 (1.5,  $25^{\circ}\text{C}$ , selected, Dilling 1977)

7230 (shake flask-LSC, Banerjee et al. 1980)

11900 (shake flask-titration/turbidity, Coca et al. 1980)

7360 (shake flask-LSC, Veith et al. 1980)

7920\* (summary of literature data, temp range  $0$ – $60^{\circ}\text{C}$ , Horvath 1982)2525 ( $30^{\circ}\text{C}$ , headspace-GC, McNally & Grob 1984)

7190 (calculated-UNIFAC activity coeff., Banerjee 1985)

8200 (shake flask-radiometric method, Lo et al. 1986)

8150 ( $20^{\circ}\text{C}$ , selected, Riddick et al. 1986)8080, 7435, 7290 (20, 35,  $50^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Barr & Newsham 1987)8670 ( $23$ – $24^{\circ}\text{C}$ , shake flask-GC, Broholm et al. 1992)8200\*, 7900 ( $19.6^{\circ}\text{C}$ ,  $29.5^{\circ}\text{C}$ , shake flask-GC/TC, measured range  $0$ – $59.2^{\circ}\text{C}$ , Stephenson 1992)

7280, 8118, 8558, 9011 (20, 30, 35, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -UNIFAC, Tse et al. 1992)  
 8108, 7030, 7694 (20, 35, 50°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 7345 (gas stripping-GC, Li et al. 1993)  
 8098 (20°C, activity coeff. by inert air stripping-GC, Hovorka & Dohnal 1997)

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):

21115, 31990 (20°C, 30°C, Rex 1906)  
 39345\* (35.0°C, vapor-liquid equilibrium, measured range 35.0–60.0°C, Scatchard & Raymond 1938)  
 26660 (interpolated from graph, temp range –30 to 170°C, McGovern 1943)  
 25700\* (interpolated-Antoine eq. regression, temp range –58.0 to 61.3°C, Stull 1947)  
 26310 (calculated-Antoine eq., Dreisbach 1959)  
 $\log(P/\text{mmHg}) = 6.90328 - 1163.0/(227.0 + t/^\circ\text{C})$ ; temp range –15 to 90°C (Antoine eq. for liquid state, Dreisbach 1959)  
 $\log(P/\text{mmHg}) = 6.93708 - 1171.2/(227.0 + t/^\circ\text{C})$ ; temp range –13 to 97°C (Antoine eq. for liquid state, Dreisbach 1961)  
 25780\* (24.598°C, temp range –10.356 to 60.319°C, Boublik & Aim 1972; quoted, Boublik et al 1984)  
 23080 (interpolated from Antoine eq., temp range –58 to 254°C, Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 7500.5/(T/K)] + 7.735083$ ; temp range –58 to 254°C (Antoine eq., Weast 1972–73)  
 26240, 18950 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log(P/\text{mmHg}) = 6.85465 - 1170.966/(226.252 + t/^\circ\text{C})$ ; temp range (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 $\log(P/\text{mmHg}) = 6.4934 - 959.444/(196.03 + t/^\circ\text{C})$ ; temp range (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 26217, 26104 (static method-differential pressure gauge, Bissell & Williamson 1975)  
 20000 (20°C, Pearson & McConnell 1975)  
 25590 (literature average, Dilling 1977)  
 21330 (20°C, Verschueren 1983)  
 26220, 32080 (calculated-Antoine eq., Boublik et al. 1984)  
 21330 (20°C, quoted, McNally & Grob 1984)  
 $\log(P/\text{mmHg}) = 6.4934 - 929.44/(196.03 + t/^\circ\text{C})$ ; temp range –36 to 61°C (Antoine eq., Dean 1985, 1992)  
 25970 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 5.96288 - 1106.94/(218.552 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 26220 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.07853 - 1170.42/(-46.98 + T/K)$ ; temp range 262–334 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 5.38327 - 948.979/(-61.73 + T/K)$ ; temp range 227–269 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.11152 - 1173.606/(-48.54 + T/K)$ ; temp range 333–416 K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 7.89882 - 2879.244/(-161.978 + T/K)$ ; temp range 410–481 K (Antoine eq.-IV, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 4.58922 - 181.802/(-325.74 + T/K)$ ; temp range 479–523 K (Antoine eq.-V, Stephenson & Malanowski 1987)  
 $\log(P/\text{mmHg}) = 56.6178 - 3.2462 \times 10^3/(T/K) - 18.7 \cdot \log(T/K) + 9.515 \times 10^{-3} \cdot (T/K) + 1.1553 \times 10^{-12} \cdot (T/K)^2$ ; temp range 210–536 K (vapor pressure eq., Yaws 1994)  
 26182 (selected summary of literature data, temp range 209.64–368.15 K, Xiang 2002)  
 32408 (30°C, vapor-liquid equilibrium VLE data, Pathare et al. 2004)

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):

314.1 (20°C, Dilling et al. 1975)  
 440.8 (calculated as  $1/K_{AW}$ ,  $C_W/C_A$ , Hine & Mookerjee 1975)  
 283.4 (20°C, McConnell et al. 1975; Pearson & McConell 1975)  
 310 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)



- $\log (k_H/\text{atm}) = 9.10 - 2103.09/(T/K)$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)  
 373\* (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)  
 $\ln (k_H/\text{atm}) = 18.97 - 4046/(T/K)$ ; temp range 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 292.0 (20°C, calculated-P/C, Mabey et al. 1982; Mills et al. 1982)  
 536.9 (batch stripping-GC, Munz & Roberts 1982; Roberts & Dändliker 1983; Roberts et al. 1985)  
 432.2 (calculated-UNIFAC activity coeff., Arbuckle 1983)  
 $\ln K_{AW} = 10.63 - 3649/(T/K)$ ; measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith et al. 1983)  
 298 (calculated-P/C, Jury et al. 1984; Jury et al. 1990)  
 337.4; 308 (20°C, EPICS-GC; batch air stripping-headspace GC, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 8.553 - 4180/(T/K)$ ; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 8.956 - 4322/(T/K)$ , temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)  
 304; 314; 486, 365 (20°C, batch air stripping-GC; calculated-P/C; quoted lit. values, Nicholson et al. 1984)  
 334, 294, 314 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 11.90 - 5200/(T/K)$ ; temp range 10–30°C (air stripping-GC, Nicholson et al. 1984)  
 343.4 (adsorption isotherm, Urano & Murata 1985)  
 372\* (EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.843 - 4612/(T/K)$ ; temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)  
 334 (EPICS-GC, Munz & Roberts 1987)  
 $\log K_{AW} = 4.990 - 1729/(T/K)$ , temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)  
 343 (gas stripping-GC, Warner et al. 1987)  
 427; 387; 372; 374; 399 (EPICS-GC; calculated-P/C; EPICS; direct concn ratio; calculated-UNIFAC activity coefficient, Ashworth et al. 1988)  
 427\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 11.41 - 5030/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 294 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 318 (calculated-P/C, Suntio et al. 1988; Mackay & Shiu 1990)  
 411 (computed value, Yaws et al. 1991)  
 199.3\* (26.5°C, tap water, EPICS-GC, measured range 26.5–47.2°C, Tancrede & Yanagisawa 1990)  
 $\log K_{AW} = 9.154 - 3051/(T/K)$ ; temp range 26.5–47.2°C (EPICS measurements, Tancrede & Yanagisawa 1990)  
 306, 592, 1046 (20, 35, 50°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 362 (activity coefficient  $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)  
 514, 513 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 379\* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)  
 177, 444 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)  
 $\ln K_{AW} = -4142/(T/K) + 0.00588 \cdot Z + 12.012$ ; with Z salinity of 0–35.5‰ and temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)  
 212, 341 (10, 20°C, gas stripping-GC, Moore et al. 1995)  
 126, 214, 352 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)  
 $\ln K_{AW} = 11.17 - 3840/(T/K)$ ; seawater of salinity of 30.4‰, temp range: 0–20°C (Moore et al. 1995)  
 261, 451 (15, 25°C, vapor liquid equilibrium-GC, Turner et al. 1996)  
 $K_{AW} = 0.0394 + 0.00486 \cdot (T/K)$ ; temp range 0–60°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)  
 312 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)  
 331.2 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 370.8 (modified EPICS method-GC, Ryu & Park 1999)  
 411; 260 (EPICS-GC; calculated-P/C, David et al. 2000)  
 307 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 5.343 - 1830/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)  
 704.5 (37°C, equilibrium headspace-GC, Batterman et al. 2002)  
 408\* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)  
 $\ln K_{AW} = 10.96 - 3821.3/(T/K)$ ; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

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:

- 1.97 (Hansch & Anderson 1967)
- 1.97 (shake flask-UV, Hansch et al. 1968; Leo et al. 1971; Hansch et al. 1975)
- 1.94 (Hansch & Leo 1979)
- 1.90 (shake flask-LSC, Banerjee et al. 1980)
- 1.90 (shake flask-LSC, Veith et al. 1980)
- 1.81 (HPLC- $k'$  correlation, McDuffie 1981)
- 2.15 (HPLC- $k'$  correlation, Wells et al. 1981)
- 1.91 (calculated-UNIFAC activity coeff., Arbuckle 1983)
- 1.90 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)
- 2.14, 2.13, 2.03 (HPLC- $k'$  correlation, Tomlinson & Hafkenscheid 1986)
- 1.66 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
- 1.97 (recommended, Sangster 1989)
- 2.00\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
- 1.86\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

- 2.80 (equilibrium head-space-GC, Abraham et al. 2001)
- 2.55; 2.53 (equilibrium headspace-GC; calculated- $K_{OW}/K_{AW}$ , Batterman et al. 2002)

Bioconcentration Factor,  $\log BCF$ :

- 0.92 (calculate- $K_{OW}$ , Veith et al. 1979; quoted, Veith et al. 1980)
- 0.78 (bluegill sunfish, Barrows et al. 1980; Bysshe 1982)
- 0.78 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982; quoted, Davies & Dobbs 1984; Suntio et al. 1988; Isnard & Lambert 1988; Saito et al. 1992)
- 0.63 (calculated- $K_{OW}$ , Mackay 1982)
- 1.41 (microorganisms-water, calculated from  $K_{OW}$ , Mabey et al. 1982)
- 0.97 (calculated-MCI  $\chi$ , Koch 1983)
- 0.78 (bluegill sunfish, LSC, Davies & Dobbs 1984)
- 2.84 (green algae, Mailhot 1987)
- 2.84 (*Selenastrum capricornutum*, Mailhot 1987)
- 0.52–1.01; 0.204–0.40; 0.46–0.49; 0.552–0.57 (rainbow trout; bluegill sunfish; large mouth bass; catfish, Howard 1990)

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

- 1.64 (calculated- $K_{OW}$ , Mabey et al. 1982)
- 1.65 (calculated-MCI  $\chi$ , Koch 1983)
- 2.15 (wastewater solids with correlation to  $K_{OW}$ , Dobbs et al. 1989)
- 1.44 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
- 1.98 (20°C, weathered shale, mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 2.79 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 1.85, 1.92 (20°C, calculated- $K_{OW}$ , Grathwohl 1990)
- 1.53 (soil, Howard 1990)
- 1.46 (selected, Jury et al. 1990)
- 1.57; 1.46; 1.54 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 1.63, 1.65, 1.63, 1.66, 1.69, 1.65, 1.70 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)

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

- 1.65, 1.40 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)

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

Volatilization: calculated  $t_{1/2} = 1.4$  min (Mackay & Wolkoff 1973);

primary transport process from the aquatic environment with  $t_{1/2} = 21$ –26 min at pH 7 and 25°C stirred at 200 rpm in an open container (Dilling et al. 1975)

evaporation rate  $k(\text{exptl}) = 13.2 \times 10^{-5} \text{ g cm}^{-2} \text{ s}^{-1}$  to still air (Chiou & Freed 1977; Chiou et al. 1980)

evaporation  $t_{1/2}(\text{exptl}) = (8.5\text{--}25.7)$  min,  $t_{1/2}(\text{calc}) = 1.46, 2.37$  min at 20–25°C,  $t_{1/2}(\text{exptl}) = 34.6$  min at 1.5°C (Dilling 1977)

$t_{1/2} = 3$ –5.6 h for different laboratory studies of evaporation from water with moderate mixing conditions (Smith et al. 1980; Rathbun & Tai 1981; Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} = 1.2$  d in Rhine River and  $t_{1/2} = 31$  d in a lake in Rhine Basin. (Zoeteman et al. 1980).

$t_{1/2} \sim 3.7$  h from water (estimated, Thomas 1982);

$t_{1/2} = 29$  min–11.3 d from rivers and streams, calculated using published  $\text{O}_2$  reaeration values; and  $t_{1/2}(\text{calc}) = 31.2$  h from rivers and streams, calculated using estimated  $\text{O}_2$  reaeration rate constant (Kaczmar et al. 1984);

predicted  $t_{1/2} = 36$  h in a river,  $t_{1/2} = 40$  h in a pond and  $t_{1/2} = 9$ –10 d in a lake (USEPA 1984; quoted, Howard 1990);

$t_{1/2} = 4$  h at 20°C was predicted from a model river of 1 m deep at flowing speed of 1 m/s with a wind velocity of 3 m/s and its Henry's law constant (Smith et al. 1980; quoted, Howard 1990);

Photolysis: not important only by UV in the stratosphere (Robbins 1976);

probably not significant in aquatic systems (Callahan et al. 1979);

photocatalyzed mineralization by the presence of  $\text{TiO}_2$  with a rate of  $4.4 \text{ ppm min}^{-1} \text{ g}^{-1}$  of catalyst (Ollis 1985).

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:

$k_{\text{OH}} = 1.01 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{\text{OH}}^* = 1.14 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  at 298 K with lifetime of 0.56 yr, measured range 245–375 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altshuller 1980)

troposphere with  $t_{1/2} = 0.19$ –0.32 yr due to reaction with OH radical (Callahan et al. 1979)

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

$k_{\text{OH}}^* = 1.01 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 249–487 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1982)

$k_{\text{OH}} = 6.6 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  of estimated at 300 K (Lyman 1982)

$t_{1/2} = 78.5$ –3140 yr from the rate constant for the reaction with OH radical (estimated, Dorfman & Adams 1973)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $0.7 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical both at 25°C (Mabey et al. 1982)

$k \leq 0.1 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

photooxidation  $t_{1/2} = 26$ –260 d, based on measured data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k = 4.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$  with reference to  $\text{CH}_3\text{CCl}_3$  (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{\text{OH}} = 1.03 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k(\text{soln}) = 1.8 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}^* = 1.03 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K, measured range 295–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

$k = (5.4 \pm 3.0) \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

$k_{\text{OH}}^* = 1.03 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

Hydrolysis: first-order rate constant  $k = 0.045 \text{ mo}^{-1}$  with  $t_{1/2} \sim 15$  months (Dilling et al. 1975; quoted, Callahan et al. 1979);

$k = 6.9 \times 10^{-12} \text{ s}^{-1}$  (Radding 1976);

hydrolysis rate constant  $k = 6.9 \times 10^{-12} \text{ s}^{-1}$  with  $t_{1/2} = 3500$  yr at 25°C and pH 7 (Mabey & Mill 1978)

no hydrolysis in acidic aqueous solutions, and rate constant in alkaline aqueous solution,  $k = 0.23 \text{ M}^{-1} \text{ h}^{-1}$  at 25°C, and  $k = 2.5 \times 10^{-9} \text{ M}^{-1} \text{ h}^{-1}$  at 25°C in neutral aqueous solutions (Mabey & Mill 1978; Mabey et al. 1982; Mills et al. 1982);

probably not a significant fate process with  $t_{1/2} = 3500$  yr, based on reported rate constant  $k = 6.9 \times 10^{-12} \text{ s}^{-1}$  at pH 7 and  $25^\circ\text{C}$  (Mabey & Mill 1978; quoted, Callahan et al. 1979; Haque et al. 1980).

Biodegradation: very slow by BOD bottle experiments (Pearson & McConnell 1975);

$t_{1/2}(\text{aq. aerobic}) = 4$  wk to 6 months by unacclimated screening tests (Kawasaki 1980; Flathman & Dahlgran 1982; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 1\text{--}4$  wk by unacclimated anaerobic screening tests (Bouwer et al. 1981; Bouwer & McCarty 1983; quoted, Howard et al. 1991);

$k = 0.5 \text{ d}^{-1}$  (Tabak et al. 1981; Mills et al. 1982).

Bioaccumulation: weak to moderate bioaccumulation; no evidence of biomagnification of trichloromethane in marine food chain (Callahan et al. 1979).

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

#### Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 23$  wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

residence time of 1.7 yr in troposphere, based on one compartment nonsteady state model (Singh et al. 1978; quoted, Lyman 1982);

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

estimated residence time in N. troposphere to be 100 d (Lyman 1982);

$t_{1/2} = 623\text{--}6231$  h, based on photooxidation half-life in air from measured reaction data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

tropospheric lifetime  $\sim 0.17$  yr (estimated, Nimitz & Skaggs 1992)

lifetime for reaction with OH radicals,  $\tau = 3.0$  yr for Polar region,  $\tau = 0.6$  yr for Middle region and  $\tau = 0.2$  yr for Tropical region in the Northern hemisphere;  $\tau = 0.3$  yr for Tropical,  $\tau = 1.0$  yr for Middle and  $\tau = 3.2$  yr for Polar region in the Southern hemisphere;  $\tau = 0.5$  yr in the Global atmosphere, based on data from 1985–1996 (Khalil & Rasmussen 1999b)

Surface water: not important for aqueous phase (Dilling et al. 1975);

$t_{1/2} = 1.0\text{--}31$  d in various location in the Netherlands in case of a first order reduction process (estimated, Zoeteman et al. 1980)

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

Ground water:  $t_{1/2} = 1344\text{--}43200$  h, based on unacclimated aqueous aerobic biodegradation and grab sample data of aerobic soil from a ground water aquifer (Wilson et al. 1983; quoted, Howard et al. 1991).

Soil:  $t_{1/2} = 10\text{--}50$  d (Ryan et al. 1988);

$t_{1/2} = 100$  d, estimated volatilization loss from soil (Jury et al. 1990)

disappearance  $t_{1/2} = 4.1$  d was calculated from first order kinetic for volatilization loss from soil mixtures (Anderson et al. 1991);

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

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

$t_{1/2} = 10\text{--}50$  d, subject plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.3.1

Reported aqueous solubilities of trichloromethane at various temperatures

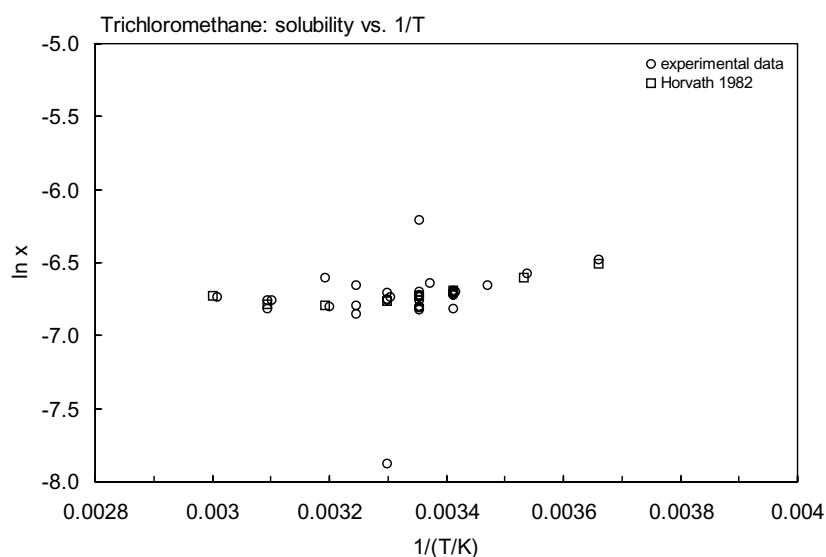
$$S/(\text{wt}\%) = 0.995 - 1.0531 \times 10^{-2} \cdot t/^{\circ}\text{C} + 7.9819 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 6.6431 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

1.

Rex 1906		Gross & Saylor 1931		Horvath 1982		Barr & Newsham 1987	
volumetric method		shake flask-IR		summary of literature data		activity coefficient	
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>
20	8220	15	8520	0	9905	20	8080
30	7760	30	7710	10	8983	35	7435
				20	8216	50	7290
				25	7920		
				30	7689		
				40	7440		
				50	7511		
				60	7940		
				eq.1	S/wt%		

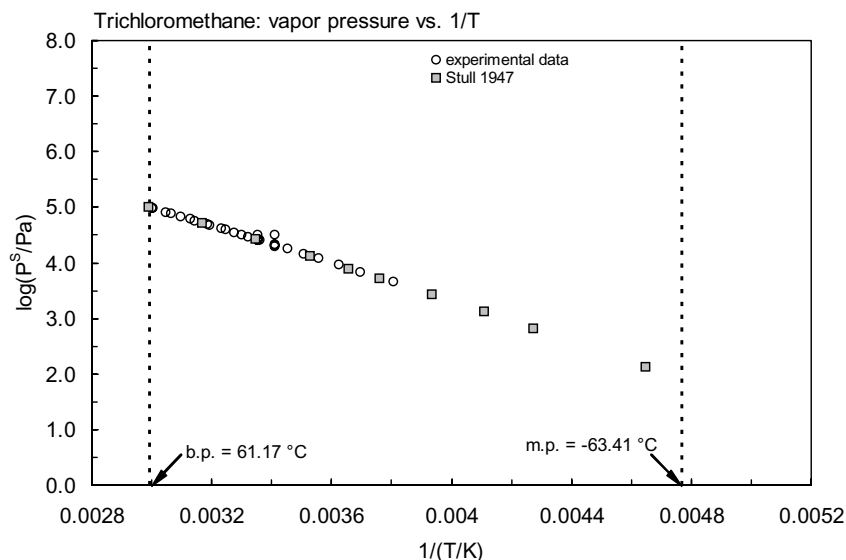
2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
shake flask-GC		activity coefficient		activity coefficient	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0	10200	20	7280	20	8108
9.5	9300	30	8118	35	7030
19.6	8200	35	8558	50	7694
29.5	7900	40	9011		
39.3	7400				
49.2	7700				
59.2	7900				

FIGURE 5.1.1.3.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for trichloromethane.

**TABLE 5.1.1.3.2**  
**Reported vapor pressures of trichloromethane 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)						
Scatchard & Raymond 1938	Stull 1947	Boublik & Aim 1972					
vapor-liquid equilibrium	summary of literature data	in Boublik et al 1984					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
35.0	39345	−58.0	133.3	−10.356	4524	46.583	61295
40.0	48023	−39.1	666.6	−2.610	6967	53.070	77125
45.0	57800	−29.7	1333	2.882	9306	60.319	98412
50.0	69218	−19.0	2666	8.010	12046		
55.0	82372	−7.10	5333	11.927	14549	bp/°C	61.203
60.0	97342	0.50	7999	16.417	17921	Antoine eq	P/kPa
		10.4	13332	20.240	21314	eq. 2	6.07945
		25.9	26664	24.598	25780	A	1170.902
		42.7	53329	28.118	29923	B	226.224
		61.3	101325	32.289	35493	C	
				36.223	41470		
		mp/°C	−65.3	40.913	49704		



**FIGURE 5.1.1.3.2** Logarithm of vapor pressure versus reciprocal temperature for trichloromethane.

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

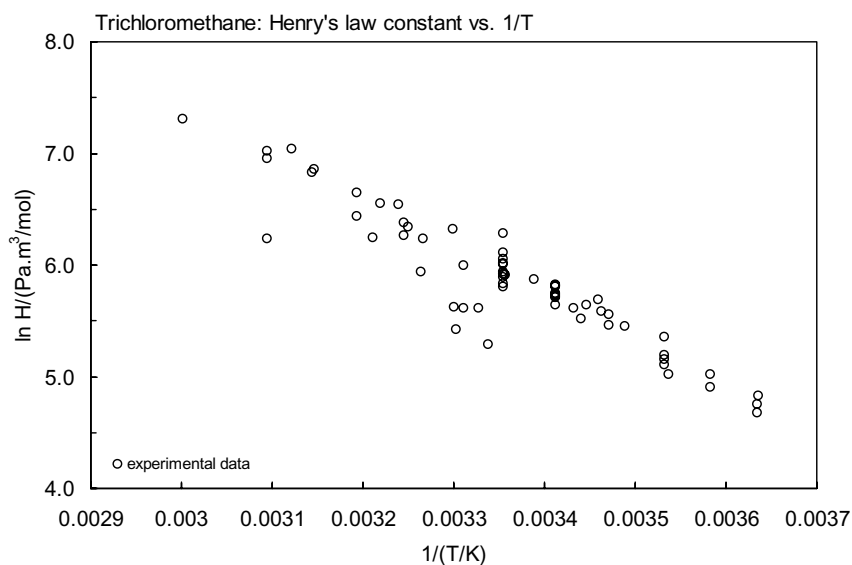
$$\begin{aligned}
\ln K_{AW} &= A - B/(T/K) & (1) & \quad \log K_{AW} = A - B/(T/K) & (1a) \\
\ln (1/K_{AW}) &= A - B/(T/K) & (2) & \quad \log (1/K_{AW}) = A - B/(T/K) & (2a) \\
\ln (k_H/atm) &= A - B/(T/K) & (3) & & \\
\ln H &= A - B/(T/K) & (4) & \quad \log H = A - B/(T/K) & (4a) \\
K_{AW} &= A - B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

1.

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancrede & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.90	125.7	9.6	152	10	174	26.5	199.3
13.5	234.7	17.5	249.3	15	236	27.4	274.9
15.7	267.6	24.8	371.9	20	336	28.9	401.8
17.1	282.7	34.6	570.5	25	427	28.9	276.2
22.0	354.7			30	561	29.7	226.6
24.9	373.5	eq. 4	H/(atm m³/mol)			29.9	277.2
25	373	A	9.843	eq. 4	H/(atm m³/mol)	33.3	382.2
		B	4612	A	11.41	35.6	693.1
eq. 3	k <sub>H</sub> /atm			B	5030	38.3	517.9
A	18.97					40	624.8
B	4046					44.7	951.2
						45	925.8
						47.2	1145
						eq. 1	K <sub>AW</sub>
						A	9.154
						B	3051

2.

Wright et al. 1992		Dewulf et al. 1995		Moore 1995		Görgényi et al. 2002	
activity coefficient		EPICS-GC		gas stripping-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)
20	306	2	116	10	212	2	108
35	592	6	135.1	20	341	6	151.3
50	1046	10	165.7			10	181.3
		18.2	276.1	In sea water 30.4‰ NaCl		16	297.8
		25	379.3	0	126	25	407.5
Bhatia & Sandler 1995				10	214	35	526.5
activity coefficient		eq. 1	K <sub>AW</sub>	20	352	40	769.9
35	514	A	12.012			50	1120
50	513	B	4142			60	1497
				Turner et al. 1996			
				vapor liquid equilibrium-GC		eq. 1	K <sub>AW</sub>
				15	261	A	10.96
				25	451	B	3821.3

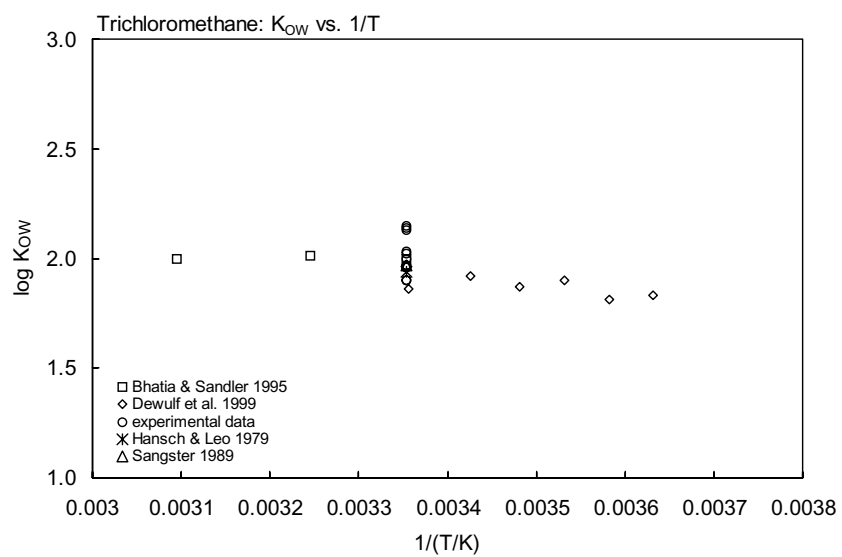


**FIGURE 5.1.1.3.3** Logarithm of Henry's law constant versus reciprocal temperature for trichloromethane.

**TABLE 5.1.1.3.4**  
Reported octanol-water partition coefficients of trichloromethane at various temperatures

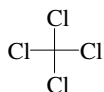
Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OW</sub>
25	2.00	2.2	1.83
35	2.01	6.0	1.815
50	2.00	10.0	1.90
		14.1	1.87
enthalpy of transfer		18.7	1.92
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$		24.8	1.86
$\log K_{OW} = A - \Delta H/2.303RT$		change in enthalpy:	
A	1.0195	$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 4.2$	
$\Delta H$	-20.2	(-4.4 to 12.8)	
		enthalpy of transfer	
		$\Delta H_{oct}/(\text{kJ mol}^{-1}) = 0.7$	
		(-7.9 to 9.3)	





**FIGURE 5.1.1.3.4** Logarithm of  $K_{OW}$  versus reciprocal temperature for trichloromethane.

## 5.1.1.4 Tetrachloromethane (Carbon tetrachloride)



Common Name: Carbon tetrachloride

Synonym: tetrachloromethane, methane tetrachloride, perchloromethane, benzinofom

Chemical Name: tetrachloromethane

CAS Registry No: 56-23-5

Molecular Formula:  $\text{CCl}_4$

Molecular Weight: 153.823

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

-22.62 (Lide 2003)

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

76.8 (Lide 2003)

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

1.594 (McGovern 1943; Dreisbach 1959, 1961; Weast 1982–83; Horvath 1982; Riddick et al. 1986)

1.6037, 1.59402, 1.58436 (15, 20,  $25^{\circ}\text{C}$ , Riddick et al. 1986)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

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

96.0 (calculated-density, Wang et al. 1992)

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

32.41, 29.96 ( $25^{\circ}\text{C}$ , bp, Riddick et al. 1986)

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

0.775 (calculated, Dreisbach 1959)

0.581 (quoted, Riddick et al. 1986)

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  $25^{\circ}\text{C}$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

800, 850 ( $20^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , volumetric method, Rex 1906)

770 (shake flask-interferometer, Gross 1929a,b)

770, 810 (15,  $30^{\circ}\text{C}$ , shake flask-interferometer, Gross & Saylor 1931)

780 (Seidell 1941)

800 (data presented in graph, temp range  $0$ – $70^{\circ}\text{C}$ , McGovern 1943; Dilling 1977)

770 ( $15^{\circ}\text{C}$ , Jones et al. 1957)

785 ( $20^{\circ}\text{C}$ , McConnell et al. 1975; Pearson & McConnell 1975)

778 ( $20^{\circ}\text{C}$ , recommended, Sørensen & Arit 1979)

800\* (measured range  $20$ – $30^{\circ}\text{C}$ , Andelman 1978)

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

700 (shake flask-titration/turbidity, Coca et al. 1980)

793.4\* (summary of literature data, Horvath 1982)

831 (calculated-UNIFAC activity coeff., Arbuckle 1983)

753 (calculated-UNIFAC activity coeff., Banerjee 1985)

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

770 (selected, Riddick et al. 1986)

780 ( $23$ – $24^{\circ}\text{C}$ , shake flask-GC, Broholm et al. 1992)

600\*, 720 ( $20.5$ ,  $31.0^{\circ}\text{C}$ , shake flask-GC/TC, measured range  $0$ – $75^{\circ}\text{C}$ , Stephenson 1992)

930, 873, 950, 982 ( $20$ ,  $30$ ,  $35$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\circ}$ -GC, Tse et al. 1992)

756, 896, 972, 1052 ( $20$ ,  $30$ ,  $35$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\circ}$ -UNIFAC, Tse et al. 1992)

700, 652, 652 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , activity coeff.  $\gamma^{\circ}$ -differential pressure transducer, Wright et al. 1992)

701, 702 ( $20^{\circ}\text{C}$ , calculated-activity coefficients, Wright et al. 1992)

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):

17170, 18810 (20°C, 30°C, Rex 1906)

11372\* (19.8°C, manometry, measured range 19.8–76.4°C, Smyth & Engel 1929)

15200 (extrapolated-Antoine eq., vapor-liquid equilibrium VLE data, measured range 30–70°C, Scatchard et al. 1939; quoted, Bissell & Williamson 1975)

$\log(P/\text{mmHg}) = 6.68148 - 1045.022/(T/K) - 99.577/(T/K)^2$ ; temp range 30–70°C (VLE data, Scatchard et al. 1939)

14530 (interpolated from graph, temp range –20 to 170°C, McGovern 1943)

14340\* (interpolated from Antoine eq. regression, temp range –50 to 76.7°C, Stull 1947)

15200 (McGlashan et al. 1954)

15100 (Moelwyn-Hughes & Missen 1957)

15360 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/\text{mmHg}) = 6.93390 - 1242.43/(230.0 + t/^\circ\text{C})$ ; temp range –15 to 138°C (Antoine eq. for liquid state, Dreisbach 1959)

15372\* (25.2°C, temp range 14.06–76.84°C, Boublik 1960; quoted, Boublik et al. 1984)

$\log(P/\text{mmHg}) = 6.94369 - 1221.1/(224.0 + t/^\circ\text{C})$ ; temp range –1 to 113°C (Antoine eq. for liquid state, Dreisbach 1961)

15220\* (twin ebulliometer, measured range 20–77°C, Hildenbrand & McDonald 1959)

15230 (Marsh 1968; quoted, Bissell & Williamson 1975)

13200 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 7628.8/(T/K)] + 7.586045$ ; temp range –50 to 276°C (Antoine eq., Weast 1972–73)

15250, 15240 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.9218 - 1235.172/(228.957 + t/^\circ\text{C})$ ; temp range 19.9–77.7°C (Antoine eq. from reported exptl. data of Hildenbrand & McDonald 1959, Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.87926 - 1212.021/(226.409 + t/^\circ\text{C})$ ; temp range 14.06–76.04°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

15195, 15184 (static method-differential pressure gauge, Bissell & Williamson 1975)

12000 (20°C, Pearson & McConnell 1975)

15230 (calculated-Antoine eq., Boublik et al. 1984)

15370, 15300 (25.2°C, quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.04073 - 1231.791/(228.51 + t/^\circ\text{C})$ ; temp range 19.9–77.7°C (Antoine eq. from reported exptl. data of Hildenbrand & McDonald 1959, Boublik et al. 1984)

$\log(P/\text{kPa}) = 5.94824 - 1177.609/(222.028 + t/^\circ\text{C})$ ; temp range 40–65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.00535 - 1212.676/(226.483 + t/^\circ\text{C})$ ; temp range 14.06–76.04°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

15170 (Daubert & Danner 1985)

$\log(P/\text{mmHg}) = 6.87926 - 1212.021/(226.41 + t/^\circ\text{C})$ , temp range not specified (Antoine eq., Dean 1985, 1992)

15360 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.10455 - 1265.632/(232.148 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

15210 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 8.214 - 2027/(T/K)$ ; temp range 208–225 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 7.946 - 1975.3/(T/K)$ , temp range 226–248 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.99114 - 1202.9/(-48.01 + T/K)$ ; temp range 262–249 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.97092 - 1195.9034/(-48.217 + T/K)$ ; temp range 349–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.22882 - 1392.458/(-19.19 + T/K)$ ; temp range 412–497 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 31.9407 - 2.6614 \times 10^3/(T/K) - 8.5763 \cdot \log(T/K) - 6.7136 \times 10^{-10} \cdot (T/K) + 2.9732 \times 10^{-6} \cdot (T/K)^2$ ; temp range 250–556 K (vapor pressure eq., Yaws 1994)

15320 (selected summary of literature data, temp range 250.33–398.15 K, Xiang 2002)

18826 (30°C, vapor-liquid equilibrium study, Pathare et al. 2004)

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

- 2912 (calculated as  $1/K_{\text{AW}} C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)  
 152.8 (calculated-bond method, Hine & Mookerjee 1975)  
 2216 ( $20^\circ\text{C}$ , McConnell et al. 1975; Pearson & McConnell 1975)  
 2776 (gas stripping-GC, Mackay et al. 1979)  
 2350 ( $20^\circ\text{C}$ , calculated-P/C, Kavanaugh & Trussell 1980, 1983)  
 $\log (H/\text{atm}) = 10.06 - 2038.25/(T/K)$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)  
 2797\* (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)  
 $\ln (k_{\text{H}}/\text{atm}) = 22.22 - 4438/(T/K)$ ; temp range  $1.0\text{--}27.2^\circ\text{C}$  (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 2160 (calculated-P/C, Mackay & Shiu 1981)  
 2330 ( $20^\circ\text{C}$ , calculated-P/C, Mabey et al. 1982)  
 2454 ( $20^\circ\text{C}$ , batch stripping, Munz & Roberts 1982)  
 2418 ( $20^\circ\text{C}$ , calculated-UNIFAC activity coeff., Arbuckle 1983)  
 3081 ( $20^\circ\text{C}$ , EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)  
 $\ln K_{\text{AW}} = 9.77 - 2918/(T/K)$ ; measured range  $5\text{--}33^\circ\text{C}$  (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)  
 $\ln K_{\text{AW}} = 11.27 - 3230/(T/K)$ ; measured range  $5\text{--}33^\circ\text{C}$  (seawater, multiply equilibrium-GC, Hunter-Smith 1983)  
 3060 (adsorption isotherm, Urano & Murata 1985)  
 2369 ( $20^\circ\text{C}$ , multiple equilibration, Munz & Roberts 1986)  
 3080\* (EPICS-GC/FID, Gossett 1987)  
 2367\* ( $20^\circ\text{C}$ , EPICS-GC/FID, measured range  $10.0\text{--}34.6^\circ\text{C}$ , Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 11.29 - 4411/(T/K)$ ; temp range  $10.0\text{--}34.6^\circ\text{C}$  (EPICS measurements, Gossett 1987)  
 2266 ( $20^\circ\text{C}$ , calculated-P/C, McKone 1987)  
 3027 (EPICS-GC, Munz & Roberts 1987)  
 $\log K_{\text{AW}} = 5.853 - 1718/(T/K)$ ; temp range  $10\text{--}30^\circ\text{C}$  (EPICS-GC measurements, Munz & Roberts 1987)  
 2900 (calculated-P/C, Warner et al. 1987)  
 228 ( $20^\circ\text{C}$ , EPICS-GC, Yurteri et al. 1987)  
 2989\* (EPICS-GC, measured range  $10\text{--}30^\circ\text{C}$ , Ashworth et al. 1988)  
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 9.739 - 3951/(T/K)$ ; temp range  $10\text{--}30^\circ\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 2330 ( $20\text{--}25^\circ\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 2980 (computed value, Yaws et al. 1991)  
 2990 (EPICS-GC, Tancréde et al. 1992)  
 2875\* (tap water, EPICS-GC, measured range  $25\text{--}47.2^\circ\text{C}$ , Tancréde & Yanagisawa 1990)  
 $\log K_{\text{AW}} = 5.569 - 1639/(T/K)$ ; temp range:  $25\text{--}47.2^\circ\text{C}$  (EPICS measurements, Tancréde & Yanagisawa 1990)  
 2067, 3415, 3871, 4580 ( $20, 30, 35, 40^\circ\text{C}$ , infinite dilution activity coeff.  $\gamma\text{-GC}$ , Tse et al. 1992)  
 2646, 4392, 6624 ( $20, 35, 50^\circ\text{C}$ , activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 3133\* ( $27.6^\circ\text{C}$ , EPICS-GC, measured range  $27.6\text{--}45^\circ\text{C}$ , Hansen et al. 1993)  
 $\ln [H/(\text{kPa}\cdot\text{m}^3/\text{mol})] = -3553/(T/K) + 13.0$ ; temp range  $27\text{--}45^\circ\text{C}$  (EPICS measurements, Hansen et al. 1993)  
 4.04, 6.0 ( $35, 50^\circ\text{C}$ , from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 2598\* (EPICS-GC/FID, measured range  $2.0\text{--}25^\circ\text{C}$ , Dewulf et al. 1995)  
 1341, 3370 ( $6.0, 25^\circ\text{C}$ , EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)  
 $\ln K_{\text{AW}} = -4073/(T/K) + 0.00814\cdot Z + 13.772$ ; with Z salinity  $0\text{--}35.5\text{‰}$ , temp range:  $2\text{--}35^\circ\text{C}$  (EPICS-GC/FID, Dewulf et al. 1995)  
 2352 ( $20^\circ\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 2612 (modified EPICS method-GC, Ryu & Park 1999)  
 2313 ( $20^\circ\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{\text{AW}} = 5.736 - 1689/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

- 2.64 (Leo et al. 1971)  
 2.62 (shake flask-GC, Chiou et al. 1977)  
 2.83 (shake flask, Hansch & Leo 1979, 1987)

- 2.73 (shake flask-LSC, Banerjee et al. 1980)
- 2.73 (shake flask-LSC, Veith et al. 1980)
- 2.94 (HPLC- $k'$  correlation, McDuffie 1981)
- 2.81, 290 (calculated from UNIFAC activity coeff. with octanol and water mutual solubility considered, not considered, Arbuckle 1983)
- 2.83 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)
- 2.03 (HPLC correlation, Eadsforth 1986)
- 2.73 (HPLC- $k'$  correlation, Tomlinson & Hafkenscheid 1986)
- 2.38 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
- 2.83 (recommended, Sangster 1989)
- 2.83 (recommended, Hansch et al. 1995)
- 2.73\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
- 2.38\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

- 2.79 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 1.24 (rainbow trout, Neely et al. 1974; Veith et al. 1979)
- 1.25 (trout muscle, calculated-ratio of rate const.  $k_1/k_2$ , Neely et al. 1974)
- 1.48 (bluegill sunfish, Barrows et al. 1980; Veith et al. 1980; Veith & Kosian 1982)
- 2.32 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)
- 1.72 (rainbow trout, Veith & Kosian 1982)
- 2.68 (activated sludge, Freitag et al. 1984)
- 2.48 (*alga chlorella fusca*-LSC, Geyer et al. 1984)
- 2.68, 2.48, < 1.0 (activated sludge, *Chlorella fusca*, golden ide, Freitag et al. 1985)
- 2.06 (calculated- $K_{OW}$ ,  $S_{OCTANOL}$ , and mp, Banerjee & Baughman 1991)

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

- 2.04 (calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.64 (calculated- $K_{OW}$ , Mabey et al. 1982)
- 1.85 (calculated-MCI  $\chi$ , Koch 1983)
- 1.70 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 1.26, 1.34, 1.70, 1.96, 2.07 (DTMA-clay, TTMA-clay, HTMA-clay, BDHA-clay, DDPa-clay, Smith et al. 1990)
- 1.69 (80% DTMA-clay at 20°C, Smith & Jaffé 1991)
- 2.16; 1.70; 2.06 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 2.20, 2.24, 2.24, 2.25, 2.28, 2.27, 2.33 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)%o
- 1.80, 1.80, 1.78 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)
- 2.01, 2.00, 2.02 (sediments: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)

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

- 1.55 (calculated-MCI  $\chi$ , Sabljic 1984)
- 1.89, 1.72 (Florida peat, OC 57.1%; Michigan muck, OC 53.1%, batch equilibrium-sorption equilibrium, Rutherford & Chiou 1992; Rutherford et al. 1992)
- 0.243, 1.866 (cellulose, extracted peat, Rutherford et al. 1992)

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

- Volatilization:  $t_{1/2} = 29$  min was determined in an open container with initial concentration of 1 mg/L when stirred at 100 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Verschueren 1983);
- Evaporation  $t_{1/2}(\text{exptl}) = 28.8$  min,  $t_{1/2}(\text{calc}) = 0.2$  min, 25.5 min from water (Dilling 1977);

ratio of evaporation rate constant to that of oxygen reaeration: 0.47 as measured value compared to 0.43 as predicted (Smith et al. 1980);

$k < 2.4 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , estimated rate constant for the reaction with OH radical at 300 K (Lyman 1982);  
 $t_{1/2} \sim 3.7 \text{ h}$  from a model river of 1 m deep for water flowing at 1 m/s with wind speed of 3 m/s and Henry's law constant (Thomas 1982; Lyman et al. 1982; quoted, Howard 1990).

Photolysis: photocatalyzed mineralization by the presence of  $\text{TiO}_2$  with the rate of 0.18 ppm/min per gram of catalyst (Ollis 1985).

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:

$k_{\text{OH}} < 1.25 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (relative rate method, Cox et al. 1976)

$k_{\text{OH}} = 1 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$  bimolecular reaction rate, with a reported tropospheric lifetime of greater than 330 yr (Cox et al. 1976; quoted, Callahan et al. 1979)

$k_{\text{OH}} < 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 2 \text{ K}$  (discharge flow-LMR, Howard & Evenson 1976a)

$k_{\text{OH}} < 1.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time  $> 11600 \text{ d}$ , loss  $\approx 0.0\%$  in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}}(\text{calc}) \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at  $25^\circ\text{C}$  (Mabey et al. 1982)

$k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water at pH 2 and  $20\text{--}23^\circ\text{C}$  (Hoigné & Bader 1983)

photooxidation half-life in air:  $1.6 \times 10^4 \text{--}1.6 \times 10^5 \text{ h}$ , based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k < 2 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

$k_{\text{OH}} < 5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

Hydrolysis: hydrolysis rate constant  $k = 4.8 \times 10^{-7} \text{ s}^{-1}$  with  $t_{1/2} = 7000 \text{ yr}$  (1 ppm),  $t_{1/2} = 7 \text{ yr}$  (1000 ppm) at  $25^\circ\text{C}$  and pH 7 (Mabey & Mill 1978)

calculated first-order  $t_{1/2} = 7000 \text{ yr}$ , based on reported rate constant  $k = 4.8 \times 10^{-7} \text{ mol}^{-1} \text{ s}^{-1}$  for 1 mg/L concentration at pH 7 and  $25^\circ\text{C}$  (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard 1990; Howard et al. 1991)

$t_{1/2} = 2,600,000 \text{ d}$  at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation:  $t_{1/2}(\text{aq. aerobic}) = 4320\text{--}8640 \text{ h}$ , based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 168\text{--}672 \text{ h}$ , based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991) and acclimated anaerobic sediment/aquifer grab sample data (Parsons et al. 1985; quoted, Howard et al. 1991).

$t_{1/2}(\text{aerobic}) = 170 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 7 \text{ d}$  in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of  $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria in water (Mabey et al. 1982).

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

$k_1 = 4.05 \text{ h}^{-1}$ ;  $k_2 = 0.229 \text{ h}^{-1}$  (trout muscle, Neely et al. 1974; quoted, Thomann 1989)

$k_1 = 4.05 \text{ mL g}^{-1} \text{ h}^{-1}$  ( $10^\circ\text{C}$ , trout gill, Neely 1979)

$k_1 = 4.10 \text{ h}^{-1}$ ;  $k_2 = 0.25 \text{ h}^{-1}$  (trout, Hawker & Connell 1985)

#### Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 10 \text{ wk}$ , when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} > 10 \text{ d}$  for the reaction with OH radical in air (Darnall et al. 1976);

estimated residence time in troposphere,  $> 330 \text{ yr}$  (CEQ 1975);

estimated residence time of 100 yr in troposphere (Singh et al. 1979);

residence time  $> 11600 \text{ d}$ , loss  $\approx 0.0\%$  in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

estimated residence time of 4–20 yr in troposphere (Lyman 1982);

$t_{1/2} = 30\text{--}50 \text{ yr}$  residence time in the troposphere (Howard 1990);

$t_{1/2} = 1.6 \times 10^4 \text{--}1.6 \times 10^5 \text{ h}$ , based on photooxidation half-life in air from measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: estimated  $t_{1/2} = 0.4\text{--}56 \text{ d}$  in various locations in the Netherlands in case of a first order reduction process;  $t_{1/2} \sim 3\text{--}30 \text{ d}$  in rivers and  $t_{1/2} = 3\text{--}300 \text{ d}$  in lakes (Zoeteman et al. 1980);

$t_{1/2} = 4320\text{--}8640 \text{ h}$ , based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

$t_{1/2}(\text{aerobic}) = 170 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 7 \text{ d}$  in natural waters (Capel & Larson 1995)

Ground water: estimated  $t_{1/2} \sim 3\text{--}300$  d (Zoeteman et al. 1980; quoted, Howard 1990);

$t_{1/2} = 168\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life and acclimated anaerobic sediment/aquifer grab sample data (Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 4320\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{calc}) = 50$  d in soil mixtures from first-order kinetic (Anderson et al. 1991).

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

**TABLE 5.1.1.4.1**

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

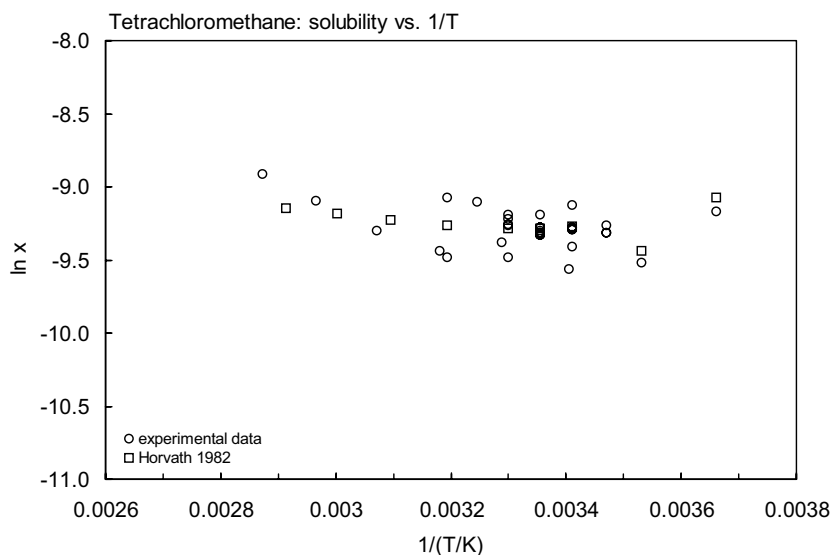
$$S/(\text{wt}\%) = 9.7842 \times 10^{-2} - 1.4942 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 3.5854 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 2.2775 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

1.

Rex 1906		Gross & Saylor 1931		Andelman 1978		Horvath 1982	
volumetric method		shake flask-IR				summary of literature data	
t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$
20	800	15	770	20	793	0	978.4
30	850	30	810	25	800	10	682.6
				30	814	20	804.8
						25	793.4
						30	791.3
						40	808.6
						50	843.0
						60	880.7
						70	908.1
						eq. 1	S/wt%

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
shake flask-GC		activity coefficient		activity coefficient	
t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$
0	890	20	930	20	700
10	630	30	873	30	652
20.5	600	35	950	40	652
31.0	720	40	982		
41.3	680				
52.5	780				
64.0	960				
75.0	1150				



**FIGURE 5.1.1.4.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for tetrachloromethane.

**TABLE 5.1.1.4.2**

**Reported vapor pressures of tetrachloromethane at various temperatures and the coefficients for the vapor pressure equations**

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Smyth & Engel 1929		Stull 1947		Hildenbrand & McDonald 1959		Boublik 1960, thesis	
static-manometer		summary of literature data		twin ebulliometer system		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
19.2	11732	–50.0	133.3	19.88	12079	14.06	9120
32.4	20798	–30.0	666.6	30.93	25211	16.66	10426
41.2	29704	–19.6	1333	56.16	51605	18.46	11876
50.0	41597	–8.20	2666	75.28	96965	21.71	13159
60.8	60368	4.30	5333	76.16	99645	25.2	15372
68.7	78180	12.3	7999	76.87	101729	29.13	18252
76.4	101325	23.0	13332	77.71	104369	33.45	21891
		38.3	26664	76.73	101325	36.98	25264
bp/°C	76.4	57.8	53329			42.07	30864
		76.7	101325			47.21	37543
				ΔH <sub>v</sub> /(kJ mol <sup>-1</sup> ) = 32.41		52.36	45367
				at 25°C		58.61	56448
						64.78	69487
				eq. 2	P/mmHg	71.43	86053
				A	6.89406	76.84	99256
				B	1219.58		
				C	227.16		
					bp/°C	76.714	
					eq. 2	P/kPa	
					A	6.00535	
					B	1212.676	
					C	226.483	



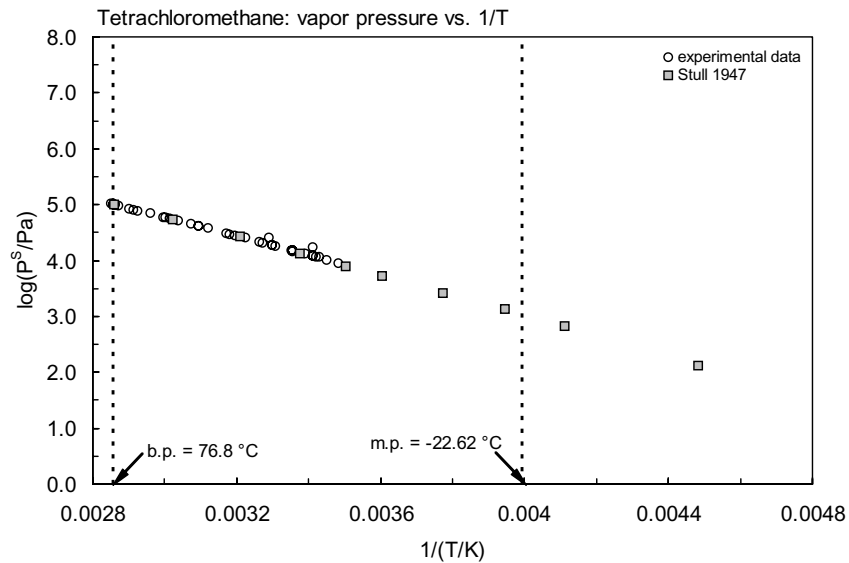


FIGURE 5.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.3  
Reported Henry’s law constants of tetrachloromethane 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(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		Gossett 1987		Ashworth et al. 1988		Tancrede & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.0	751.6	10.0	1337.5	10	1500	25	2875
1.3	752.2	17.5	2138	15	1935	26.5	2666
11.0	1312	24.8	3080	20	2351	27.4	3248
13.0	1568	34.6	4661	25	2989	28.9	3315
21.0	2335			30	3830	28.9	3466
22.0	2406	eq. 4	H/(atm m³/mol)			29.7	3525
27.1	2866	A	11.29	eq. 4	H/(atm m³/mol)	29.9	3527
25	2797	B	4411	A	9.739	33.3	4713
				B	3951	35.6	4390
eq. 3	k <sub>H</sub> /atm					38.3	5334
A	22.22					40	5546
B	4438					44.7	5416
						45	6993
						47.2	7484
						eq. 1	K <sub>AW</sub>
						A	5.569
						B	1639

(Continued)

TABLE 5.1.1.4.3 (Continued)

2.

Tse et al. 1992		Wright et al. 1992		Hansen et al. 1993		Dewulf et al. 1995	
activity coefficient		activity coefficient		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
20	2067	20	2646	27.6	3133	2.0	835
30	3415	35	4550	35.0	4550	6.0	912
35	3871	50	6624	45.0	6343	10.0	1055
40	4580					18.2	1926
				eq. 4	H/(kPa m³/mol)	25.0	2598
				A	13.0		
				B	3553	eq. 1	K <sub>AW</sub>
						A	13.722
						B	4073

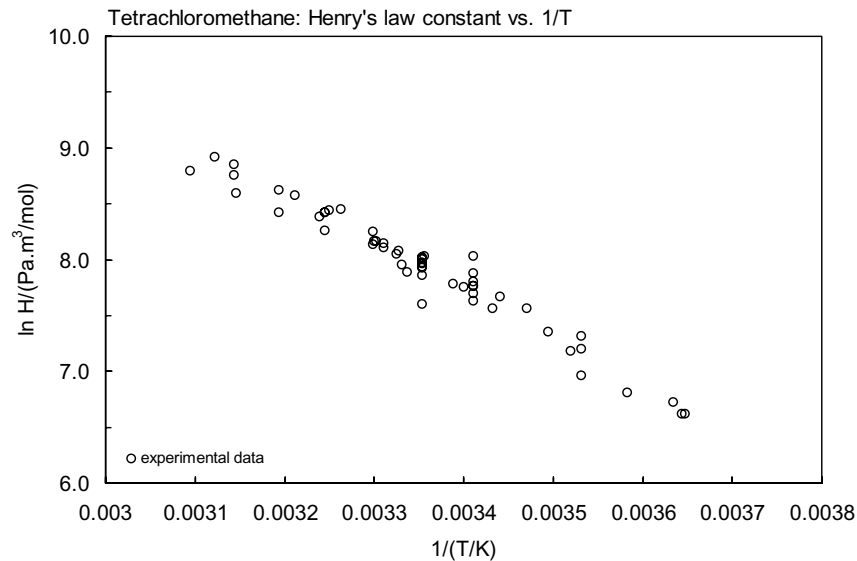


FIGURE 5.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.4

Reported octanol-water partition coefficients of tetrachloromethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OW</sub>
25	2.73	2.2	2.39
35	2.74	6.0	2.38
50	2.73	10.0	2.50
		14.1	2.44
		18.7	2.47
		24.8	2.38

change in enthalpy:  
 $\Delta H_{OW}/(\text{kJ mol}^{-1}) = 1.3$   
 (−12.1 to 14.6)

enthalpy of transfer  
 $\Delta H_{oct}/(\text{kJ mol}^{-1}) = -0.5$   
 (−13.9 to 12.8)

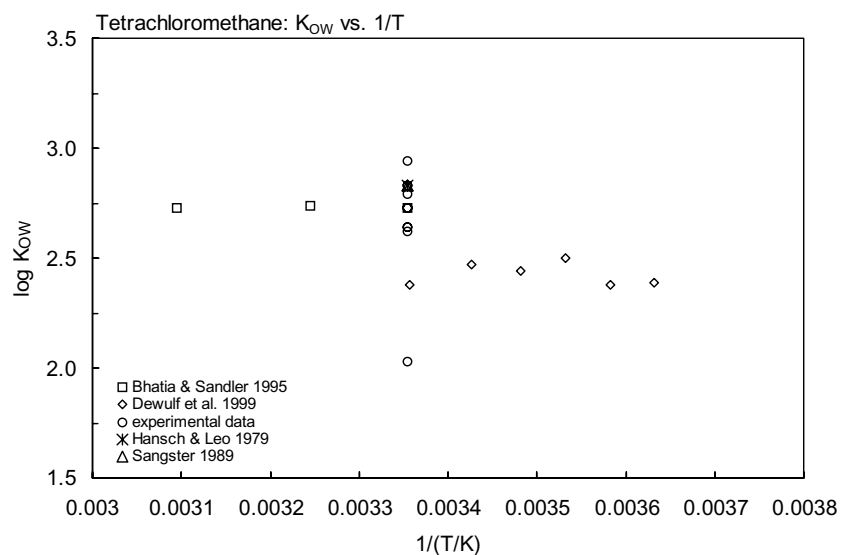


FIGURE 5.1.1.4.4 Logarithm of K<sub>OW</sub> versus reciprocal temperature for tetrachloromethane.

## 5.1.1.5 Chloroethane (Ethyl chloride)



Common Name: Ethyl chloride

Synonym: chloroethane, monochloroethane

Chemical Name: chloroethane, ethyl chloride, monochloroethane, hydrochloric ether, muriatic ether

CAS Registry No: 75-00-3

Molecular Formula:  $C_2H_5Cl$ ,  $CH_3CH_2Cl$

Molecular Weight: 64.514

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

-138.4 (Lide 2003)

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

12.30 (McGovern 1943; Weast 1982–83; Dean 1985; Howard 1990; Lide 2003)

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

0.8978 (Weast 1982–83)

0.92390, 0.8960, 0.88981 (0, 20,  $25^{\circ}C$ , Riddick et al. 1986)

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

72.0 (calculated-density, Wang et al. 1992)

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

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

27.8, 24.652 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

4.45 (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):

5735 ( $12.5^{\circ}C$ , shake flask, Fühner 1924)

7580 (Seidell 1940)

4500 ( $0^{\circ}C$ , McGovern 1943; Dean 1985)

5710 ( $20^{\circ}C$ , Neely 1976)

5700 ( $20^{\circ}C$ , selected, Dilling 1977)

5678\* ( $20^{\circ}C$ , summary of literature data, Horvath 1982)

5740 ( $20^{\circ}C$ , Verschuere 1977, 1983)

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):

136630 (data presented in graph, temp range  $-50$  to  $\sim 105^{\circ}C$ , McGovern 1943)

187000\* (extrapolated-Antoine eq. regression, summary of literature data, Stull 1947)

101436\* ( $12.51^{\circ}C$ , static method-Hg manometer, measured range  $-55.88$  to  $12.51^{\circ}C$ , Gordon & Giauque 1948)

160000 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.94914 - 1012.77/(236.47 + t/^{\circ}C)$ ; temp range  $-50$  to  $70^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

$\log (P/mmHg) = 6.94914 - 1012.77/(236.67 + t/^{\circ}C)$ , pressure range of 10 to 1500 mmHg, (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/mmHg) = [-0.2185 \times 6310.6/(T/K)] + 7.660205$ ; temp range  $-89.8$  to  $180.5^{\circ}C$  (Antoine eq., Weast 1972–73)

160000 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 6.98647 - 1030.007/(238.612 + t/^{\circ}C)$ ; temp range  $-55.94$  to  $12.5^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

149400 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.11833 - 1033.161/(236.956 + t/^{\circ}C)$ ; temp range  $-55.94$  to  $12.5^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.98647 - 1030.01/(238.61 + t/^{\circ}\text{C})$ ; temp range  $-56$  to  $12.2^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)  
 159880 (selected, Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 6.09088 - 1020.63/(237.57 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 160000 (calculated-Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.07404 - 1012.771/(-36.48 + T/\text{K})$ ; temp range  $207$ – $305$  K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.14258 - 1053.998/(-30.686 + T/\text{K})$ ; temp range  $285$ – $344$  K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.4495 - 1248.788/(-3.798 + T/\text{K})$ ; temp range:  $334$ – $413$  K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.70739 - 1465.734/(29.696 + T/\text{K})$ ; temp range  $403$ – $460$  K (Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P/\text{mmHg}) = 28.3448 - 2.0788 \times 10^3/(T/\text{K}) - 7.5387 \cdot \log (T/\text{K}) - 1.6384 \times 10^{-11} \cdot (T/\text{K}) + 4.055 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
 temp range  $137$ – $460$  K (vapor pressure eq., Yaws 1994)

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

860 (calculated as  $1/K_{\text{AW}}$ ,  $C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)  
 1140 (calculated, Dilling 1977)  
 1145 (calculated-P/C, Mackay & Shiu 1981, 1990)  
 1125\* ( $24.8^{\circ}\text{C}$ , EPICS-GC/FID, measured range  $10.3$ – $34.6^{\circ}\text{C}$ , Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 5.974 - 3120/(T/\text{K})$ ; temp range:  $10.3$ – $34.6^{\circ}\text{C}$  (EPICS measurements, Gossett 1987)  
 1226\* (EPICS-GC/FID, measured range  $10$ – $30^{\circ}\text{C}$ , Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 4.265 - 2580/(T/\text{K})$ ; temp range  $10$ – $30^{\circ}\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 1270 (calculated-QSAR, Nirmalakhandan & Speece 1988)  
 942 ( $20$ – $25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 701 (computed value, Yaws et al. 1991)  
 1019 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 3.406 - 1110/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

1.54 (Leo et al. 1971)  
 1.39 (calculated- $\pi$  substituent const., Hansch et al. 1968; Hansch & Leo 1979)  
 1.43 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1987)  
 1.43 (recommended, Sangster 1989, 1993)  
 1.43 (recommended, Hansch et al. 1995)

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

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

0.86, 0.67 (estimated- $K_{\text{OW}}$ , S, Lyman et al. 1982; quoted, Howard et al. 1990)  
 0.99 (microorganisms-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)

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

2.16, 1.52 (estimated- $K_{\text{OW}}$ , S, Lyman et al. 1982; quoted, Howard 1990)  
 1.17 (sediment-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)  
 1.40 (soil, selected, Jury et al. 1990)

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

Volatilization: estimated experimental  $t_{1/2} = 21$  min for  $1$  mg/L to evaporate from aqueous solution stirred at  $200$  rpm in an open container of depth  $65$  mm at  $25^{\circ}\text{C}$  (Dilling et al. 1975);  
 Evaporation  $t_{1/2}(\text{exptl}) = 23.1$  min,  $t_{1/2}(\text{calc}) = 0.5$  min,  $16.7$  min from water (Dilling 1977);  
 volatilization  $t_{1/2} = 2.5$  h from a model river of  $1$  m deep, based on Henry's law constant (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} = 5.6, 1.1,$  and  $4.5$  d from representative pond, river and lake were estimated based on oxygen reaeration ratio of 0.645 (Mabey et al. 1982; quoted, Howard 1990);

$t_{1/2} = 30$  d for volatilization loss from soil (Jury et al. 1990).

#### 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 and/or the Arrhenius expression see reference:

$k_{OH} = (3.9 \pm 0.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K and the calculated lifetime of about  $2.6 \times 10^8$  s or 30 d (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980)

$k_{OH} = (2.37 \pm 0.32) \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  or  $(3.94 \pm 0.53) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 297 K (flash photolysis-resonance fluorescence, Paraskevopoulos et al. 1978)

$k_{OH} = 2.3 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , estimated at 300 K (Lyman 1982)

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

$k_{O_3} = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984) photooxidation half-life of 160–1604 h, based on measured rate constants for the reaction with OH radical in air (Atkinson 1985; quoted, Howard 1990; Howard et al. 1991)

$k_{OH} = 3.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

$k_{OH}^* = (4.08 \pm 0.31) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 294.8 K, measured range 294.8–788.7 K (laser photolysis/laser induced fluorescence, Kasner et al. 1990)

Hydrolysis:  $k = 2.0 \times 10^{-7} \text{ s}^{-1}$  was estimated for reaction at pH 7 and 25°C with a maximum  $t_{1/2} = 40$  d (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982);

$k = 2.10 \times 10^{-7} \text{ s}^{-1}$  with  $t_{1/2} = 38$  day at 25°C and pH 7 (Mabey & Mill 1978)

estimated  $t_{1/2} = 38$  d at 25°C was based on an exptl  $t_{1/2} = 1.68$  h at 100°C with ethanol and HCl being the hydrolysis product (Mabey & Mill 1978; quoted, Haque et al. 1980; Howard 1990; Howard et al. 1991);

$k = 4.5 \times 10^{-5} \text{ h}^{-1}$  at pH 7 and 25°C with a calculated  $t_{1/2} = 1.8$  yr (Jeffers et al. 1989; quoted, Ellington 1989); abiotic hydrolysis or dehydrohalogenation  $t_{1/2} = 1.3$  month (Olsen & Davis 1990).

#### Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 168\text{--}672$  h, based on aqueous aerobic screening test data for 1-chloropropane and 1-chlorobutane (Gerhold & Malaney 1966; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688$  h, based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991)

$k = 0.02 \text{ yr}^{-1}$  with  $t_{1/2} = 10$  d and  $k = 0.001 \text{ yr}^{-1}$  with  $t_{1/2} = 700$  d (Olsen & Davis 1990).

#### Biotransformation:

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

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetime of about  $2.6 \times 10^8$  s or 30 d (Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980);

$t_{1/2} = 160\text{--}1604$  h, based on photooxidation half-life in air from measured rate constants for the gas phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 0.04 yr (Nimitz & Skaggs 1992).

Surface water:  $t_{1/2} = 168\text{--}672$  h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Ground water:  $t_{1/2} = 336\text{--}1344$  h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

#### Sediment:

Soil:  $t_{1/2} = 10\text{--}50$  d (Ryan et al. 1988);

$t_{1/2} = 30$  d, volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 168\text{--}672$  h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota:  $t_{1/2} = 10\text{--}50$  d, subject to plant uptake by soil through volatilization (Ryan et al. 1988).

TABLE 5.1.1.5.1  
Reported aqueous solubilities and vapor pressures of chloroethane at various temperatures

$S/(wt\%) = 0.5842 - 1.6863 \times 10^{-3} \cdot (t/^{\circ}C) + 9.3949 \times 10^{-5} \cdot (t/^{\circ}C)^2 - 2.5316 \times 10^{-6} \cdot (t/^{\circ}C)^3$  (1)

Aqueous solubility		Vapor pressure			
Horvath 1982		Stull 1947		Gordon & Giauque 1948	
summary of literature data		summary of literature data		static method-Hg manometer	
t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	P/Pa
0	5842	−89.8	133.3	−55.88	2993
10	5742	−73.9	666.6	−43.64	6726
20	5678	−65.8	1333	−35.44	10992
eq. 1	S/wt%	−56.8	2666	−28.085	16549
		−47.0	5333	−19.99	25119
		−40.6	7999	−13.48	34379
		−32.0	13332	−7.64	44878
		−18.6	26664	−1.878	57621
		−3.90	53329	3.448	17859
		12.4	101325	6.481	81100
				10.48	94708
				12.51	101436
				mp/K =	134.80
		bp/K =	285.37		
				log P = A − B/(T/K) − C·(T/K) + D·(T/K) <sup>2</sup>	
				P/cmHg	
				A	10.54417
				B	1777.378
				C	0.0115789
				D	1.06734 × 10 <sup>5</sup>
				ΔH <sub>fus</sub> /(kJ mol <sup>−1</sup> ) = 4.452	
				ΔH <sub>v</sub> /(kJ mol <sup>−1</sup> ) = 24.65	
				at 285.37 K	

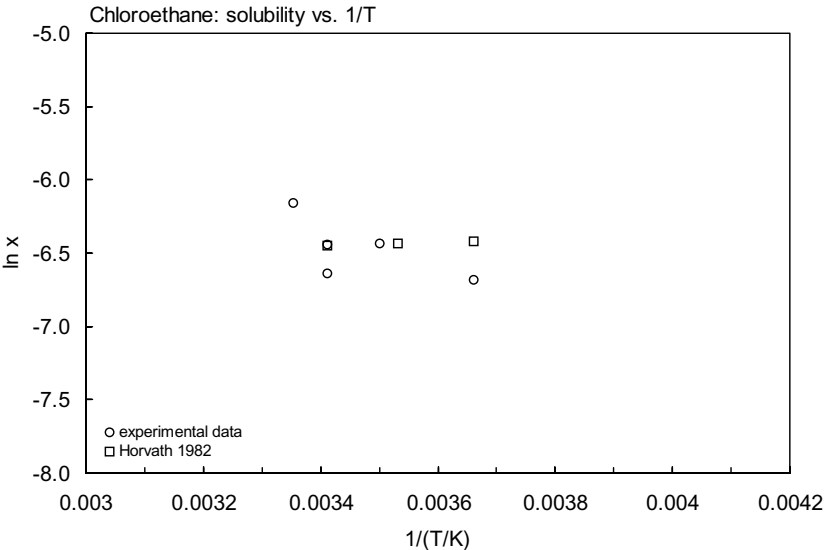


FIGURE 5.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chloroethane.

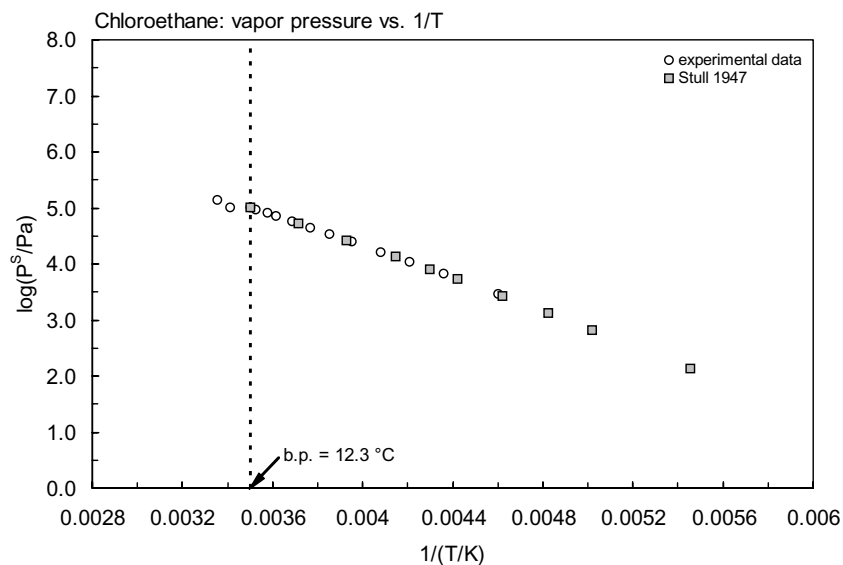
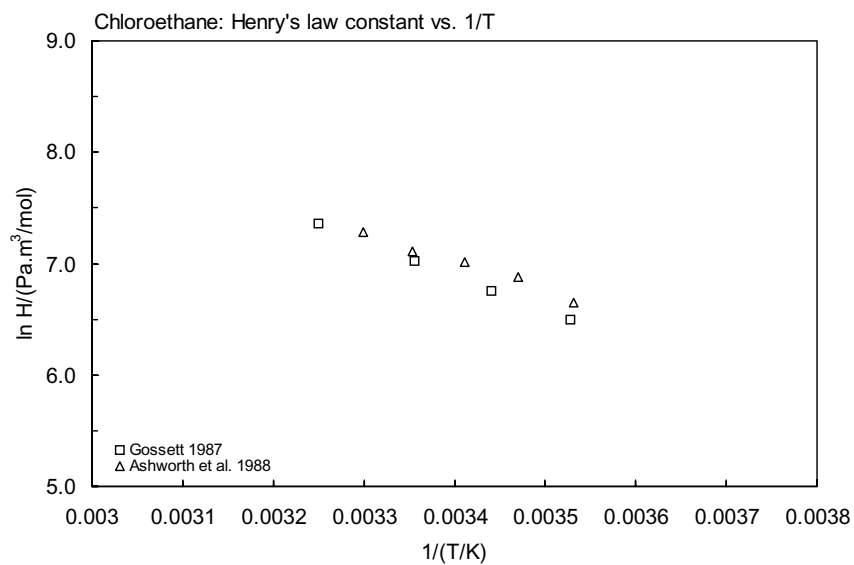


FIGURE 5.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for chloroethane.

TABLE 5.1.1.5.2  
Reported Henry’s law constants of chloroethane 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Gossett 1987			Ashworth et al. 1988		
EPICS-GC			EPICS-GC		
t/°C	H/(Pa m <sup>3</sup> /mol)		t/°C	H/(Pa m <sup>3</sup> /mol)	
10.3	660		10	769	
17.5	857.2		15	970.7	
24.8	1125		20	1115	
34.6	1571		25	1226	
			30	1449	
eq. 4a	H/(atm m <sup>3</sup> /mol)		eq. 4a	H/(atm m <sup>3</sup> /mol)	
A	7.385		A	4.265	
B	3286		B	2580	





**FIGURE 5.1.1.5.3** Logarithm of Henry's law constant versus reciprocal temperature for chloroethane.

## 5.1.1.6 1,1-Dichloroethane



Common Name: 1,1-Dichloroethane

Synonym: ethylidene chloride, ethylidene dichloride

Chemical Name: 1,1-dichloroethane

CAS Registry No: 75-34-3

Molecular Formula:  $C_2H_4Cl_2$ ,  $CH_3CHCl_2$

Molecular Weight: 98.959

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

−96.9 (Lide 2003)

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

57.3 (Weast 1982–83, Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

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

1.1757 (Dreisbach 1961; Horvath 1982; Weast 1982–83; Dean 1985)

1.1755, 1.1679 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

84.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

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

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

30.62, 28.6 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

7.87 (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):

5500\* ( $20^{\circ}C$ , volumetric method, measured range  $0$ – $30^{\circ}C$ , Rex 1906)

5060 (shake flask-interferometer, Gross 1929; quoted, Horvath 1982)

5555 (volumetric method, Wright & Schaffer 1932)

5060\* ( $20^{\circ}C$ , shake flask, measured range  $0$ – $50^{\circ}C$ , Van Arkel & Vles 1936)

5060 (Seidell 1941)

4800\* (shake flask, measured range  $10$ – $70^{\circ}C$ , Walraevens et al. 1974)

$\log [S/(mol/L)] = 2070/(T/K) - 15.116 + 0.0230 \cdot (T/K)$ , temp range  $10$ – $70^{\circ}C$ , Walraevens et al. 1974

5100 (literature average, Dilling 1977, 1982)

4767\* (summary of literature data, temp range  $0$ – $80^{\circ}C$ , Horvath 1982)

4834 ( $30^{\circ}C$ , headspace-GC analysis, McNally & Grob 1983)

4589 ( $30^{\circ}C$ , headspace-GC analysis, McNally & Grob 1984)

5030 ( $20^{\circ}C$ , selected, Riddick et al. 1986)

5090, 4910, 5090 ( $20$ ,  $35$ ,  $50^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Barr & Newsham 1987)

4842, 4984 (predicted-MCI  $\chi$  and polarizability, Nirmalakhandan & Speece 1988)

5240, 5317, 5406 ( $20$ ,  $30$ ,  $40^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

6560, 7300, 8085 ( $20$ ,  $30$ ,  $40^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -UNIFAC, Tse et al. 1992)

4998, 4434, 5236 ( $20$ ,  $35$ ,  $45^{\circ}C$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

5196\* ( $20^{\circ}C$ , activity coeff. by inert air stripping-GC, measured range  $10$ – $50^{\circ}C$ , Hovorka & Dohnal 1997)

5040\* (recommended, temp range  $0$ – $50^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 9.4136 - 5.7249 \times 10^{-2} \cdot (T/K) + 9.17839 \times 10^{-5} \cdot (T/K)^2$ , temp range  $273$ – $323\ K$  (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

24300, 37000 ( $20^{\circ}C$ ,  $30^{\circ}C$ , Rex 1906)

- 30000\* (Antoine eq. regression, temp range  $-60.7$  to  $57.4^{\circ}\text{C}$ , Stull 1947)  
 22001\* ( $17.62^{\circ}\text{C}$ , static-Hg manometer, measured range  $-38.76$  to  $17.62^{\circ}\text{C}$ , Li & Pitzer 1956)  
 30400 (calculated-Antoine eq., Dreisbach 1961)  
 $\log(P/\text{mmHg}) = 6/9853 - 1171.42/(228.12 + t/^{\circ}\text{C})$ ; temp range  $-15$  to  $82^{\circ}\text{C}$  (Antoine eq. for liquid state, Dreisbach 1961)  
 26000 (calculated-Antoine eq., Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 7288.0/(T/K)] + 7.629952$ ; temp range  $-60.7$  to  $261.5^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)  
 30260 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log(P/\text{mmHg}) = 6.97702 - 1174.022/(229.06 + t/^{\circ}\text{C})$ ; temp range  $-38.8$  to  $17.6^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 30260 (Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.10983 - 1177.636/(229.409 + t/^{\circ}\text{C})$ ; temp range  $-38.8$  to  $17.5^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log(P/\text{mmHg}) = 6.9971 - 1174.02/(229.08 + t/^{\circ}\text{C})$ ; temp range  $-39$  to  $16^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)  
 30360 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 6.16780 - 1201.05/(231.27 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 30360 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.1102 - 1171.42/(-45.03 + T/K)$ ; temp range  $258$ – $365$  K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.14443 - 1216.12/(-36.569 + T/K)$ ; temp range  $323$ – $535$  K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.22839 - 1288.092/(-24.381 + T/K)$ ; temp range  $363$ – $535$  K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 24440, 37240 54990 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , quoted from DIPPR, Tse et al. 1992)  
 $\log(P/\text{mmHg}) = 33.380 - 2.6102 \times 10^3/(T/K) - 9.1336 \cdot \log(T/K) - 2.8838 \times 10^{-11} \cdot (T/K) + 3.7323 \times 10^{-6} \cdot (T/K)^2$ ;  
 temp range  $176$ – $523$  K (vapor pressure eq., Yaws 1994)  
 $\log(P/\text{kPa}) = 6.110022 - 1171.420/(T/K - 45.03)$  (from database of CData 1991, Hovorka & Dohnal 1997)

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

- 595 (calculated- $1/K_{\text{AW}}$  ( $C_{\text{W}}/C_{\text{A}}$ ) reported as exptl., Hine & Mookerjee 1975)  
 595 (calculated- $P/C$ , Dilling 1977)  
 $\log(k_{\text{H}}/\text{atm}) = 8.87 - 1902.37/(T/K)$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)  
 569\* (EPICS-GC/FID, measured range  $9.6$ – $34.6^{\circ}\text{C}$ , Gossett 1987)  
 $\ln[H/(\text{atm m}^3/\text{mol})] = 9.637 - 4128/(T/K)$ ; temp range  $9.6$ – $34.6^{\circ}\text{C}$  (EPICS measurements, Gossett 1987)  
 552 (gas stripping-GC, Warner et al. 1987)  
 633\* (EPICS-GC/FID, measured range  $10$ – $30^{\circ}\text{C}$ , Ashworth et al. 1988)  
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.484 - 3137/(T/K)$ ; temp range  $10$ – $30^{\circ}\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 436 ( $20$ – $25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 584 (calculated- $P/C$ , Mackay & Shiu 1990)  
 595 (computed value, Yaws et al. 1991)  
 436 ( $20^{\circ}\text{C}$ , quoted from Gossett 1987, Tse et al. 1992)  
 466, 709, 1034 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)  
 477, 995, 1226 ( $20$ ,  $35$ ,  $45^{\circ}\text{C}$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)  
 588, 1125, 1844 ( $25$ ,  $35$ ,  $50^{\circ}\text{C}$ , from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 511\* (EPICS-GC/FID, measured range  $2.0$ – $25^{\circ}\text{C}$ , Dewulf et al. 1995)  
 246, 627 ( $6.0$ ,  $25^{\circ}\text{C}$ , EPICS-GC, natural sea water with salinity of  $35\%$ , Dewulf et al. 1995)  
 $\ln K_{\text{AW}} = -3975/(T/K) + 0.00768 \cdot Z + 11.727$ ; with  $Z$  salinity  $0$ – $35.5\%$ , temp range:  $2$ – $35^{\circ}\text{C}$ , (EPICS-GC/FID, Dewulf et al. 1995)  
 526 ( $20^{\circ}\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 466\* ( $20^{\circ}\text{C}$ , equilibrium air stripping-GC, measured range  $10$ – $50^{\circ}\text{C}$ , Hovorka & Dohnal 1997)  
 500 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{\text{AW}} = 4.416 - 1498/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

592\* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)  
 $\ln K_{AW} = 10.09 - 3447.7/(T/K)$ ; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

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:

- 1.79 (shake flask-GC, Hansch et al. 1975, Hansch & Leo 1987)
- 1.92 (Hansch & Leo 1979)
- 1.79 (recommended, Sangster 1993)
- 1.89 (calculated-activity coefficients, Tse & Sandler 1994)
- 1.82\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
- 1.79 (recommended, Hansch et al. 1995)
- 1.75\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

- 2.41 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 1.20 (estimated-S, Lyman et al. 1982)
- 1.28 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)

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

- 1.60 (estimated-S, Lyman et al. 1982)
- 1.48 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)
- 1.66 (soil, selected, Jury et al. 1990)
- 1.43, 1.46, 1.43, 1.48, 1.50, 1.49, 1.55 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)

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

Volatilization: estimated experimental  $t_{1/2} = 22$  min for initial concentration of 1.0 mg/L when stirred at 200 rpm in water at approx. 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);  
 Evaporation  $t_{1/2}(\text{exptl}) = 32.2$  min,  $t_{1/2}(\text{calc}) = 0.98$  min, 21.2 min from water (Dilling 1977);  
 $t_{1/2} = 6\text{--}9$  d in a typical pond,  $t_{1/2} = 5\text{--}8$  d in a typical lake, and  $t_{1/2} = 24\text{--}32$  h in a typical river (Smith et al. 1980; quoted, Howard 1990);  
 ratio of rate of evaporation to that of oxygen reaeration: measured value of 0.57 compared to that predicted value of 0.47 (Smith et al. 1980);  
 $t_{1/2} = 45$  d for the volatilization loss from soil (Jury et al. 1990).

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:

$k_{OH} = (2.6 \pm 0.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980; Howard 1990)

$k_{OH} = 2.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 44 d, loss of 2.3% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{OH} < 1.6 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  for the reaction with OH radical at 300 K (Lyman 1982)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $1.0 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical both at 25°C (Mabey et al. 1982; quoted, Ma et al. 1990)

photooxidation  $t_{1/2} = 247\text{--}2468$  h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis:  $k = 1.15 \times 10^{-7} \text{ M}^{-1} \text{ h}^{-1}$  for neutral process by analogy to dichloromethane (Mabey et al. 1982);

$k = 1.29 \times 10^{-6} \text{ h}^{-1}$  at pH 7 and 25°C with calculated  $t_{1/2} = 61$  yr (Jeffers et al. 1989; quoted, Ellington 1989).

Biodegradation:  $t_{1/2}(\text{aq. aerobic}) = 768\text{--}3696$  h, based on estimated methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a ground water aquifer

(Wilson et al. 1983; quoted, Howard et al. 1991);  $t_{1/2}(\text{aq. anaerobic}) = 3072\text{--}14784$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} > 60$  d (Olsen & Davis 1990).

Biotransformation:

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

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetime of 1.5 months based on reaction with OH radical (Callahan et al. 1979; Altshuller 1980; Howard 1990);

residence time of 44 d, loss of 2.3% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 247\text{--}2468$  h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991); estimated tropospheric lifetime of 0.02 yr (Nimitz & Skaggs 1992).

Surface water:  $t_{1/2} = 768\text{--}3696$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater:  $t_{1/2} = 1344\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life and sub-soil grab sample data from a groundwater aquifer (Wilson et al. 1983; quoted, Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 10\text{--}50$  d (Ryan et al. 1988);

$t_{1/2} = 768\text{--}3696$  h, based on methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a groundwater aquifer (Wilson et al. 1983; quoted, Howard et al. 1991);

$t_{1/2} = 45$  d, volatilization loss from soil (Jury et al. 1990).

Biota:  $t_{1/2} < 2$  d of elimination from whole body of bluegill sunfish (USEPA 1980; quoted, Howard 1990);

$t_{1/2} = 10\text{--}50$  d, subject to plant uptake via volatilization (Ryan et al. 1988).

**TABLE 5.1.1.6.1**

**Reported aqueous solubilities of 1,1-dichloroethane at various temperatures**

$$S/(\text{wt}\%) = 0.5826 - 7.8236 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 1.5268 \times 10^{-4} \cdot (t/^{\circ}\text{C})^2 - 3.6609 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 9.4136 - 5.7249 \times 10^{-2} \cdot (T/\text{K}) + 9.17839 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Rex 1906		Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982	
volumetric method		shake flask		shake flask-GC		summary of literature data	
t/ $^{\circ}\text{C}$	S/g·m <sup>-3</sup>	t/ $^{\circ}\text{C}$	S/g·m <sup>-3</sup>	t/ $^{\circ}\text{C}$	S/g·m <sup>-3</sup>	t/ $^{\circ}\text{C}$	S/g·m <sup>-3</sup>
0	6560	0	5940	10	5030	0	5826
10	5950	20	5060	20	4830	10	5193
20	5500	35	4820	25	4800	20	4843
30	5400	50	5190	30	4810	25	4766
				40	4960	30	4754
				50	5280	40	4905
				60	5790	50	5274
				70	8520	60	5838
				80	7510	70	6575
						80	7465
						eq.1	S/wt%

(Continued)

TABLE 5.1.1.6.1 (Continued)

2.

Barr & Newsham 1987		Wright et al. 1992		Hovorka & Dohnal 1997		Horvath & Getzen 1999a	
infinite dilution activity coeff.		activity coefficient		activity coefficient		recommended, IUPAC-NIST	
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>
20	5090	20	4998	10	5627	0	6240
35	4910	35	4434	20	5196	5	5910
50	5090	45	5236	30	5236	10	5620
				35	5266	15	5380
				40	5395	20	5190
				45	5576	25	5040
				50	5812	30	4930
						35	4880
						40	4870
						45	4900
						50	4980
						eq. 2	S/wt%
						temp range 273–323 K	

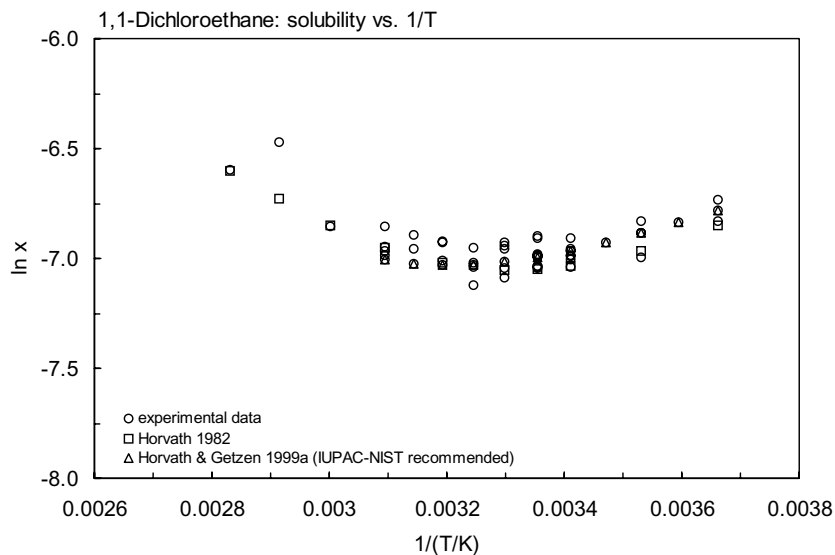


FIGURE 5.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.2  
Reported vapor pressures of 1,1-dichloroethane 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)				
Stull 1947	Li & Pitzer 1956				
summary of literature data	static-Hg manometer				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−60.7	133.3	−38.76	858.6	11.34	16536
−41.9	666.6	−29.61	1649	17.50	21876
−32.3	1333	−20.21	3020	17.62	22001
−21.9	2666	−19.18	3234		
−10.2	5333	−18.16	3301	mp/°C	−96.98
−2.90	7999	−17.69	3517		
7.20	13332	−16.82	3716	eq. 2	P/cmHg
22.4	26664	−12.61	4772	A	6.1560
39.8	53329	−12.20	4869	B	1258.1
57.4	101325	−2.23	8425	C	26.0
		1.18	10077	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 7.87$	
mp/°C	−96.7	11.10	16333	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 31.02$	

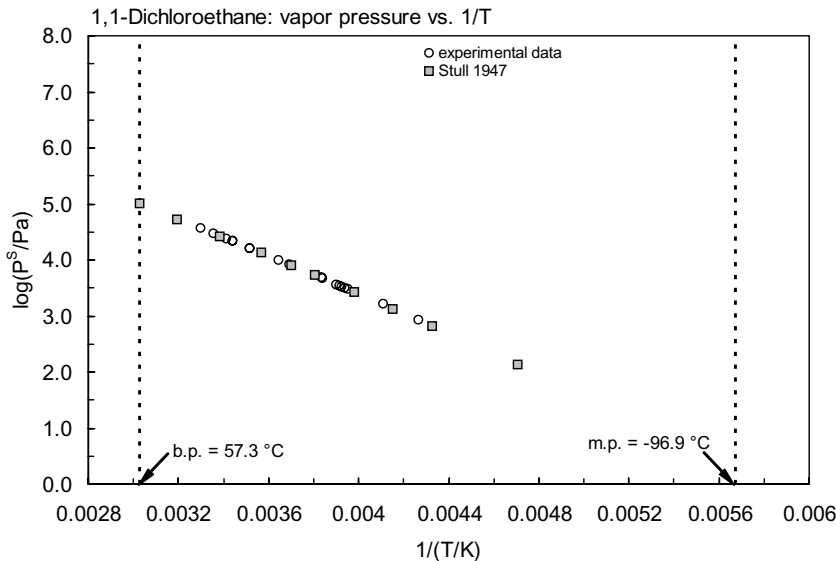


FIGURE 5.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.3

Reported Henry's law constants of 1,1-dichloroethane at various temperatures and temperature dependence equations

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

1.

Gossett 1987		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
EPICS-GC		EPICS-GC		activity coefficient		activity coefficient	
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)
9.6	251.3	10	373	20	466	20	477
17.5	394.2	15	460	30	709	35	995
24.8	569.4	20	570	40	1034	45	1226
34.6	820.7	25	631				
		30	786				
eq. 4	H/(atm m <sup>3</sup> /mol)	eq. 4	H/(atm m <sup>3</sup> /mol)				
A	8.637	A	5.484				
B	4128	B	3137				

2.

Bhatia & Sandler 1995		Dewulf et al. 1995		Hovorka & Dohnal 1997		Görgényi et al. 2002	
activity coefficient		EPICS-GC		equilibrium air stripping-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)
25	588	2	152.1	10	273	2	174
35	1125	6	195.2	20	466	6	240.4
50	1844	10	194.7	30	692	10	283.9
		18.2	378.2	35	851	18	452.4
		25	510.6	40	1010	25	592.4
				45	1172	30	760.9
		eq. 1	K <sub>AW</sub>	50	1338	40	1059
		A	11.727			50	1472
		B	3975			60	1907
						eq. 1	K <sub>AW</sub>
						A	10.09
						B	3447.7



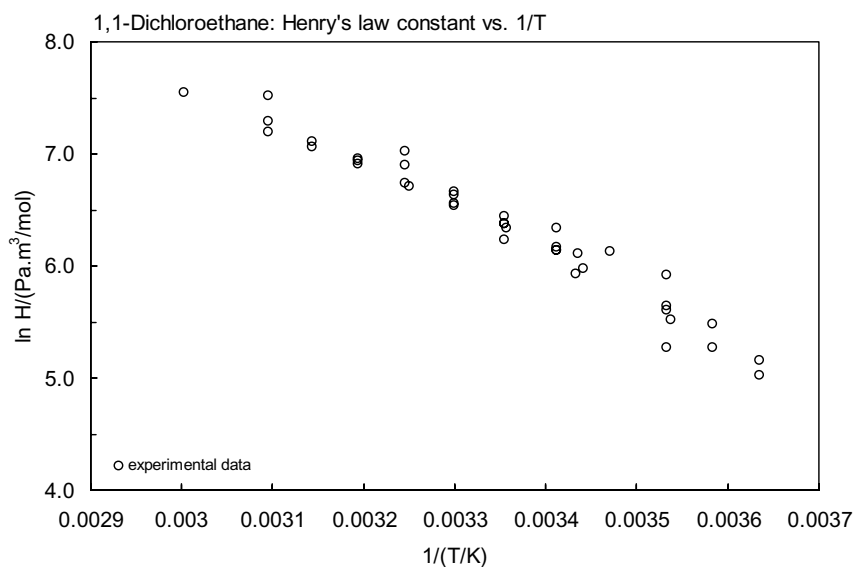
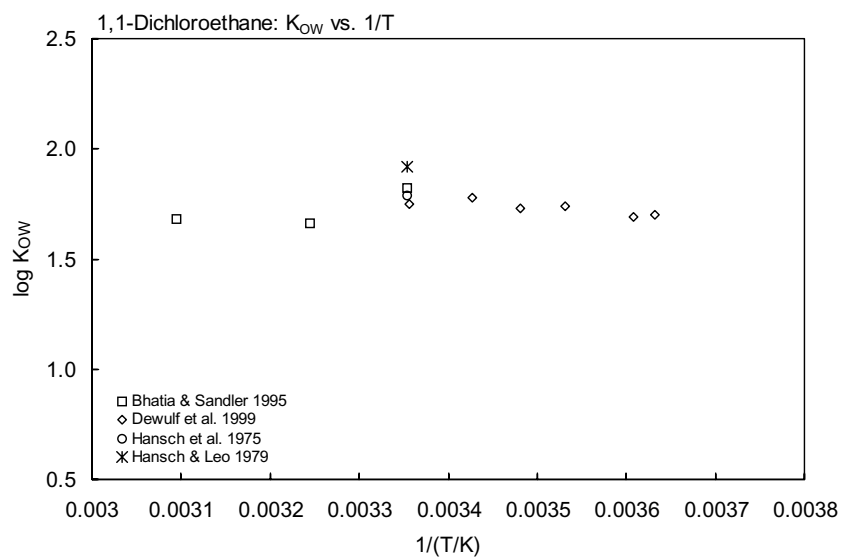


FIGURE 5.1.1.6.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.4

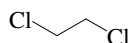
Reported octanol-water partition coefficients of 1,1-dichloroethane at various temperatures

Bhatia & Sandler 1995		DeWulf et al. 1999	
relative GC-RT technique		EPICS-GC	
$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$	$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$
25	1.82	2.2	1.70
35	1.66	4.0	1.69
50	1.68	10.0	1.74
		14.1	1.73
		18.7	1.78
		24.8	1.75
change in enthalpy:			
$\Delta H_{\text{OW}}/(\text{kJ mol}^{-1}) = 5.2$			
(0.0 to 10.4)			
enthalpy of transfer			
$\Delta H_{\text{OCT}}/(\text{kJ mol}^{-1}) = 2.5$			
(-2.7 to 7.7)			



**FIGURE 5.1.1.6.4** Logarithm of  $K_{OW}$  versus reciprocal temperature for 1,1-dichloroethane.

## 5.1.1.7 1,2-Dichloroethane



Common Name: 1,2-Dichloroethane

Synonym: ethylene chloride, ethylene dichloride, glycol dichloride, sym-dichloroethane, Dutch oil, EDC

Chemical Name: 1,2-dichloroethane

CAS Registry No: 107-06-2

Molecular Formula:  $C_2H_4Cl_2$ ,  $CH_2ClCH_2Cl$

Molecular Weight: 98.959

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

−35.7 (Lide 2003)

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

85.3 (Lide 2003)

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

1.2531, 1.2458 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959; Dean 1985)

1.25209, 1.24637 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

78.0 (calculated-density, Wang et al. 1992)

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

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

35.15, 32.02 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

1.982 (calculated, Dreisbach 1959)

2.112 (quoted, Riddick et al. 1986)

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

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

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):

8690\* ( $20^{\circ}C$ , volumetric method, measured range  $0-30^{\circ}C$ , Rex 1906)

8650 (shake flask-interferometer, Gross 1929)

8720, 9000 ( $15^{\circ}C$ ,  $30^{\circ}C$ , shake flask-interferometer, Gross & Saylor 1931)

8696 (volumetric method, Wright & Schaffer 1932)

8490\* ( $20^{\circ}C$ , shake flask, measured range  $0-56^{\circ}C$ , Van Arkel & Vles 1936)

8620 (Seidell 1940)

8400 (data presented in graph, temp range  $0-70^{\circ}C$ , McGovern 1943; Horvath 1982)

8610\* (shake flask-GC, temp range  $0-80^{\circ}C$ , Walraevens et al. 1974)

$\log [S/(mol/L)] = 2070/(T/K) - 15.369 + 0.0247 \cdot (T/K)$ ; temp range  $0-80^{\circ}C$  (Walraevens et al. 1974)

8800 (shake flask-GC, McConnell et al. 1975)

8800 ( $20^{\circ}C$ , Pearson & McConnell 1975)

8570, 8390, 10250 (3, 20,  $34^{\circ}C$ , shake flask-GC/ECD, Chiou & Freed 1977)

8450 (shake flask-GC, Chiou et al. 1979)

8630 ( $20^{\circ}C$ , recommended, Sørensen & Arit 1979)

7987 (shake flask-LSC, Banerjee et al. 1980)

10600 (shake flask-titration, Coca & Diza 1980)

11000 (shake flask-titration/turbidity, Coca et al. 1980)

8000 (shake flask-LSC, Veith et al. 1980)

8608\* (summary of literature data, temp range  $0-80^{\circ}C$ , Horvath 1982)

3506 ( $30^{\circ}C$ , shake flask-headspace-GC, McNally & Grob 1984)

8044 (calculated-UNIFAC activity coeff., Banerjee 1985)

8100 (Dean 1985, Riddick et al. 1986)

8782, 9102, 9960 (20, 35,  $50^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Barr & Newsham 1987)

7200\* ( $19.7^{\circ}C$ , shake flask-GC/TC, measured range  $0-80^{\circ}C$ , Stephenson 1992)

8500, 9013, 9163 (20, 30,  $40^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

7809, 8727, 9209 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -UNIFAC, Tse et al. 1992)  
 9400, 9209, 9835 (20, 35, 50°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 6537 (20°C, activity coeff.  $\gamma^\infty$  by inert air stripping-GC, Hovorka & Dohnal 1997)  
 8600\* (recommended, temp range 0–100°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)  
 $S/(wt\%) = 17.9147 - 0.11684 \cdot (T/K) + 2.0003 \times 10^{-4} \cdot (T/K)^2$ , temp range 273–373 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)404

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):

8130, 12980 (20°C, 30°C, Rex 1906)  
 10519\* (isotenoscope method, measured range –30.82 to 99.4°C, Pearce & Peters 1929)  
 $\log (P/\text{mmHg}) = 128.756 - 4481.12/(T/K) - 52.3092 \cdot \log (T/K) + 0.07153 \cdot (T/K) - 4.1847 \times 10^{-5} \cdot (T/K)^2$ ; temp range 243–363 K (isotenoscope method, Pearce & Peters 1929)  
 10660 (McGovern 1943)  
 10740\* (interpolated-Antoine eq., regression, temp range –30.8 to 99.4°C, Stull 1947)  
 10700 (calculated-Antoine eq., Dreisbach 1959)  
 $\log (P/\text{mmHg}) = 7.18431 - 1358.5/(252.0 + t/^\circ\text{C})$ ; temp range 6–161°C (Antoine eq. for liquid state, Dreisbach 1959)  
 10150 (calculated-Antoine eq., Weast 1972–73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 7950.7/(T/K)] + 7.708405$ ; temp range –44.5 to 285°C (Antoine eq., Weast 1972–73)  
 10500 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log (P/\text{mmHg}) = 7.0253 - 1271.254/(222.927 + t/^\circ\text{C})$ ; temp range –30.82 to 99.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 8520 (McConnell et al. 1975)  
 8400 (Pearson & McConnell 1975)  
 13282\*, 65145 (30, 70°C, vapor-liquid equilibrium VLE data, measured range 28.75–85.54°C, Gutsche & Knapp 1982)  
 $\ln (P/\text{kPa}) = 14.142372 - 2896.480/[(T/K) - 52.506]$ ; temp range 301.9–357.69 K (vapor-liquid equilibrium VLE data, Gutsche & Knapp 1982)  
 10500 (Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.16284 - 1278.323/(223.694 + t/^\circ\text{C})$ ; temp range –30.82 to 99.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.13975 - 1256.68/(220.504 + t/^\circ\text{C})$ ; temp range 28.75–84.54°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{mmHg}) = 7.0253 - 1271.3/(222.9 + t/^\circ\text{C})$ ; temp range –31 to 99°C (Antoine eq., Dean 1985, 1992)  
 11110 (selected, Riddick et al. 1986)  
 11100 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.07712 - 1247.8/(-50.15 + T/K)$ ; temp range 279–434 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.53278 - 1599.07/(-3.303 + T/K)$ ; temp range 356–558 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.07287 - 1245.488/(-50.392 + T/K)$ ; temp range 279–374 K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.40918 - 1505.414/(-14.406 + T/K)$ ; temp range 368–524 K (Antoine eq.-IV, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.5198 - 2129.577/(T/K)$ ; temp range 523–561 K (Antoine eq.-V, Stephenson & Malanowski 1987)  
 10462 (resistance measurements-Antoine eq., Foco et al. 1992)  
 8270, 13320, 16720 (20, 30, 35°C, quoted from DIPPR, Tse et al. 1992)  
 $\log (P/\text{mmHg}) = 48.4226 - 3.1803 \times 10^3/(T/K) - 15.37 \cdot \log (T/K) + 7.2935 \times 10^{-3} \cdot (T/K) + 2.6844 \times 10^{-14} \cdot (T/K)^2$ ; temp range 237–561 K (vapor pressure eq., Yaws 1994)

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):

133.1 (exptl.,  $1/K_{AW} (C_W/C_A)$ , Hine & Mookerjee 1975)  
 92.3 (calculated- $C_W/C_A$ , McConnell et al. 1975; Pearson & McConnell 1975)

- 99.0, 123.9 (exptl., calculated-P/C, Dilling 1977)  
 111.3 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)  
 174\* (27.0°C, equilibrium cell-concn ratio-GC/FID, measured range 1.0–27.0°C, Leighton & Calo 1981)  
 $\ln(k_H/\text{atm}) = 18.51 - 3482/(T/K)$ ; temp range: 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 110 (recommended, Mackay & Shiu 1981)  
 111.5 (gas stripping-GC, Warner et al. 1987)  
 143\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln[H/(\text{atm}\cdot\text{m}^3/\text{mol})] = -1.371 - 1522/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 92.0 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 70.8 (computed value, Yaws et al. 1991)  
 101, 152, 182 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^\circ$ -GC, Tse et al. 1992)  
 110, 185, 319 (20, 35, 50°C, activity coeff.  $\gamma^\circ$ -differential pressure transducer, Wright et al. 1992)  
 122.5 ( $\gamma^\circ$  from gas stripping-GC, Li et al. 1993)  
 5.30, 8.99 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 102.1\* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)  
 55.9, 123 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)  
 $\ln K_{AW} = -4329/(T/K) + 0.00473\cdot Z + 11.377$ ; with Z salinity 0–35.5‰, temp range: 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)  
 110 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 95.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)  
 185.2 (EPICS-GC, Ayuttaya et al. 2001)  
 102 (20°C, selected from reported experimentally determined values, Staudinger & Roberts 2001)  
 $\log K_{AW} = 4.434 - 1705/(T/K)$  (summary of literature 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:

- 1.48 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979, 1987)  
 1.45 (shake flask-LSC, Banerjee et al. 1980; Veith et al. 1980)  
 1.58, 1.54 (calculated-octanol and water mutual solubility not considered, calculated-octanol and water mutual solubility considered, Arbuckle 1983)  
 1.44 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)  
 1.48 (recommended, Sangster 1993)  
 1.55 (calculated-from activity coefficients, Tse & Sandler 1994)  
 1.51\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)  
 1.48 (recommended, Hansch et al. 1995)  
 1.46\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

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

- 2.78 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 0.30 (bluegill sunfish, Barrows et al. 1980)  
 0.301 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)  
 0.954 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982; quoted, Ma et al. 1990)  
 0.30 (bluegill sunfish, Davies & Dobbs; quoted, Sabljic 1987; Ma et al. 1990)

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

- 1.28 (soil, equilibrium sorption isotherm, Chiou et al. 1979)  
 1.51 (soil, quoted from Chiou et al. 1979, Karickhoff 1981)  
 1.06, 1.19, 1.48 (estimated- $K_{OW}$ , estimated-S and mp, estimated-S, Karickhoff 1981)  
 2.18 (estimated- $K_{OW}$ , Lyman et al. 1982;)  
 1.15 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 1.09 (BUA 1987; quoted, Brüggemann et al. 1991)

1.34 (soil, selected, Jury et al. 1990)

1.64, 1.645, 1.64, 1.68, 1.70, 1.65, 1.68 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)

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

1.28, 1.50 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)

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

Volatilization: estimated experimental half-life of volatilization from aqueous solution of 1 mg/L to be  $(28 \pm 1)$  min when stirred at 200 rpm in water at approx. 25°C in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation  $t_{1/2}(\text{exptl}) = 28.0$  min,  $t_{1/2}(\text{calc}) = 4.5$  min, 24.5 min from water (Dilling 1977)

rate of evaporation  $k = 2.4 \text{ g m}^{-2} \text{ s}^{-1}$  (Environment Canada 1984);

$t_{1/2} = 90$  d, estimated volatilization loss from soil (Jury et al. 1990).

Photolysis: photocatalyzed mineralization by the presence of  $\text{TiO}_2$  with the rate of 1.1 ppm/min per gram of catalyst (Ollis 1985)

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:

$k_{OH} = (2.2 \pm 0.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow-laser magnetic resonance, Howard & Everson 1976b; quoted, Callahan et al. 1979)

$k_{OH} = 0.1 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  and  $t_{1/2} = 234$  h (Radding et al. 1977; quoted, Callahan et al. 1979)

$k_{OH} = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with residence time of 53 d, loss of 1.9% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH} = 1.3 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , estimated, at 300 K (Lyman 1982)

$k < 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k < 1 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radicals at 25°C (Mabey et al. 1982)

photooxidation  $t_{1/2} = 292\text{--}2917$  h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k(\text{aq.}) \leq 0.05 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 21°C, with a  $t_{1/2} \geq 8$  d at pH 7 (Yao & Haag 1991).

Hydrolysis:

$k = 5 \times 10^{-13} \text{ s}^{-1}$  with a max.  $t_{1/2} = 50,000$  yr at pH 7 and 25°C from experimental data at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979);

$k = 1.80 \times 10^{-9} \text{ h}^{-1}$  for neutral process (Mabey et al. 1982; quoted, Ma et al. 1990)

$t_{1/2}(\text{abiotic})$  or  $t_{1/2}(\text{dehydrohalogenation}) = 50$  months (Mabey et al. 1983; quoted, Olsen & Davis 1990)

$k(\text{neutral}) = .63 \text{ yr}^{-1}$  with first-order  $t_{1/2} = 1.1$  yr (Kollig et al. 1987; quoted, Howard et al. 1991)

$k = 1.1 \times 10^{-6} \text{ h}^{-1}$  at pH 7 and 25°C with calculated  $t_{1/2} = 72$  yr (Jeffers et al. 1989; quoted, Ellington 1989; Brüggemann et al. 1991)

$t_{1/2} = 400$  d at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: relatively undegradable (Lyman et al. 1982; quoted, Brüggemann et al. 1991)

$k < 1.4 \times 10^{-5} \text{ min}^{-1}$  disappearance rate in sediment-water sample, with  $t_{1/2} > 35$  d (Jafvert & Wolfe 1987)

$t_{1/2}(\text{aq. aerobic}) = 2400\text{--}4320$  h, based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 9600\text{--}17280$  h (Howard et al. 1991)

$t_{1/2} > 60$  d (Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 100$  d,  $t_{1/2}(\text{anaerobic}) = 400$  d in natural waters (Capel & Larson 1995)

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

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

Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 17$  wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

lifetime of 1.7 months at 296 K based on reaction with OH radical (Callahan et al. 1979);

residence time of 53 d, loss of 1.9% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 292\text{--}2917$  h, based on photooxidation half-life in air from measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water:  $t_{1/2} = 2400\text{--}4320$  h, based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991);

$t_{1/2} > 35$  d in sediment-water sample (Jafvert & Wolfe 1987)

$t_{1/2}(\text{aerobic}) = 100$  d,  $t_{1/2}(\text{anaerobic}) = 400$  d in natural waters (Capel & Larson 1995)

measured rate constant  $k \leq 0.05 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 21°C, with  $t_{1/2} \geq 8$  d at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 2400\text{--}8640$  h, based on unacclimated grab sample of aerobic soil from ground water aquifers and estimated aqueous aerobic biodegradation half-life (Wilson et al. 1983; Howard et al. 1991).

Sediment:  $t_{1/2} > 35$  d in Bar-H sediment-water sample (Jafvert & Wolfe 1987)

Soil:  $t_{1/2} = 10\text{--}50$  d (Ryan et al. 1988);

$t_{1/2} = 90$  d, estimated volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 2400\text{--}4320$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

$t_{1/2} = 10\text{--}50$  d, subject to plant uptake via volatilization (Ryan et al. 1988).

**TABLE 5.1.1.7.1**

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

$$\log [S/(\text{mol/L})] = -A + 2070/(T/K) + B(T/K) \quad (1)$$

$$S/(\text{wt}\%) = 0.888 - 4.0468 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 9.37388 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 9.8465 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (2)$$

$$S/(\text{wt}\%) = 17.9147 - 0.11684 \cdot (T/K) + 2.0003 \times 10^{-4} \cdot (T/K)^2 \quad (3)$$

1.

Rex 1906		Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982	
volumetric method		shake flask		shake flask		summary of literature data	
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>
0	9220	0	8370	10	8520	0	8880
10	8650	20	8490	20	8490	10	8579
20	8690	36	8950	25	8610	20	8524
30	8904	56	10300	30	8800	25	8608
				40	9440	30	8775
				50	10460	40	9391
				60	11920	50	10430
				70	13950	60	11951
				80	16720	70	14014
						80	16678
Gross & Saylor 1931							
shake flask-IR							
t/°C	S/g·m <sup>-3</sup>						
15	8720			eq. 1	S/(mol/L)		
30	9000			A	15.369	eq. 1	S/wt%
				B	0.0247		

\*data calculated by Horvath 1982

(Continued)

TABLE 5.1.1.7.1 (Continued)

2.

Barr & Newsham 1987		Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
infinite dilution activity coeff.		shake flask-GC		activity coefficient		activity coefficient	
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>
20	8782	0	8200	20	8500	20	9400
35	9102	9.3	7700	30	9013	35	9209
50	9960	19.7	7200	40	9163	50	9835
		29.7	8100				
		39.4	9800				
		50.3	10600				
		61.0	10800				
		70.6	11300				
		80.7	10600				

3.

Horvath & Getzen 1999a					
recommended, IUPAC-NIST					
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0	9240	40	9410	80	15990
5	8910	45	9890	85	17270
10	8680	50	10460	90	18640
15	8550	55	11130	95	20110
20	8520	60	11900	100	21680
25	8600	65	12780		
30	8770	70	13750	eq. 2	S/wt%
35	9040	75	14820	temp range 273–373 K	

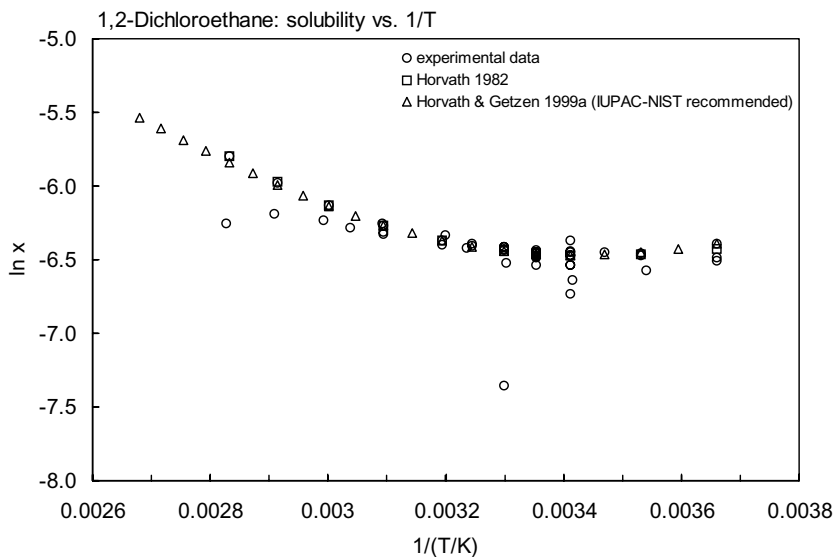


FIGURE 5.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,2-dichloroethane.



TABLE 5.1.1.7.2

Reported vapor pressures of 1,2-dichloroethane 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)			
Pearce & Peters 1929		Stull 1947		Gutsche & Knapp 1982	
isoteniscope method		summary of literature data		Bourdon-tube manometer	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-30.82	427	-44.5	133.3	28.75	12530
-24.92	613	-24.0	666.6	38.65	19521
-19.32	860	-13.6	1333	46.39	27004
-15.02	1093	-2.40	2666	51.72	33373
-10.42	1547	10.0	5333	56.63	40285
-5.12	2120	18.1	7999	60.79	47009
0.070	2800	29.4	13332	64.19	53158
5.09	3760	45.7	26664	67.62	60006
10.07	4893	64.0	53329	70.24	65669
15.52	6546	82.4	101325	73.85	74207
20.21	8279			76.36	80633
25.25	10639	mp/ $^{\circ}\text{C}$	-35.3	78.67	86926
30.23	13452			80.80	93115
35.24	16839			82.74	98997
39.79	20425			84.54	104743
45.13	25544				
51.12	31304			eq. 3	P/kPa
55.22	37997			A	14.142372
60.28	45969			B	2896.480
65.27	55035			C	52.506
70.27	65448				
75.36	77220				
80.43	91046				
85.45	105938				
91.03	124603				
bp/ $^{\circ}\text{C}$	84.1				
$\Delta H_v/(\text{kJ mol}^{-1}) = 32.41$ at bp					
vapor pressure eq. see <a href="#">ref.</a>					

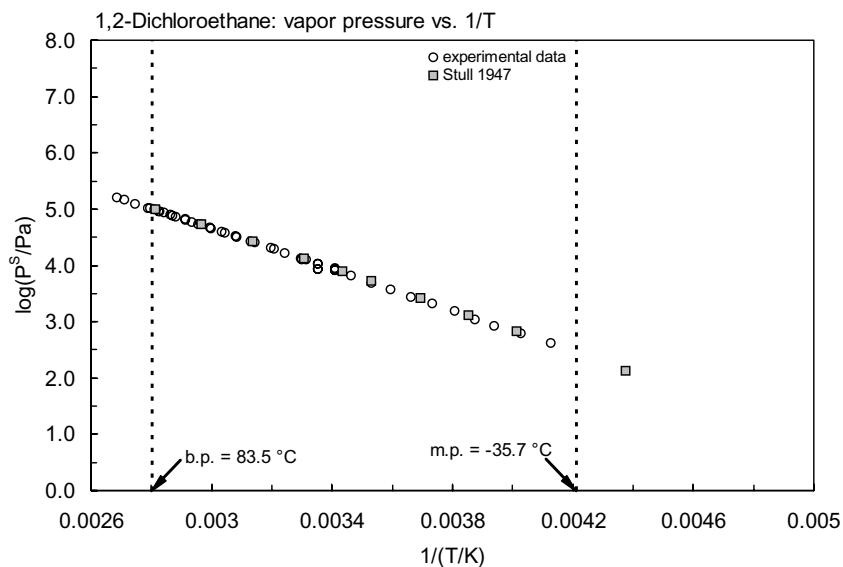


FIGURE 5.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloroethane.

TABLE 5.1.1.7.3  
Reported Henry’s law constants of 1,2-dichlorethane 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
Leighton & Calo 1981		Ashworth et al. 1988		Dewulf et al. 1995	
equilibrium cell-GC		EPICS-GC		EPICS-GC	
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)
1.0	55.85	10	118.6	2.0	32.03
1.3	56.34	15	131.7	6.0	42.47
11.0	84.92	20	148.95	10.0	39.55
21.0	125.6	25	142.87	18.2	75.4
22.0	139.7	30	176.3	25.0	102.1
27.2	174.1				
25	119.3	eq. 4	H/(atm m <sup>3</sup> /mol)	eq. 1	K <sub>AW</sub>
		A	-1.371	A	11.377
eq. 3	H/atm	B	1522	B	4329
A	16.05				
B	3539				

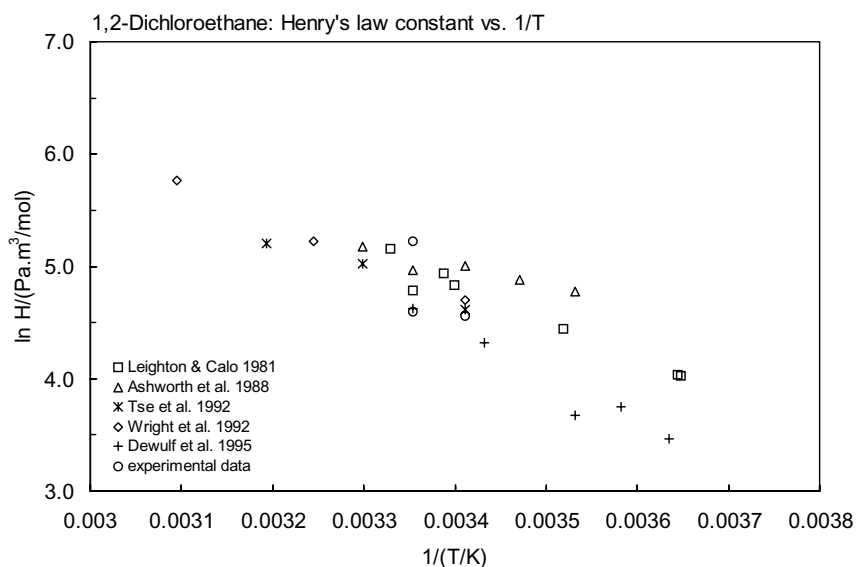
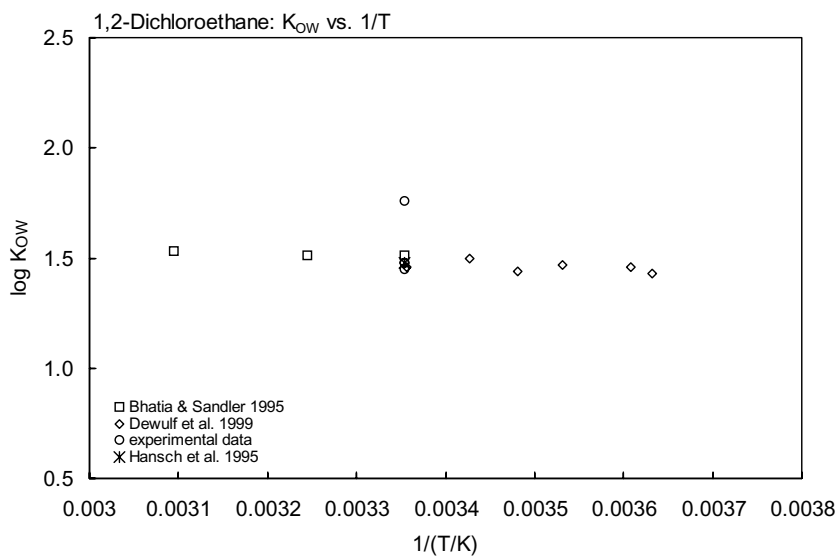


FIGURE 5.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dichloroethane.

**TABLE 5.1.1.7.4**  
Reported octanol-water partition coefficients of 1,2-dichloroethane at various temperatures

Bhatia & Sandler 1995		DeWulf et al. 1999	
relative GC-RT technique		EPICS-GC	
$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$	$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$
25	1.51	2.2	1.43
35	1.51	4.0	1.46
50	1.53	10.0	1.47
		14.1	1.44
		18.7	1.50
		24.8	1.46
change in enthalpy:			
$\Delta H_{\text{OW}} / (\text{kJ mol}^{-1}) = 3.3$			
(-2.1 to 8.6)			
enthalpy of transfer			
$\Delta H_{\text{oct}} / (\text{kJ mol}^{-1}) = 0.2$			
(-5.2 to 5.5)			



**FIGURE 5.1.1.7.4** Logarithm of  $K_{OW}$  versus reciprocal temperature for 1,2-dichloroethane.

## 5.1.1.8 1,1,1-Trichloroethane



Common Name: 1,1,1-Trichloroethane

Synonym: methyl chloroform, chlorotene, Genklene, Baltana

Chemical Name: 1,1,1-trichloroethane

CAS Registry No: 71-55-6

Molecular Formula:  $\text{CH}_3\text{CCl}_3$

Molecular Weight: 133.404

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

−30.01 (Lide 2003)

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

74.09 (Lide 2003)

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

1.3390 (Dreisbach 1961; Horvath 1982; Weast 1982–83; McNally & Grob 1984)

1.3381, 1.3299 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Riddick et al. 1986)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

99.0, 52.0 (calculated-density, intrinsic volume-van der Waals method, Abernethy et al. 1988)

100.0 (calculated-density, Wang et al. 1992)

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

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

32.74, 29.74 ( $25^{\circ}\text{C}$ , bp, Dreisbach 1961)

32.39, 29.708 ( $25^{\circ}\text{C}$ , bp, Riddick et al. 1986)

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

2.35 (Riddick et al. 1986)

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

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

Water Solubility ( $\text{g}/\text{m}^3$  or  $\text{mg}/\text{L}$  at  $25^{\circ}\text{C}$  or as indicated or as indicated and reported temperature dependence equations.

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

1320\* ( $20^{\circ}\text{C}$ , shake flask, measured range  $0$ – $50^{\circ}\text{C}$ , Van Arkel & Vles 1936)

1304 (Seidell 1940)

1490\* (shake flask-GC, measured range  $10$ – $80^{\circ}\text{C}$ , Walraevens et al. 1974)

$\log [S/(\text{mol}/\text{L})] = 2070/(T/\text{K}) - 14.860 + 0.020 \cdot (T/\text{K})$ ; temp range 2630353 K (shake flask, Walraevens et al. 1974)

480 ( $20^{\circ}\text{C}$ , shake flask-GC, Pearson & McConnell 1975; McConnell et al. 1975)

880, 720 (1.5,  $25^{\circ}\text{C}$ , average literature values, Dilling 1977)

1360 (shake flask, Chiou et al. 1979)

1320 ( $20^{\circ}\text{C}$ , recommended, Sørensen & Arit 1979)

100 (shake flask-titration, Coca & Diaz 1980)

1334 (shake flask-LSC, Banerjee et al. 1980)

1150, 1200 ( $23.5^{\circ}\text{C}$ , elution chromatography, Schwarz 1980)

1850\* ( $20^{\circ}\text{C}$ , elution chromatography, measured range  $10$ – $30^{\circ}\text{C}$ , Schwarz & Miller 1980)

1334; 278.7 (shake flask-LSC; calculated-f const., Veith et al. 1980)

1260 (calculated-group contribution as per Irmann 1965, Horvath 1982)

1485\* (summary of literature data, temp range  $0$ – $80^{\circ}\text{C}$ , Horvath 1982)

3200 (calculated-UNIFAC activity coeff., Arbuckle 1983)

479.8 ( $30^{\circ}\text{C}$ , headspace-GC, McNally & Grob 1984)

1334 (calculated-UNIFAC activity coeff., Banerjee 1985)

1320 ( $20^{\circ}\text{C}$ , selected, Riddick et al. 1986)

1310, 1194, 1267 ( $20$ ,  $35$ ,  $50^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Barr & Newsham 1987)

1252 ( $23$ – $24^{\circ}\text{C}$ , shake flask-GC, Broholm et al. 1992)

700\* ( $20.2^{\circ}\text{C}$ , shake flask-GC/TC, measured range  $0$ – $71.5^{\circ}\text{C}$ , Stephenson 1992)

1260, 1353, 1370 (20, 30, 40°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 1413, 1392, 1454, 1489 (20, 30, 35, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)  
 2935, 3228, 3536, 3749 (20, 30, 35, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -UNIFAC, Tse et al. 1992)  
 1758 ( $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)  
 1250 (shake flask-GC, Broholm & Feenstra 1995)  
 1380 (20°C, activity coeff.  $\gamma^\infty$  by inert air stripping-GC, Hovorka & Dohnal 1997)  
 1290\* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)  
 $S/(\text{wt}\%) = 1.09092 - 6.52776 \times 10^{-3} \cdot (T/K) + 1.10747 \times 10^{-5} \cdot (T/K)^2$ , temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

12159\* (17.68°C, static method-Hg manometer, measured range 268–290 K, Rubin et al. 1944)  
 $\log(P/\text{cmHg}) = 6.92013 - 1729/(T/K)$ ; temp range 268–290 K (Hg manometer, Rubin et al. 1944)  
 16190\* (interpolated from Antoine eq. regression, temp range –52 to 74.1°C, Stull 1947)  
 16100 (calculated-Antoine eq., Dreisbach 1961)  
 $\log(P/\text{mmHg}) = 6.94983 - 1217.0/(225.0 + t/^\circ\text{C})$ ; temp range –3 to 111°C (Antoine eq. for liquid state, Dreisbach 1961)  
 16170 (calculated-Antoine eq., Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 8012.7/(T/K)] + 7.955902$ ; temp range –52 to 74.1°C (Antoine eq., Weast 1972–73)  
 16490\* (ebulliometry, measured range –77.15 to 25°C, Ambrose et al. 1975)  
 16490 (ebulliometry, measured –77.15 to 25°C, Boublik et al. 1984)  
 17800 (calculated-Antoine eq., Boublik et al. 1973, 1984)  
 $\log(P/\text{mmHg}) = 8.64344 - 2136.621/(302.769 + t/^\circ\text{C})$ ; temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 12800 (20°C, Pearson & McConnell 1975; McConnell et al. 1975)  
 17800, 16490 (calculated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 7.78612 - 2147.034/(303.568 + t/^\circ\text{C})$ ; temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.13297 - 1260.034/(231.327 + t/^\circ\text{C})$ ; temp range –77.2 to 25°C (Antoine eq. from reported exptl. data of Ambrose et al. 1973, Boublik et al. 1984)  
 $\log(P/\text{mmHg}) = 8.6434 - 2136.6/(302.8 + t/^\circ\text{C})$ ; temp range –6 to 17°C (Antoine eq., Dean 1985, 1992)  
 16490 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 5.98755 - 1182.527/(222.594 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 16490 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 5.98755 - 1182.527/(-50.256 + T/K)$ ; temp range; 295–372 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.00452 - 1193.604/(-48.734 + T/K)$ ; temp range 349–408 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.36873 - 1474.394/(-8.08 + T/K)$ ; temp range 399–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 16530, 960 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)  
 13150, 20520, 25300, 30940 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)  
 $\log(P/\text{mmHg}) = 36.5468 - 2.821 \times 10^3/(T/K) - 10.205 \cdot \log(T/K) - 2.6369 \times 10^{-9} \cdot (T/K) + 3.7075 \times 10^{-6} \cdot (T/K)^2$ ; temp range 243–545 K (vapor pressure eq., Yaws 1994)

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):

1638 (calculated as  $1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)  
 3433 (20°C, McConnell et al. 1975)  
 2800, 2875 (exptl., calculated-P/C, Dilling 1977)  
 2025 (20°C, batch stripping-GC, Mackay et al. 1979)  
 730 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)  
 $\log(k_{\text{H}}/\text{atm}) = 9.39 - 1992.95/(T/K)$ , (least-square regression of data from lit., Kavanaugh & Trussell 1980)  
 1996\* (equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)

- $\ln (k_H/\text{atm}) = 21.68 - 4375/(T/K)$ ; temp range 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 1520 (20°C, batch air stripping, Munz & Roberts 1982)  
 836, 1317, 2155 (10, 20, 30°C, multiple equilibrium-GC, Munz 1985)  
 606.9 (20°C, predicted-UNIFAC activity coeff., Arbuckle 1983)  
 1319\* (multiple equilibrium technique-GC, temp range 5–33°C, Hunter-Smith et al. 1983)  
 $\ln K_{AW} = 9.15 - 2915/(T/K)$ ; measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)  
 $\ln K_{AW} = 13.04 - 3905/(T/K)$ ; measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith 1983)  
 1743 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)  
 1337, 1358 (20°C, EPICS-GC/FID, batch air stripping-GC, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 10.21 - 4262/(T/K)$ ; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.975 - 4186/(T/K)$ ; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)  
 498.5 (adsorption isotherm, Urano & Murata 1985)  
 1360 (20°C, multiple equilibration, Munz & Roberts 1986; quoted, Yurteri et al. 1987)  
 $\log K_{AW} = 5.327 - 1636/(T/K)$ ; temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)  
 498.5 (gas stripping-GC, Warner et al. 1987)  
 1345, 1413\* (20, 25°C, EPICS-GC/FID, measured range 9.6–24.6°C, Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.777 - 4133/(T/K)$ ; temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)  
 1572 (20°C, EPICS, Yurteri et al. 1987)  
 1763\* (EPICS-GC, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 7.351 - 3399/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 1317 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 1578\* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)  
 $\ln (1/K_{AW}) = -2.52 + 950/(T/K)$ ; temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)  
 1277, 2027, 2381, 2847 (20, 30, 35, 40°C, from measured activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)  
 1380, 1998, 2952 (20, 30, 40°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 1763\* (26.3°C, EPICS-GC, measured range 26.3–44.8°C, Hansen et al. 1993)  
 $\ln [H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -3120/(T/K) + 11.0$ ; temp range 26.3–45°C (EPICS-GC, Hansen et al. 1993)  
 1783\* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)  
 1507\* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)  
 800, 2010 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)  
 $\ln K_{AW} = -3834/(T/K) + 0.00897 \cdot Z + 12.351$ ; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID measurements, Dewulf et al. 1995)  
 1387 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 2072 (vapor-liquid equilibrium-GC, Turner et al. 1996)  
 $K_{AW} = 0.204 + 0.0182 \cdot (T/K) + 0.000173 \cdot (T/K)^2$ ; temp range 0–35°C (vapor-liquid equilibrium-GC with additional lit. data, Turner et al. 1996)  
 1280 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)  
 1614, 1750, 1415; 1380 (direct calculated method, gas-phase EPICS method, liquid-phase EPICS method; quoted lit. Chiang et al. 1998)  
 1370 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{AW} = 5.163 - 1588/(T/K)$  (summary of literature 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:

- 2.17 (Tute 1971)  
 2.49 (shake flask, Hansch & Leo 1979; Hansch & Leo 1985)  
 2.47 (shake flask-LSC, Banerjee et al. 1980)  
 2.47 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)  
 2.35, 2.29 (calculated-UNIFAC with octanol and water mutual solubility not considered, calculated-UNIFAC with octanol and water mutual solubility considered, Arbuckle 1983)  
 1.96 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)  
 2.49 (recommended, Sangster 1993)  
 2.60 (calculated-activity coefficients, Tse & Sandler 1994)

- 2.47\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)  
 2.20\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

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

- 2.70 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 1.40 (calculated- $K_{OW}$ , Veith et al. 1979; Veith et al. 1980)  
 0.954 (bluegill sunfish, Veith et al. 1980)  
 0.954 (bluegill sunfish, Barrows et al. 1980)  
 1.908 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 0.950 (bluegill sunfish, Veith & Kosian 1982)  
 1.70 (calculated-MCI  $\chi$ , Koch 1983)

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

- 2.02 (soil, equilibrium sorption isotherm, Chiou et al. 1979)  
 2.25 (quoted from Chiou et al. 1979, Karickhoff 1981, 1985)  
 2.08, 2.04, 2.02 (estimated- $K_{OW}$ , estimated-S and mp, estimated-S, Karickhoff 1981)  
 2.182 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 2.20 (soil, best estimate, Karickhoff 1985)  
 1.70 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)  
 2.26 (20°C, soil, Chiou et al. 1988)  
 1.65 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)  
 2.22 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)  
 3.02 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)  
 2.053 (soil, selected, Jury et al. 1990)  
 1.95, 1.98, 1.99, 2.01, 1.98, 2.03 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)  
 3.20 (soil, calculated-universal solvation model, Winget et al. 2000)  
 2.16 (soil: organic carbon  $OC \geq 0.1\%$ , average, Delle Site 2001)

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

- 2.02, 1.55 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)

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

- Volatilization: evaporation  $t_{1/2}(\text{exptl}) = 21$  min,  $t_{1/2}(\text{calc}) = 0.34$  min from water (Dilling et al. 1975)  
 $t_{1/2}(\text{exptl}) \sim (20 \pm 3)$  min at 25°C for an aqueous solution of 1 mg L<sup>-1</sup> when stirred at 200 rpm in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);  
 Evaporation  $t_{1/2}(\text{exptl}) = (17.3\text{--}24.9)$  min,  $t_{1/2}(\text{calc}) = 0.19$  min, 23.7 min at 20–25°C, and  $t_{1/2} = 30.2$  min at 15°C from water (Dilling 1977);  
 estimated  $t_{1/2} \sim 3.7$  h from water (Thomas 1982);  
 $k = 0.029$  d<sup>-1</sup>,  $t_{1/2} = 24$  d in spring at 8–16°C,  $k = 0.058$  d<sup>-1</sup>,  $t_{1/2} = 12$  d in summer at 20–22°C,  $k = 0.063$  d<sup>-1</sup>,  $t_{1/2} = 11$  d in winter at 3–7°C for the periods when volatilization appears to dominate, and  $k = 0.60$  d<sup>-1</sup>,  $t_{1/2} = 11.5$  d with HgCl<sub>2</sub>, and  $k = 0.072$  d<sup>-1</sup>,  $t_{1/2} = 9.6$  d without HgCl<sub>2</sub> in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);  
 estimated  $t_{1/2} \sim 365$  d for volatilization loss from soil to be 365 d (Jury et al. 1990).

Photolysis: not expected to be important (Howard et al. 1991).

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 and/or the Arrhenius expression see reference:

- $k_{OH} = 3.36 \times 10^{-14}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a troposphere life time of 1.1 yr at 298 K (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)  
 $k_{OH} = (1.5 \pm 0.3) \times 10^{-14}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296 K (discharge flow-resonance fluorescence, Howard & Evenson 1976b)



$k_{\text{OH}}^* = (2.19 \pm 0.26) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 275–405 K, with calculated lifetime of 3.8–6.0 yr in troposphere (discharge flow system-resonance fluorescence, Chang & Kaufman 1977)

$k_{\text{OH}} = (1.59 \pm 0.16) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K with lifetime of 13 yr (flash photolysis-resonance fluorescence, Watson et al. 1977; quoted, Callahan et al. 1979; Altshuller 1980)

$k_{\text{OH}}^* = (1.06 \pm 0.09) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 293 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)

$k_{\text{OH}}^* = (1.08 \pm 0.20) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 222–363 K (flash photolysis resonance fluorescence, Kurylo et al. 1979)

$k_{\text{OH}} = 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , with an estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k = 9.0 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , estimated at 300 K (Lyman 1982)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $1.0 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation  $t_{1/2} = 5393\text{--}53929 \text{ h}$ , based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 1.3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}}^* = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Prinn et al. 1987; quoted, Bunce et al. 1991)

$k_{\text{O}_3}(\text{aq.}) \leq 0.012 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 22°C, with  $t_{1/2} \geq 32 \text{ d}$  at pH 7 (Yao & Haag 1991).

Hydrolysis:  $k = 0.12 \text{ month}^{-1}$  with  $t_{1/2}(\text{exptl.}) = 6 \text{ months}$  at pH 7 and 25°C (Dilling et al. 1975; quoted, Callahan et al. 1979; Mabey et al. 1979; Neely 1985);

$k = 0.96 \text{ yr}^{-1}$  at pH 7 and 25°C with a first-order hydrolysis  $t_{1/2} = 0.73 \text{ yr}$  (Kollig et al. 1987);

$k = (1.93 \pm 0.40) \times 10^{-8} \text{ s}^{-1}$  in distilled water contained 0.1% w/w  $\text{CH}_2\text{O}$  as sterilant with 39% conversion,

$k = (2.04 \pm 0.47) \times 10^{-8} \text{ s}^{-1}$  in autoclaved distilled water with 40% conversion and

$k = (1.80 \pm 0.90) \times 10^{-8} \text{ s}^{-1}$  in sediment contained 0.1% w/w  $\text{CH}_2\text{O}$  as sterilant with 25% conversion at 25°C, calculated  $t_{1/2} = 350 \text{ d}$  at 25°C (Haag & Mill 1988)

$t_{1/2} = 6 \text{ months}$ , abiotic hydrolysis or dehydrohalogenation half-life (Olsen & Davis 1990)

$t_{1/2} = 0.73 \text{ yr}$ , based on reported rate constant at pH 7 at 25°C (Howard et al. 1991)

Biodegradation:

$k = 0.043 \text{ d}^{-1}$  in fresh water plus sediment incubated under anaerobic conditions (Wood et al. 1981; quoted, Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 3360\text{--}6552 \text{ h}$ , based on unacclimated aerobic seawater grab sample data and sub-soil sample data from a ground water aquifer (Pearson & McConnell 1975; Wilson et al. 1983; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 13440\text{--}26208 \text{ h}$ , based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 26 \text{ wk}$ , when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

estimated troposphere residence time of 1.1 yr for reaction with OH radical (CEQ 1975);

estimated N. troposphere residence time of 7.2 yr by one compartment non-steady state model (Singh et al. 1978);

estimated troposphere residence time of 8–10 yr by two compartment non-steady state model (Singh 1977; Singh et al. 1979);

lifetime of 8 yr in troposphere (Altshuller 1980);

estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

atmospheric lifetime  $\tau = 6.3 \text{ yr}$  (Prinn et al. 1987);

troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Bunce et al. 1991)

$t_{1/2} = 5393\text{--}53929$  h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

estimated tropospheric lifetime of 7.8 yr and 6.1 yr by rigorous calculations (Nimitz & Skaggs 1992).

Surface water:  $t_{1/2} = 24$  d in the spring at 8–16°C,  $t_{1/2} = 12$  d in the summer at 20–22°C,  $t_{1/2} = 11$  d in the winter at 3–7°C when volatilization dominates, and  $t_{1/2} = 11.5$  d and 9.6 d for experiments with and without  $\text{HgCl}_2$  as poison, respectively, in September 9–15 in marine mesocosm experiment (Wakeham et al. 1983);

calculated hydrolysis  $t_{1/2} = 350$  d at 25°C (Haag & Mill 1988);

$t_{1/2} = 3360\text{--}6552$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$k(\text{exptl}) \leq 0.012 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 22°C, with  $t_{1/2} \geq 32$  d at pH 7 (Yao & Haag 1991).

Ground water: estimated  $t_{1/2} \sim 1.0$  yr in the groundwater of the Netherlands (Zoeteman et al. 1981);

$t_{1/2} = 3360\text{--}13104$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life and sub-soil grab sample data from a ground water aquifer (Howard et al. 1991; Wilson et al. 1983).

Sediment: measured  $t_{1/2} = 450$  d at 25°C, based on neutral and base-catalyzed hydrolysis rates studied in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil:  $t_{1/2} = 365$  d, estimated volatilization loss (Jury et al. 1990);

$t_{1/2} = 3360\text{--}6552$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

**TABLE 5.1.1.8.1**

**Reported aqueous solubilities of 1,1,1-trichloroethane at various temperatures**

$$S/(\text{wt}\%) = 0.1910 - 2.2811 \times 10^{-3} \cdot (t/^\circ\text{C}) + 2.5529 \times 10^{-5} \cdot (t/^\circ\text{C})^2 - 2.4775 \times 10^{-8} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 1.09092 - 6.52776 \times 10^{-3} \cdot (T/\text{K}) + 1.10747 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Schwarz & Miller 1980		Horvath 1982	
shake flask		shake flask-GC		elution chromatography		summary of literature data	
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>
0	1590	10	1730	10	1800	0	1910
20	1320	20	1550	20	1850	10	1707
35	1260	25	1490	30	1590	20	1554
50	1280	30	1440			25	1495
		40	1390			30	1449
		50	1380			40	1390
		60	1410			50	1377
		70	1480			60	1407
		80	1590			70	1479
						80	1592
						eq. 1	S/wt%

TABLE 5.1.1.8.1 (Continued)

2.

Barr & Newsham 1987		Stephenson 1992		Tse et al 1992		Horvath & Getzen 1999a	
activity coefficient		shake flask-GC		activity coefficient		recommended, IUPAC-NIST	
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>
20	1310	0	1470	20	1413	0	1340
35	1194	20.2	700	30	1392	5	1320
50	1267	31.6	760	35	1454	10	1300
		41.1	1010	40	1489	15	1290
		51.3	1060			20	1290
		61.5	1030			25	1290
		71.5	1140			30	1300
				Wright et al. 1992		35	1310
				activity coefficient		40	1330
				t/°C	S/g·m <sup>-3</sup>	45	1350
				20	1260	50	1380
				30	1353		
				40	1370		
						eq. 2 S/wt% temp range 273–323 K	

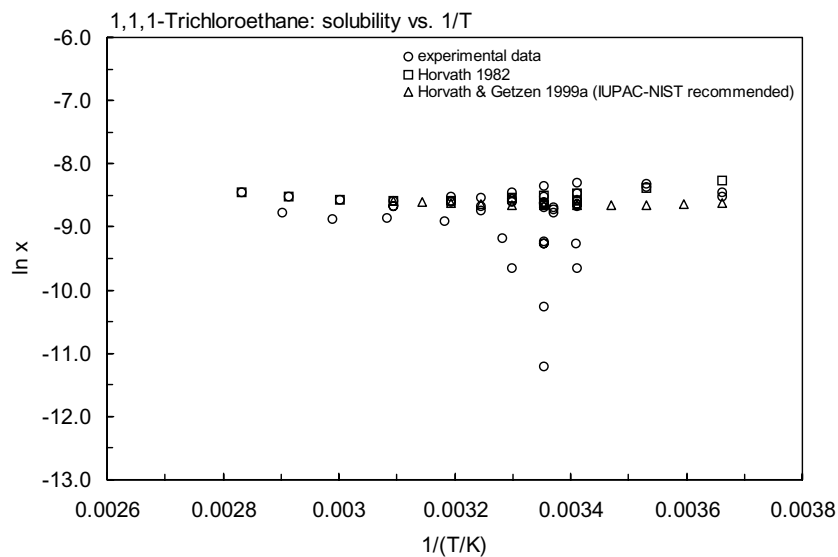


FIGURE 5.1.1.8.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.2

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

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

Rubin et al. 1944		Stull 1947		Ambrose et al. 1975	
static-mercury manometer		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-5.534	3840	-52.0	133.3	-77.15	20
-0.207	5160	-32.0	666.6	-55.15	100
5.12	6733	-21.9	1333	-25.85	1000
11.33	9239	-10.8	2666	14.15	10000
16.93	12159	1.6	5333	25.0	16490
		9.5	7999		
mp/K	240.2	20.0	13332		
		36.2	26664		
eq. 1	P/cmHg	54.6	53329		
A	6.92013	74.1	101325		
B	1729				
		mp/°C	-30.6		

$\Delta H_v/(\text{kJ mol}^{-1}) = 33.42$   
at 286.53 K

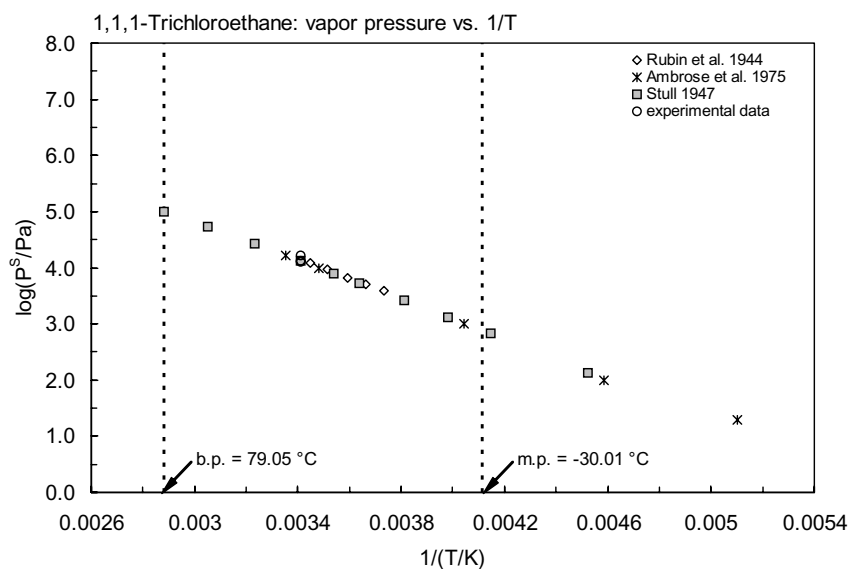


FIGURE 5.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.3

Reported Henry's law constants of 1,1,1-trichloroethane at various temperatures and temperature dependence equations

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

1.

Leighton & Calo 1981		Hunter-Smith 1983		Gossett 1987		Ashworth et al. 1988	
equilibrium cell-GC		multiple equilibrium-GC		EPICS-GC		EPICS-GC	
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)
1.0	541.7	5	612	9.6	771	10	978
1.0	543.3	10	749	17.5	1216	15	1165
1.2	555.9	15	912	24.8	1743	20	1479
2.5	597.9	20	1102	34.6	2523	25	1763
7.0	763.3	25	1324			30	2138
10.0	919.2	33	1738	eq. 4	H/(atm m <sup>3</sup> /mol)	eq. 4	H/(atm m <sup>3</sup> /mol)
12.0	1016			A	9.777	A	7.351
12.0	1039			B	4133	B	3399
12.9	1069						
14.0	1190						
18.0	1398						
18.0	1447						
18.0	1464						
19.0	1511						
19.2	1526						
19.5	1437						
24.3	1874						
25.2	1995						
25.3	2026						
26.0	1988						
26.0	2064						
26.1	1958						
$\ln (k_H/\text{atm}) = A - B/(T/K)$							
A	21.68						
B	4375						

2.

Kolb et al. 1992		Tse et al. 1992		Wright et al. 1992		Hansen et al. 1993	
equilibrium headspace-GC		activity coefficient		activity coefficient		EPICS-GC	
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)
40	1578	20	1277	20	1380	26.3	1763
60	1884	30	2027	30	1998	35.0	2412
70	2264	35	2381	40	2952	44.8	3232
80	2488	40	2847				
						eq. 4	H/(kPa m <sup>3</sup> /mol)
eq. 2	1/K <sub>AW</sub>					A	11 ± 0.30
A	-2.52					B	3120 ± 93
B	-950						

(Continued)

TABLE 5.1.1.8.3 (Continued)

3.

Robbins et al. 1993		Dewulf et al. 1995	
static headspace-GC		EPICS-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
25	1783	2.0	152.1
30	2209	6.0	195.2
40	2675	10.0	194.7
45	3597	18.2	378.2
50	4164	25.0	510.6
		eq. 1	K <sub>AW</sub>
		A	12.351
		B	3834

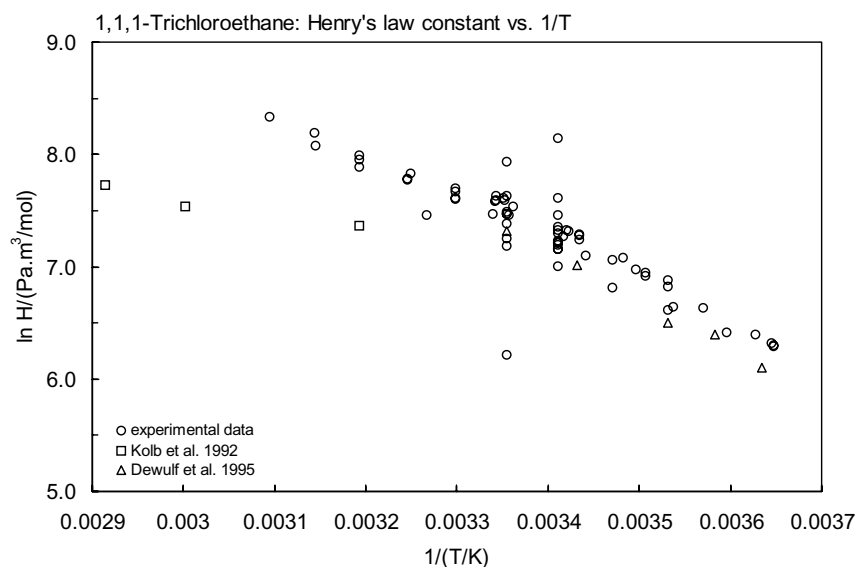


FIGURE 5.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.4

Reported octanol-water partition coefficients of 1,1,1-trichloroethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		shake flask-GC	
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OW</sub>
25	2.47	2.2	2.18
35	2.50	6.0	2.18
50	2.52	10.0	2.28
		14.1	2.24
		18.7	2.285
		24.8	2.20
enthalpy of transfer			
ΔH/(kJ mol <sup>-1</sup> ) = -20.2			
log K <sub>OW</sub> = A - ΔH/2.303RT			
A	1.0195		
ΔH	-20.2		

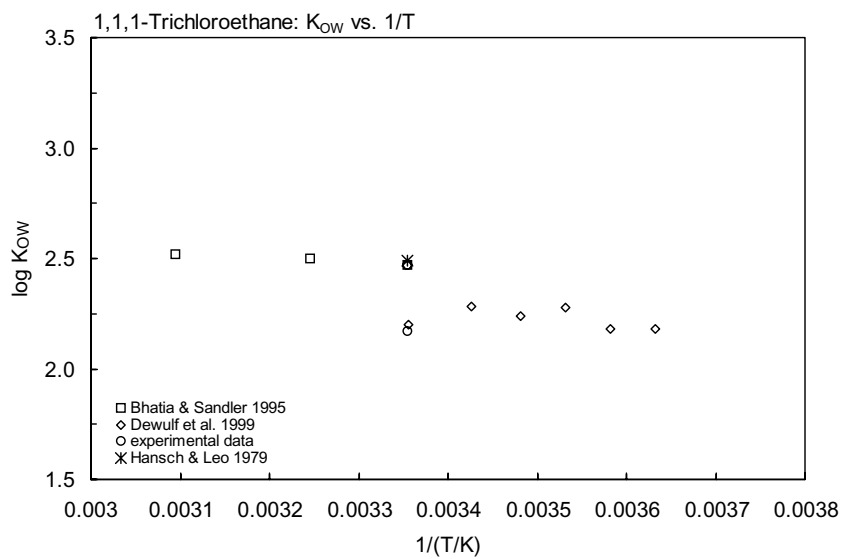
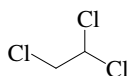


FIGURE 5.1.1.8.4 Logarithm of  $K_{OW}$  versus reciprocal temperature for 1,1,1-trichloroethane.

## 5.1.1.9 1,1,2-Trichloroethane



Common Name: 1,1,2-Trichloroethane

Synonym: vinyl trichloride

Chemical Name: 1,1,2-trichloroethane

CAS Registry No: 79-00-5

Molecular Formula:  $\text{CH}_2\text{ClCHCl}_2$ 

Molecular Weight: 133.404

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

-36.3 (Lide 2003)

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

113.8 (Lide 2003)

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

1.440 (Dreisbach 1959; Weast 1982–83; Verschuereen 1983;)

1.43931, 1.43213( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Riddick et al. 1986)Molar Volume ( $\text{cm}^3/\text{mol}$ ):

93.0 (calculated-density, Wang et al. 1992)

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

Enthalpy of Vaporization,  $\Delta H_v$  ( $\text{kJ}/\text{mol}$ ):46.77, 37.07 ( $25^{\circ}\text{C}$ , bp, Dreisbach 1961)40.28, 34.23 ( $25^{\circ}\text{C}$ , bp, Riddick et al. 1986)Enthalpy of Fusion,  $\Delta H_{\text{fus}}$  ( $\text{kJ}/\text{mol}$ ):

11.543 (Dreisbach 1959; quoted, Riddick et al. 1986)

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

3704 (volumetric method, Wright &amp; Schaffer 1932)

4580\* (shake flask, measured range  $0$ – $55^{\circ}\text{C}$ , Van Arkel & Vles 1936)

4418 (Seidell 1940)

4400 (data presented in graph, temp range  $0$ – $70^{\circ}\text{C}$ , McGovern 1943)

4400 (shake flask-refractive index and density, Treybal et al. 1946)

4380\* (shake flask-GC, measured range  $0$ – $80^{\circ}\text{C}$ , Walraevens et al. 1974) $\log [S/(\text{mol}/\text{L})] = 2070/(T/K) - 15.285 + 0.0230 \cdot (T/K)$ ; temp range  $0$ – $80^{\circ}\text{C}$  (Walraevens et al. 1974)

4420 (literature average, Dilling 1977)

4500 ( $20^{\circ}\text{C}$ , Verschuereen 1977, 1983)4370 ( $20^{\circ}\text{C}$ , recommended, Sørensen & Arit 1979)

5100 (shake flask-titration/turbidity, Coca &amp; Diaz 1980, Coca et al. 1980)

1490 (shake flask-LSC, Veith et al. 1980)

4394\* (summary of literature data, temp range  $0$ – $80^{\circ}\text{C}$ , Horvath 1982)4365 ( $30^{\circ}\text{C}$ , headspace-GC, McNally & Grob 1984)

4800 (Dean 1985)

4941, 4876, 5183 ( $20$ ,  $35$ ,  $50^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Barr & Newsham 1987)2858, 1469 (predicted-MCI  $\chi$  and polarizability, Nirmalakhandan & Speece 1988)4580\* ( $31.3^{\circ}\text{C}$ , shake flask-GC/TC, measured range  $0$ – $90.8^{\circ}\text{C}$ , Stephenson 1992)4813, 5035, 5205 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)2574, 2960, 3378 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -UNIFAC, Tse et al. 1992)4877, 5257, 6075 ( $20$ ,  $35$ ,  $50^{\circ}\text{C}$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)4460 ( $20^{\circ}\text{C}$ , activity coeff.  $\gamma^{\infty}$  by inert air stripping-GC, Hovorka & Dohnal 1997)



4590\* (tentative values, temp range 0–55°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(\text{wt}\%) = 2.89796 - 1.8585 \times 10^{-2} \cdot (T/K) + 3.48961 \times 10^{-5} \cdot (T/K)^2$ , temp range 273–328 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

26664\* (73.5°C, ebulliometry, measured range 73.5–113.5°C, Treybal et al. 1946)

3090\* (Antoine eq. regression, temp range –24 to 113.9°C, Stull 1947)

19114\* (49.97°C, ebulliometry, measured range 49.97–113.67°C, Dreisbach & Shrader 1949)

2998 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/\text{mmHg}) = 6.84165 - 1262.6/(205.0 + t/^\circ\text{C})$ ; temp range 30–186°C (Antoine eq. for liquid state, Dreisbach 1959)

3217 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.96527 - 1351.0/(217.0 + t/^\circ\text{C})$ ; temp range 29–155°C (Antoine eq. for liquid state, Dreisbach 1961)

3088 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 9163.2/(T/K)] + 8.079996$ ; temp range –24 to 113.9°C, (Antoine eq., Weast 1972–73)

2910 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/\text{mmHg}) = 6.95185 - 1314.41/(209.197 + t/^\circ\text{C})$ ; temp range 49.97–113.7°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)

3066 (literature average, Dilling 1977)

2533, 4266 (20, 30°C, Verschuereen 1983)

$\log(P/\text{kPa}) = 6.13975 - 1313.598/(209.106 + t/^\circ\text{C})$ ; temp range 49.97–113.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

$\log(P/\text{mmHg}) = 6.95185 - 1314.41/(209.20 + t/^\circ\text{C})$ ; temp range 50–114°C (Antoine eq., Dean 1985, 1992)

2998 (selected lit., Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.10301 - 1332.6/(211.38 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

3218 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.09017 - 1351.0/(-56.15 + T/K)$ ; temp range 302–428 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.13875 - 1351.685/(-59.953 + T/K)$ ; temp range 316–384 K (Antoine eq., Stephenson & Malanowski 1987)

2369, 4012, 6590 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)

$\log(P/\text{mmHg}) = 25.0845 - 2.7368 \times 10^3/(T/K) - 5.9182 \cdot \log(T/K) + 2.5155 \times 10^{-10} \cdot (T/K) + 1.1831 \times 10^{-6} \cdot (T/K)^2$ ; temp range 237–602 K (vapor pressure eq., Yaws 1994)

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):

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

94.2 (calculated-P/C, Dilling 1977)

78.4 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

122, 120 (calculated-P/C, recommended, Mackay & Shiu 1981, 1990)

81.4\* (24.3°C, equilibrium cell-concn ratio-GC/FID, measured range 2.5–26.1°C, Leighton & Calo 1981)

$\ln(k_H/\text{atm}) = 16.20 - 3690/(T/K)$ ; temp range 2.5–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

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

$\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 9.320 - 4943/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

74.97 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

97.34 (computed value, Yaws et al. 1991)

70.9, 115.5, 172.3 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)

67.1, 136, 234 (20, 35, 50°C, activity coeff  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)

82\* (26.2°C, EPICS-GC, measured range 26.2–44.8°C, Hansen et al. 1993)

$\ln[H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -5091/(T/K) + 17.0$ ; temp range 26.2–45°C (EPICS-GC measurements, Hansen et al. 1993)

- 1.30, 2.48 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 122 (quoted from Howard 1989–1991, Capel & Larson 1995)  
 66.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)  
 65.7 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 66.78 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 5.219 - 1989/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

- 2.17 (calculated as per Tute 1971, Callahan et al. 1979; Ryan et al. 1988)  
 2.38 (Hansch & Leo 1979)  
 1.89 (shake flask, Log P Database, Hansch & Leo 1987)  
 1.89 (recommended, Sangster 1993)  
 2.07 (calculated-activity coefficients, Tse & Sandler 1994)  
 1.98\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)  
 1.89 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

- 3.40 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- < 1.0 (Kawasaki 1980; quoted, Howard 1990)  
 1.519 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 1.23 (quoted, Isnard & Lambert 1988)  
 1.049 (calculated- $K_{OW}$ , McCarty et al. 1992)

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

- 1.845 (sandy soil column, Wilson et al. 1981)  
 1.748 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 3.20; 1.90 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)  
 1.88 (soil: organic carbon OC  $\geq 0.1\%$ , average, Delle Site 2001)

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

Volatilization:  $t_{1/2} = 21$  min, estimated from lab. experiment of initial 1 mg/L in water stirred at 200 rpm at 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Howard 1990)

Evaporation  $t_{1/2}(\text{exptl}) = 35.1$  min,  $t_{1/2}(\text{calc}) = 6.1$  min, 30.1 min from water (Dilling 1977)

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 and/or the Arrhenius expression see reference:  
 $k_{OH}^* = (3.18 \pm 0.06) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)  
 $k_{OH} = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , with estimated residence time of 35 d, loss of 2.8% in 1 d 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  $k = 3.0 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)  
 photooxidation  $t_{1/2} \sim 196\text{--}1956$  h, based on measured rate constants for reaction with hydroxyl radical in air (estimated, Atkinson 1985; quoted, Howard et al. 1991)  
 $k_{OH}^* = (3.18 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K, measured range 277–461 K (discharge flow-resonance fluorescence, Jeong et al. 1984)  
 $k_{O_3}(\text{aq.}) \leq 0.08 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 22°C, with  $t_{1/2} \geq 5$  d at pH 7 (Yao & Haag 1991).  
 $k_{OH}(\text{aq.}) = 1.1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

## Hydrolysis:

$k = 1.2 \times 10^{-7} \text{ h}^{-1}$  at 25°C and pH 7 (estimated, Mabey et al. 1982)

$k = 5.9 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 3263 \text{ h}$ , based on alkaline catalyzed hydrolysis reaction at pH 9 and 25°C;  
 $t_{1/2} = 37 \text{ yr}$ , based on hydrolysis rate constant measured at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard 1990; Howard et al. 1991)

$t_{1/2}(\text{abiotic})$  or  $t_{1/2}(\text{dehydrohalogenation}) = 170 \text{ months}$  (Olsen & Davis 1990)

$t_{1/2} = 14000 \text{ d}$  at pH 7,  $t_{1/2} = 0.14 \text{ d}$  at pH 12 in natural waters (Capel & Larson 1995)

## Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 4320\text{--}8760 \text{ h}$ , based on the extremely low or no biodegradation which was observed in screening tests and a river die-away test (Tabak et al. 1981; Kawasaki 1980; Mudder & Musterman 1982; quoted, Howard 1990; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 17280\text{--}35040 \text{ h}$ , based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991)

$k = 0.04 \text{ yr}^{-1}$  with  $t_{1/2} = 24 \text{ d}$  (Wood et al. 1985; quoted, Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 180 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 720 \text{ d}$  in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant  $k = 3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

$k_1 = 0.763 \text{ h}^{-1}$  (flagfish, calculated-BCF  $\times k_2$ , McCarty et al. 1992)

$k_2 = 0.0676 \text{ h}^{-1}$  (flagfish, estimated from one compartment first-order kinetic, McCarty et al. 1992)

## Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  for the reaction with OH radical in air (Darnall et al. 1976);

photodecomposition  $t_{1/2} = 15.9 \text{ h}$  with NO under simulated atmospheric conditions (Dilling et al. 1976);

estimated residence time of 35 d, loss of 2.8% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 196\text{--}1956 \text{ h}$ , based on measured rate constants for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: estimated  $t_{1/2} = 1.9 \text{ d}$  in surface waters in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 3263\text{--}8760 \text{ h}$ , based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous degradation half-life (Howard et al. 1991)

Biodegradation  $t_{1/2}(\text{aerobic}) = 100 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 400 \text{ d}$  and hydrolysis  $t_{1/2} = 14000 \text{ d}$  at pH 7,  $t_{1/2} = 0.14 \text{ d}$  at pH 12 in natural waters (Capel & Larson 1995)

$k(\text{exptl}) \leq 0.08 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 22°C, with  $t_{1/2} \geq 5 \text{ d}$  at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 3263\text{--}117520 \text{ h}$ , based on estimated hydrolysis half-life pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and data from estimated unacclimated aerobic aqueous biodegradation half-life as well as a ground water die-away study in which no biodegradation was observed (Wilson et al. 1984; quoted, Howard et al. 1991).

## Sediment:

Soil:  $t_{1/2} = 3263\text{--}8760 \text{ h}$ , based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991) and a soil column test in which no biodegradation was observed (Wilson et al. 1981; quoted, Howard et al. 1991).

## Biota:

TABLE 5.1.1.9.1

Reported aqueous solubilities of 1,1,2-trichloroethane at various temperatures

$$S/(\text{wt}\%) = 0.48137 - 2.9594 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 4.3162 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 3.2190 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

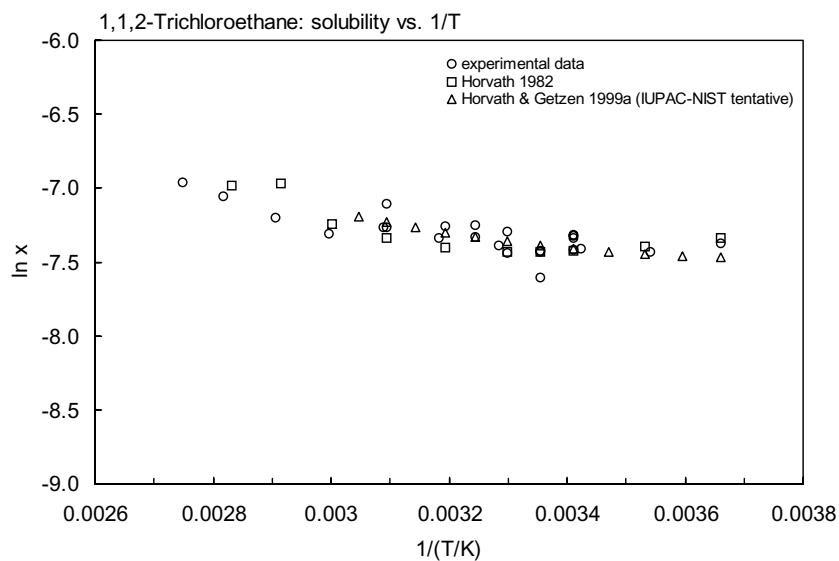
$$S/(\text{wt}\%) = 2.89796 - 1.8585 \times 10^{-2} \cdot (T/\text{K}) + 3.48961 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982		Barr & Newsham 1987	
shake flask				summary of literature data		activity coefficient	
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>
0	4660	10	4600	0	4814	20	4941
20	4360	20	4410	10	4546	35	4876
25	4580	25	4380	20	4420	50	5183
55	5320	30	4390	25	4394		
		40	4530	30	4401		
		50	4830	40	4527		
		60	5290	50	4815		
		70	5950	60	5287		
		80	6860	70	6961		
				80	6857		
				eq. 1	S/wt%		

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999a	
shake flask-GC		activity coefficient		activity coefficient		tentative, IUPAC-NIST	
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>
0	4640	20	4813	20	4877	0	4250
9.2	4390	30	5035	35	5257	5	4280
31.3	4580	40	5205	50	6075	10	4330
41	4830					15	4400
50.6	5180					20	4490
60.5	4970					25	4590
710	5550					30	4710
81.7	6380					35	4850
90.8	7030					40	5000
						45	5170
						50	5360
						55	5570
						eq. 2	S/wt%
						temp range 263–328 K	

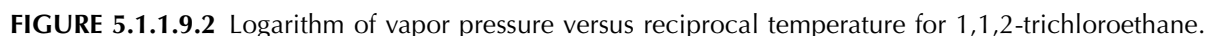


**FIGURE 5.1.1.9.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,1,2-trichloroethane.

**TABLE 5.1.1.9.2**

Reported vapor pressures of 1,1,2-trichloroethane at various temperatures

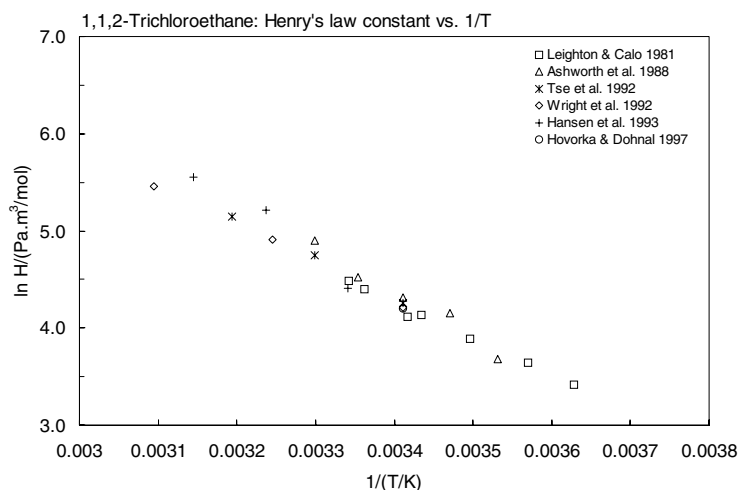
Treybal et al. 1946		Stull 1947		Dreisbach & Shrader 1949	
ebulliometry		summary of literature data		ebulliometry	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
73.5	26664	-24.0	133.3	49.97	19114
80.3	34397	-2.0	666.6	61.29	16500
82.4	37064	8.3	1333	85.99	42066
83.8	38530	21.6	2666	100.34	67661
85.6	41597	35.2	5333	113.67	101325
96.2	59328	44.0	7999		
104.6	77594	55.7	13332		
108.7	87326	73.3	26664		
109.8	90393	93.0	53329		
111.3	94392	113.9	101325		
113.5	101325				



**Reported Henry's law constants of 1,1,2-trichloroethane at various temperatures and temperature dependence equations**

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

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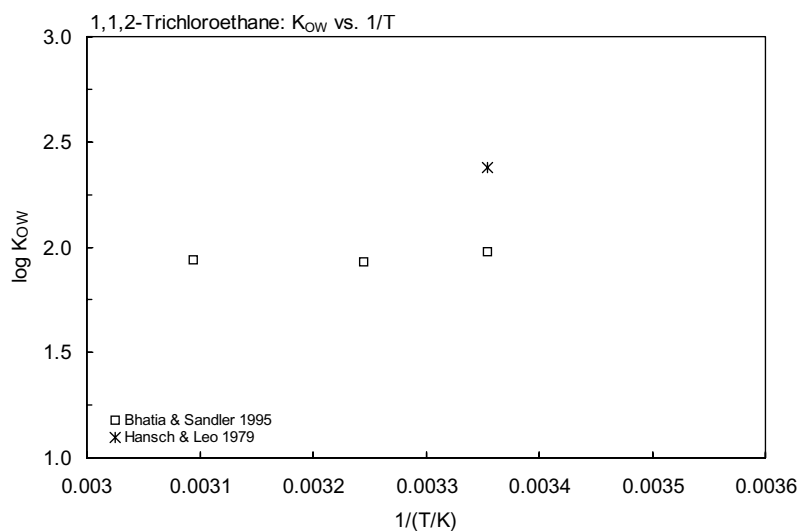


**FIGURE 5.1.1.9.3** Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2-trichloroethane.

**TABLE 5.1.1.9.4**

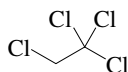
**Reported octanol-water partition coefficients of 1,1,2-trichloroethane at various temperatures**

Bhatia & Sandler 1995	
relative GC-RT technique	
$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$
25	1.98
35	1.93
50	1.94
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2.$	
$\log K_{\text{OW}} = A - \Delta H/2.303RT$	
A	1.0195
$\Delta H$	-20.2



**FIGURE 5.1.1.9.4** Logarithm of  $K_{\text{OW}}$  versus reciprocal temperature for 1,1,2-trichloroethane.

## 5.1.1.10 1,1,1,2-Tetrachloroethane



Common Name: 1,1,1,2-Tetrachloroethane

Synonym:

Chemical Name: 1,1,1,2-tetrachloroethane

CAS Registry No: 630-20-6

Molecular Formula:  $\text{CH}_2\text{ClCCl}_3$

Molecular Weight: 167.849

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

-70.2 (Lide 2003)

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

130.2 (Lide 2003)

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

1.5406 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

1.5328 ( $25^{\circ}\text{C}$ , Dreisbach 1961)

1.4819 (Dean 1985)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

109.0 ( $20^{\circ}\text{C}$ , calculated-density)

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

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

34.78, 42.18 (normal boiling point,  $25^{\circ}\text{C}$ , Dreisbach 1961)

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

1090\* ( $20^{\circ}\text{C}$ , shake flask, measured range  $0$ – $50^{\circ}\text{C}$ , Van Arkel & Vles 1936)

1110 (Seidell 1940)

1100\* (shake flask, temp range  $10$ – $80^{\circ}\text{C}$ , Walraevens et al. 1974)

$\log [S/(\text{mol}/\text{L})] = 2070/(T/\text{K}) - 16.165 + 0.0236 \cdot (T/\text{K})$ , temp range  $283$ – $353$  K (Walraevens et al. 1974)

1100 (interpolation of literature values, Dilling 1977)

215, 200, 202 (3, 20,  $34^{\circ}\text{C}$ , shake flask-GC, Chiou & Freed 1977)

1110\* (summary of literature data, temp range  $0$ – $80^{\circ}\text{C}$ , Horvath 1982)

1206, 1280, 1292, 1321 (20, 30, 35,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

1178, 1382, 1492, 1607 (20, 30,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -UNIFAC, Tse et al. 1992)

1005, 1093, 1056 (20, 30,  $40^{\circ}\text{C}$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

1070\* (recommended, temp range  $0$ – $50^{\circ}\text{C}$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(\text{wt}\%) = 2.17896 - 1.3966 \times 10^{-3} \cdot (T/\text{K}) + 2.93282 \times 10^{-5} \cdot (T/\text{K})^2$ , temp range  $273$ – $323$  K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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

1767\* (Antoine eq. regression, temp range  $58$ – $200^{\circ}\text{C}$ , Stull 1947)

8851\* ( $59.31^{\circ}\text{C}$ , ebulliometry, measured range  $59.31$ – $130.2^{\circ}\text{C}$ , Dreisbach & Shrader 1949)

1578 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/\text{mmHg}) = 6.97560 - 1410.7/(214.0 + t/^{\circ}\text{C})$ ; temp range  $43$ – $174^{\circ}\text{C}$  (Antoine eq. for liquid state, Dreisbach 1961)

1778 (calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 9296.5/(T/\text{K})] + 7.938042$ ; temp range  $-16.3$  to  $130.5^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)

1604 (calculated-Antoine eq., Boublik et al. 1973, 1984)



$\log(P/\text{mmHg}) = 6.89875 - 1365.876/(209.744 + t/^{\circ}\text{C})$ ; temp range 59–130°C (Antoine eq. from reported exptl. data of data of Dreisbach & Shrader 1949, Boublik et al. 1973)

1853 (20°C, interpolation of literature values, Dilling 1977)

$\log(P/\text{kPa}) = 6.02534 - 1366.919/(209.861 + t/^{\circ}\text{C})$ ; temp range 59.31–130.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

$\log(P/\text{mmHg}) = 6.89875 - 1365.88/(209.74 + t/^{\circ}\text{C})$ ; temp range 59–130°C (Antoine eq., Dean 1985, 1992)

1578 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.1005 - 1410.7/(-59.15 + T/\text{K})$ ; temp range 316–417 K (Antoine eq., Stephenson & Malanowski 1987)

1201, 2120, 2765, 3575 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)

$\log(P/\text{mmHg}) = -1.0712 - 2.5074 \times 10^3/(T/\text{K}) + 6.1536 \cdot \log(T/\text{K}) - 1.8763 \times 10^{-2} \cdot (T/\text{K}) + 1.0462 \times 10^{-5} \cdot (T/\text{K})^2$ ; temp range 203–624 K (vapor pressure eq., Yaws 1994)

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

272.7 (calculated-P/C, Dilling 1977)

283, 280 (calculated-P/C, recommended, Mackay & Shiu 1981)

172, 2, 284, 365, 486 (20, 30, 35, 40°C, infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

196, 320, 560 (20, 30, 40°C, activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

0.496, 0.80 (30, 40°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

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

3.03 (calculated, Müller & Klein 1992)

2.62, 2.62 (30, 40°C, infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

Bioconcentration Factor,  $\log BCF$ :

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

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

Volatilization:  $t_{1/2} = 43$  min for the evaporation from dilute aqueous solution (Dilling et al. 1975)

Evaporation  $t_{1/2}(\text{exptl}) = 42.3$  min,  $t_{1/2}(\text{calc}) = 2.01$  min, 48.8 min from water (Dilling 1977)

Photolysis:

Oxidation:

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:

$k_{OH} < 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time  $> 1160$  d, loss  $< 0.1\%$  in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photooxidation  $t_{1/2} = 2236\text{--}22361$  h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:  $k = 1.2 \text{ M}^{-1} \text{ s}^{-1}$  for reaction at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991);

$k = 4320 \text{ M}^{-1} \text{ h}^{-1}$  for base reaction at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991);

abiotic hydrolysis or dehydrohalogenation  $t_{1/2} = 384$  months (Mabey et al. 1983; quoted, Olsen & Davis 1990).

Biodegradation: aqueous aerobic  $t_{1/2} = 672\text{--}4320$  h, based on acclimated river die-away rate data for 1,1,2,2-tetrachloroethane (Mudder 1981; quoted, Howard et al. 1991), unacclimated sea water (Pearson & McConnell 1975; quoted, Howard et al. 1991) and sub-soil grab sample data for a ground water aquifer for 1,1,1-trichloroethane (Wilson et al. 1983; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2688\text{--}17280$  h, based on aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976) residence time  $> 1160$  d, loss  $< 0.1\%$  in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical with OH radical (Singh et al. 1981)

$t_{1/2} = 2236\text{--}22361$  h, based on an estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 1.9 yr (Nimitz & Skaggs 1992).

Surface water:  $t_{1/2} = 16\text{--}1604$  h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 16\text{--}1604$  h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 16\text{--}1604$  h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Biota:

**TABLE 5.1.1.10.1**

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

$$S/(\text{wt}\%) = 0.11968 - 7.87116 \times 10^{-4} \cdot (t/^{\circ}\text{C}) + 1.42253 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 7.24354 \times 10^{-8} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

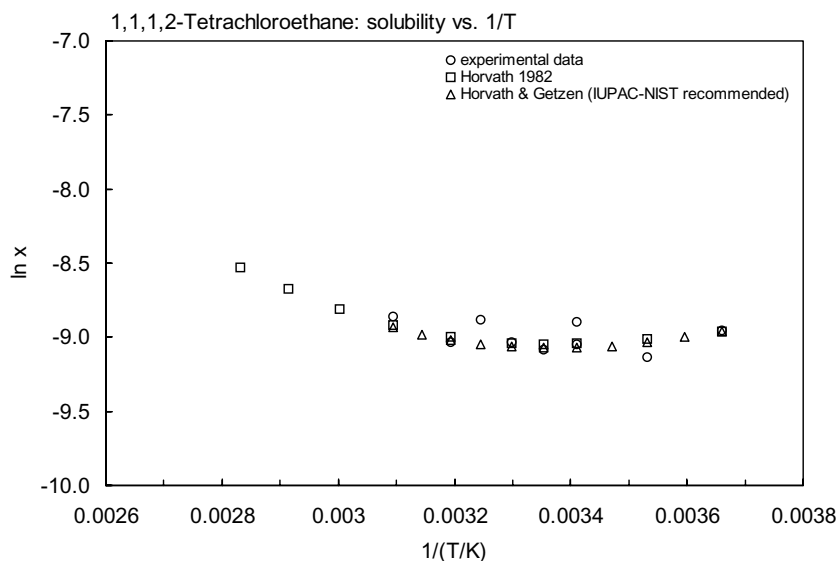
$$S/(\text{wt}\%) = 2.17896 - 1.3966 \times 10^{-3} \cdot (T/\text{K}) + 2.93282 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982		Tse et al. 1992	
shake flask		shake flask-GC		summary of literature data		activity coefficient	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	1200	10	1130	0	1197	20	1206
20	1090	20	1100	10	1133	30	1280
35	1150	25	1100	20	1102	35	1292
50	1250	30	1110	25	1100	40	1321
		40	1160	30	1108		
		50	1250	40	1156		
		60	1390	50	1249		
		70	1590	60	1393		
		80	1850	70	1591		
				80	1848		
				eq. 1	$S/\text{wt}\%$		

2.

Wright et al. 1992		Horvath & Getzen 1999a	
activity coefficient		recommended, IUPAC-NIST	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
20	1005	0	1200
30	1093	5	1150
40	1056	10	1110
		15	1080
		20	1070
		25	1070
		30	1080
		35	1100
		40	1130
		45	1170
		50	1230
		eq. 2	$S/\text{wt}\%$
		temp range 273–323 K	



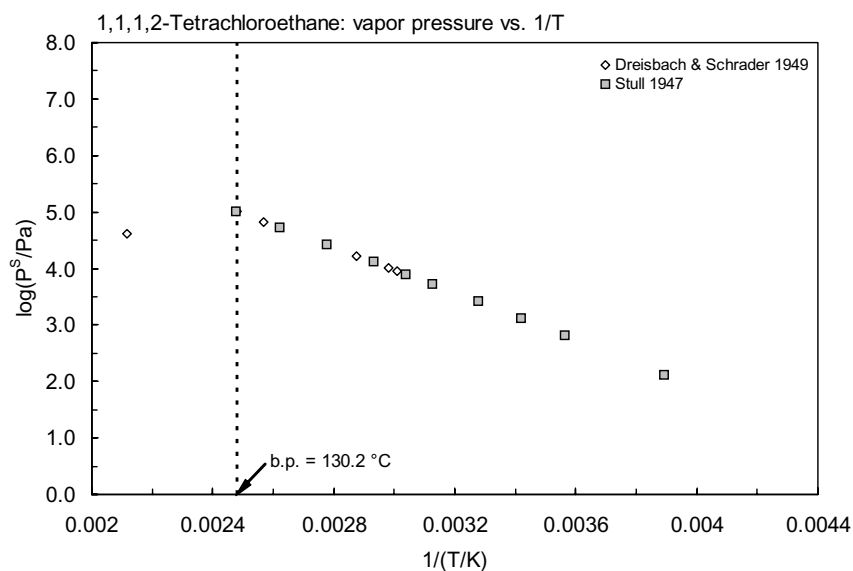
**FIGURE 5.1.1.10.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

**TABLE 5.1.1.10.2**

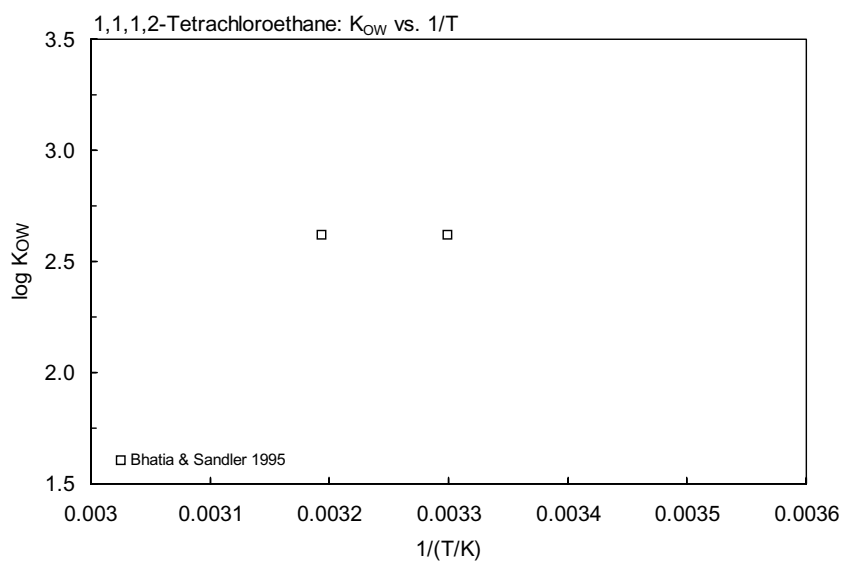
Reported vapor pressures and octanol-water partition coefficients of 1,1,1,2-tetrachloroethane at various temperatures and the coefficients for the vapor pressure equations

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

Vapor pressure				log $K_{OW}$	
Stull 1947		Dreisbach & Shrader 1949		Bhatia & Sandler 1995	
summary of literature data		ebulliometry		relative GC-RT technique	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	log $K_{OW}$
-16.3	133.3	59.31	8851	30	2.62
7.40	666.6	62.39	10114	40	2.62
19.3	1333	74.47	16500		
32.1	2666	199.69	42066		enthalpy of transfer
46.7	5333	115.99	67881		$\Delta H/(\text{kJ mol}^{-1}) = -20.2.$
56.0	7999	130.2	101325		
68.0	13332				$\log K_{OW} = A - \Delta H/2.303RT$
87.2	26664				A 1.0195.
108.2	53329				$\Delta H$ -20.2
130.5	101325				
mp/ $^{\circ}\text{C}$	-68.7				

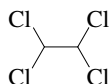


**FIGURE 5.1.1.10.2** Logarithm of vapor pressure versus reciprocal temperature for 1,1,1,2-tetrachloroethane.



**FIGURE 5.1.1.10.3** Logarithm of  $K_{OW}$  versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

## 5.1.1.11 1,1,2,2-Tetrachloroethane



Common Name: 1,1,2,2-Tetrachloroethane

Synonym: sym-tetrachloroethane, acetylene tetrachloride

Chemical Name: 1,1,2,2-tetrachloroethane

CAS Registry No: 79-34-5

Molecular Formula:  $C_2H_2Cl_4$ ,  $CHCl_2CHCl_2$

Molecular Weight: 167.849

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

−42.4 (Lide 2003)

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

145.2 (Lide 2003)

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

1.5953 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

1.59449, 1.58666 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

105.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

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

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

44.89, 36.18 ( $25^{\circ}C$ , at normal boiling point, Dreisbach 1961)

45.78, 38.65 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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 and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

2857 (volumetric method, Wright & Schaffer 1932)

2880, 3360 ( $20$ ,  $55.6^{\circ}C$ , Van Arkel & Vles 1936)

2850 (Seidell 1940)

2900 (data presented in graph, temp range  $0$ – $70^{\circ}C$ , McGovern 1943)

2960\* (shake flask-GC, measured range  $10$ – $80^{\circ}C$ , Walraevens et al. 1974)

$\log [S/(mol/L)] = 2070/(T/K) - 16.316 + 0.0222 \cdot (T/K)$ , temp range  $283$ – $353\ K$  (Walraevens et al. 1974)

3790, 3220, 3210 ( $3$ ,  $20$ ,  $34^{\circ}C$ , shake flask-GC, Chiou & Freed 1977)

3000 (literature average, Dilling 1977)

3230 (shake flask-GC, Chiou et al. 1979)

3041 ( $37^{\circ}C$ , shake flask-GC, Sato & Nakijima 1979)

2880 ( $20^{\circ}C$ , recommended, Sørensen & Arit 1979)

2970 (shake flask-LSC, Banerjee et al. 1980)

2960 ( $23.5^{\circ}C$ , elution chromatography, Schwartz 1980)

3850\* ( $20^{\circ}C$ , elution chromatography, measured range  $10$ – $30^{\circ}C$ , Schwarz & Miller 1980)

2985 (shake flask-LSC, Veith et al. 1980)

2962\* (summary of literature data, temp range  $0$ – $80^{\circ}C$ , Horvath 1982)

866.4 (calculated-UNIFAC activity coeff., Arbuckle 1983)

2915 ( $30^{\circ}C$ , headspace-GC, McNally & Grob 1984)

2985 (calculated-UNIFAC activity coeff., Banerjee 1985)

2870 ( $20^{\circ}C$ , selected, Riddick et al. 1986)

2355, 2695, 3008 ( $20$ ,  $35$ ,  $50^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Barr & Newsham 1987)

2910\* ( $20^{\circ}C$ , shake flask-GC/TC, measured range  $0$ – $90.8^{\circ}C$ , Stephenson 1992)

2481, 2503, 2917, 3008 ( $20$ ,  $30$ ,  $35$ ,  $40^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

778, 918, 994, 1074 ( $20$ ,  $30$ ,  $35$ ,  $40^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -UNIFAC, Tse et al. 1992)

2422, 3140, 2612 (20, 30, 40°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 2570 (20°C, activity coeff.  $\gamma^\infty$  by equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 2830\* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)  
 $S/(\text{wt}\%) = 4.87975 - 3.0937 \times 10^{-3} \cdot (T/K) + 5.20513 \times 10^{-5} \cdot (T/K)^2$ , temp range 276–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

827\* (static method, extrapolated, measured range 31.1–146.7°C, Nelson 1930)  
 $\log(P/\text{mmHg}) = 8.06938 - 2167.83/(T/K)$ ; temp range 31.1–146.7°C (static method, Nelson 1930)  
 850\* (Antoine eq. regression, temp range 65–243.5°C, Stull 1947)  
 560\* (Ramsay-Young method, measured range 25–130°C, Matthews et al. 1950)  
 793 (calculated-Antoine eq., Dreisbach 1961)  
 $\log(P/\text{mmHg}) = 6.98240 - 1465.1/(211.0 + t/^\circ\text{C})$ ; temp range 55–191°C (Antoine eq. for liquid state, Dreisbach 1961)  
 851 (interpolated-Antoine eq., Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 9917.1/(T/K)] + 8.072583$ ; temp range –3.8 to 146°C (Antoine eq., Weast 1972–73)  
 582 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log(P/\text{kPa}) = 6.63168 - 1228.062/(179.972 + t/^\circ\text{C})$ ; temp range 25–120°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 867 (literature average, Dilling 1977)  
 585 (calculated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 5.77919 - 1240.857/(181.401 + t/^\circ\text{C})$ ; temp range 25–130°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 2133 (McNally & Grob 1984)  
 $\log(P/\text{mmHg}) = 6.6317 - 1228.1/(279.9 + t/^\circ\text{C})$ ; temp range 25–130°C (Antoine eq., Dean 1985, 1992)  
 793 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 6.1295 - 1444.3/(205.1 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 793 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.1073 - 1465.1/(-62.15 + T/K)$ ; temp range 328–464 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 5.98931 - 1365.692/(-76.476 + T/K)$ ; temp range 377–419 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 440, 848, 1154, 2550 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)  
 $\log(P/\text{mmHg}) = 56.2356 - 4.4615 \times 10^3/(T/K) - 1.6556 \cdot \log(T/K) - 3.5724 \times 10^{-10} \cdot (T/K) + 4.0425 \times 10^{-6} \cdot (T/K)^2$ ; temp range 229–645 K (vapor pressure eq., Yaws 1994)

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):

46.2 (exptl.  $1/K_{AW} (C_W/C_A)$ , Hine & Mookerjee 1975)  
 47.1 (calculated-P/C, Dilling 1977)  
 35.38\* (22.0°C, equilibrium cell-GC, measured range 11.0–27.2°C, Leighton & Calo 1981)  
 48.5, 48.0 (calculated-P/C, recommended, Mackay & Shiu 1981)  
 25.3\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 1.726 - 2810/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 38.5 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 33.45 (computed value, Yaws et al. 1991)  
 30.4, 50.7, 60.8, 91.2 (20, 30, 35, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)  
 40.3, 57.06, 120 (20, 30, 40°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 34.4 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 34.12 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 2.493 - 1255/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

2.56 (calculated as per Tute 1971, Callahan et al. 1979)  
 2.39 (shake flask-LSC, Banerjee et al. 1980)

- 2.39 (shake flask-LSC, Veith et al. 1980)  
 2.79, 2.84 (calculated-UNIFAC with octanol and water mutual solubility considered, calculated-UNIFAC with octanol and water mutual solubility not considered; Arbuckle 1983)  
 2.39 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)  
 2.93 (recommended, Sangster 1993)  
 2.39 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 0.9–1.0 (bluegill sunfish, Barrows et al. 1980; Kawasaki 1980)  
 0.90 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)  
 1.96 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 0.91 (fathead minnow, Veith & Kosian 1982)  
 2.03 (calculated- $K_{OW}$ , McCarty et al. 1992)

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

- 1.66 (soil, equilibrium sorption isotherm, Chiou et al. 1979)  
 1.90 (silt loam, quoted from Chiou et al. 1979; Karickhoff 1981; Howard 1990)  
 2.00, 1.80, 1.87 (estimated- $K_{OW}$ , estimated-S and mp, estimated-S, Karickhoff 1981)  
 2.07 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 3.60 (soil, calculated-universal solvation model; Winget et al. 2000)

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

- 1.66, 1.90 (quoted, calculated-MCI  $\chi$ , Sabljic 1984)

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

Volatilization: estimated experimental  $t_{1/2}$  = 56 min for initial concentration of 1 mg/L when stirred at 200 rpm in water at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation  $t_{1/2}(\text{exptl})$  = 55.2 min,  $t_{1/2}(\text{calc})$  = 12.0 min, 40.5 min from water (Dilling 1977);

estimated  $t_{1/2}$  ~ 6.3 h for a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated Henry's law constant (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2}$  ~ 3.5 d for a model pond was based on the effect of adsorption (USEPA 1987; quoted, Howard 1990).

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:

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 2.0 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)

$k_{OH} < 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , estimated as toxic chemical residence time > 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 213\text{--}2131 \text{ h}$ , based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis:  $k = 1.2 \times 10^{-7} \text{ h}^{-1}$  at 25°C and pH 7 (estimated, Mabey et al. 1982);

$t_{1/2}(\text{abiotic})$  or  $t_{1/2}(\text{dehydrohalogenation}) = 10 \text{ months}$  (Mabey et al. 1983; quoted, Olsen & Davis 1990)

$t_{1/2}(\text{abiotic}) = 3.3 \text{ months}$  (Cooper et al. 1987; quoted, Olsen & Davis 1990);

$k = 2.3 \times 10^7 \text{ M}^{-1} \text{ yr}^{-1}$  at pH 9 and 25°C with  $t_{1/2} = 1.1 \text{ d}$  in alkaline soil, and  $k = 111 \text{ d}$  at pH 7 (Kollig et al. 1987; quoted, Howard 1990)

$k = 1.8 \text{ M}^{-1} \text{ s}^{-1}$  for base-catalyzed reaction at 25°C and pH 7 with  $t_{1/2} = 45 \text{ d}$ ;  $k = 6480 \text{ M}^{-1} \text{ h}^{-1}$  for base reaction at pH 9 and 25°C;  $k = (27.6 \pm 4.0) \times 10^{-8} \text{ s}^{-1}$  in sediment with 61% conversion (Haag & Mill 1988)

Biodegradation:  $k = (7.3 \pm 0.1) \times 10^{-5} \text{ min}^{-1}$  with  $t_{1/2} = 6.6 \text{ d}$  in sediment-water sample (Jafvert & Wolfe 1987)

$t_{1/2}(\text{abiotic}) > 800 \text{ d}$  for the reaction with photochemically produced hydroxyl radical (Singh et al. 1981; quoted, Howard 1990)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320 \text{ h}$ , based on acclimated river die-away rate data (Mudder 1981; quoted, Howard et al. 1991)

$t_{1/2}$ (aq. anaerobic) = 168–672 h, based on anaerobic sediment grab sample data (Jafvert & Wolfe 1987) and anaerobic screening test data (Hallen et al. 1986; quoted, Howard et al. 1991).

Biotransformation: estimated rate constant of  $3 \times 10^{-12}$  mL cell<sup>-1</sup> h<sup>-1</sup> for bacteria (Mabey et al. 1982).

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

$k_1 = 13.2$  h<sup>-1</sup> (flagfish, calculated-BCF  $\times k_2$ , McCarty et al. 1992)

$k_2 = 0.123$  h<sup>-1</sup> (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4$ –24 h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); estimated as toxic chemical residence time > 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 213$ –2131 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water:  $t_{1/2} = 6.6$  d in sediment-water sample (Jafvert & Wolfe 1987);

$t_{1/2} = 45$  d at pH 7 and 25°C, based on based-catalyzed hydrolysis rate constant (Haag & Mill 1988);

$t_{1/2} = 10.7$ –1056 h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Ground water:  $t_{1/2} = 10.7$ –1056 h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Sediment:  $t_{1/2} = 6.6$  d in Bar-H sediment-water sample (Jafvert & Wolfe 1987);

measured  $t_{1/2} = 29$  d at 25°C, based on neutral and base-catalyzed hydrolysis rates studies in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

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

$t_{1/2} = 10.7$ –1056 h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

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

$t_{1/2} < 10$  d, subject to plant uptake via volatilization (Ryan et al. 1988).

**TABLE 5.1.1.11.1**

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

$$\log S/(\text{mol/L}) = -15.316 + 2070/(T/K) + B(T/K) \quad (1)$$

$$S/(\text{wt}\%) = 0.32934 - 2.10434 \times 10^{-3} \cdot (t/^\circ\text{C}) + 2.54796 \times 10^{-5} \cdot (t/^\circ\text{C})^2 + 1.86126 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (2)$$

$$S/(\text{wt}\%) = 4.87975 - 3.0937 \times 10^{-3} \cdot (T/K) + 5.20513 \times 10^{-5} \cdot (T/K)^2 \quad (3)$$

1.

Walraevens et al. 1974		Schwarz & Miller 1980		Horvath 1982		Barr & Newsham 1987	
shake flask-GC		elution chromatography		summary of literature data		activity coefficient	
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	3200	10	3720	0	3299	20	2235
20	3010	20	3850	10	3116	35	2595
25	2960	30	3670	20	2995	50	3008
30	2940			25	2962		
40	2980			30	2948		
50	3120			40	2984		
60	3360			50	3118		
70	3710			60	3356		
80	4200			70	3713		
				80	4199		
eq. 1	S/(mol/L)						
A	15.316						
B	0.0222			eq. 2	S/wt%		



TABLE 5.1.1.11.1 (Continued)

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999a	
shake flask-GC		activity coefficient		activity coefficient		recommended, IUPAC-NIST	
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>
0	3170	20	2481	20	2422	5	3020
9.5	2900	30	2503	30	3140	10	2830
20	2910	35	2917	40	2612	15	2870
29.7	2920	40	3008			25	2840
39.6	3010					30	2830
50.1	3160					35	2850
61	3570					40	2890
70.5	3850					45	3060
80.6	4250					50	3160
90.8	4740						

eq. 3                      S/wt%  
temp range 276–323 K

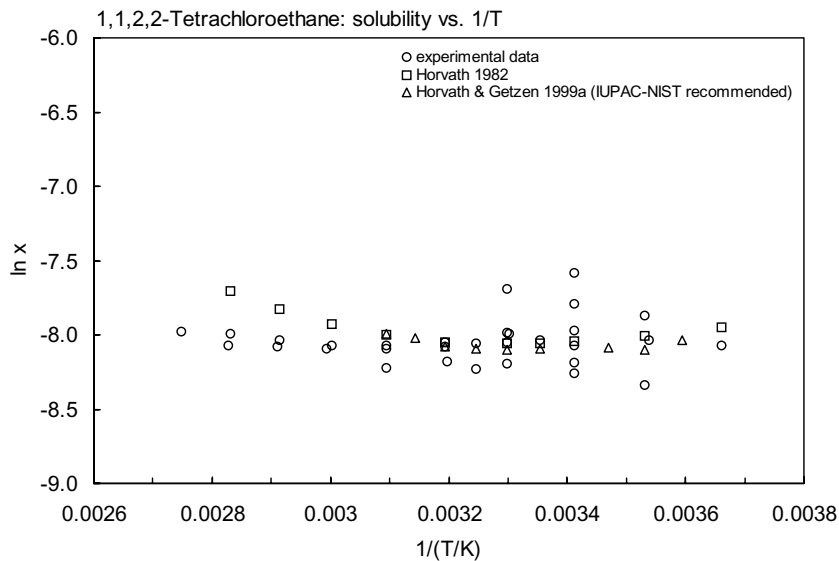


FIGURE 5.1.1.11.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

TABLE 5.1.1.11.2

Reported vapor pressures of 1,1,2,2-tetrachloroethane 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)			
Nelson 1930		Stull 1947		Matthews et al. 1950	
static method		summary of literature data		Ramsay-Young method	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
31.1	1000	-3.80	133.3	25.0	560
34.6	1067	20.7	666.6	30.0	667
39.3	1533	33.0	1333	35.0	1080
44.3	2200	46.2	2666	40.0	1493
50.4	3120	60.8	5333	45.0	2000
57.8	4253	70.0	7999	50.0	2680
64.6	5893	83.2	13332	55.0	3480
72.3	8293	102.2	26664	60.0	4440
79.0	10879	124.0	53329	65.0	5626
85.0	13865	145.9	101325	70.0	6933
89.9	16785			75.0	8533
94.9	20438	mp/ $^{\circ}\text{C}$	-36	80.0	10666
99.9	24611			85.0	13066
105	29851			90.0	16079
109.1	34770			95.0	19532
114.9	41730			100	23665
119.9	47703			105	28331
120.1	48569			110	33130
124.5	54865			115	38930
130.4	66328			120	45663
135.2	92139			135	53329
141.5	102285			130	62795
146.7	106938				
20	626.6*			bp/K	420.4
25	826.6*			$\Delta H_v = 38.42 \text{ kJ/mol at bp}$	
				Kirchhoff, Rankine, Dupre eq.	
eq. 1	P/mmHg			eq. 4	P/mmHg
A	8.08938			A	35.117
B	2167.83			B	3646
				C	8.981

\*extrapolated

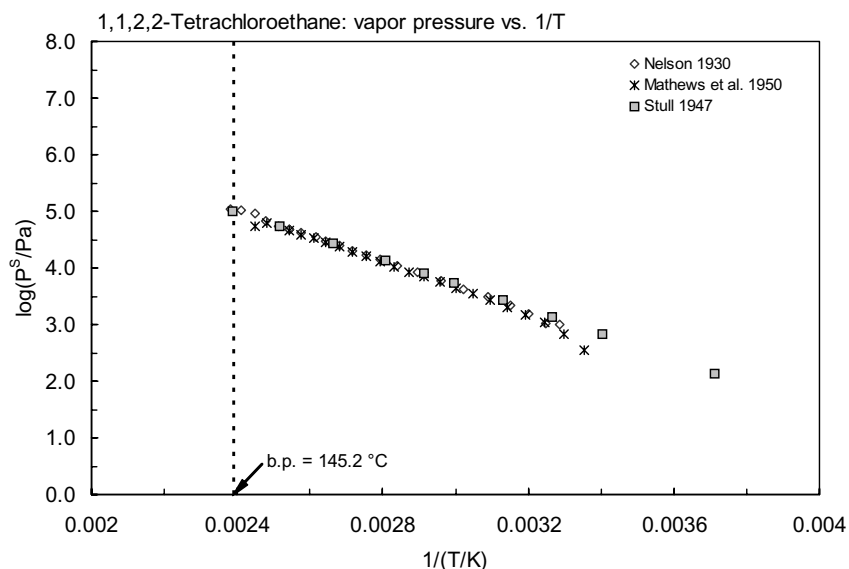


FIGURE 5.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

TABLE 5.1.11.3

Reported Henry's law constants of 1,1,2,2-tetrachloroethane at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1)$$

$$\log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2)$$

$$\log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

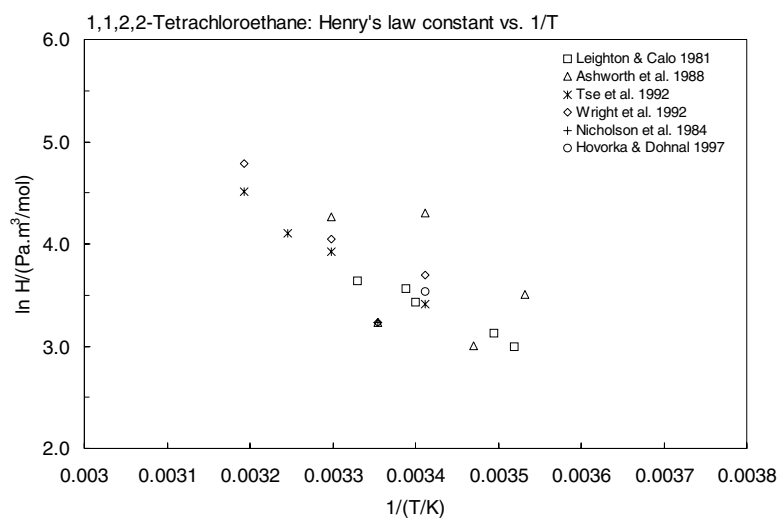
$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4)$$

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

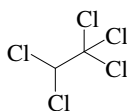
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

Leighton & Calo 1981		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
equilibrium cell-GC		EPICS-GC		activity coefficient		activity coefficient	
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)
11.0	19.95	10	33.44	20	30.4	20	40.3
13.0	22.83	15	20.27	30	50.7	30	57.06
21.0	31.06	20	73.97	35	60.8	40	120
22.0	35.38	25	25.33	40	91.2		
27.2	38.19	30	70.93				
eq. 3	H/atm	eq. 4a	H/(atm m <sup>3</sup> /mol)				
A	14.91	A	1.726				
B	3547	B	2810				



**FIGURE 5.1.1.11.3** Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

## 5.1.1.12 Pentachloroethane



Common Name: Pentachloroethane

Synonym: 1,1,1,2,2-pentachloroethane, pentalin

Chemical Name: pentachloroethane

CAS Registry No: 76-01-7

Molecular Formula:  $C_2HCl_5$ ,  $CHCl_2CCl_3$

Molecular Weight: 202.294

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

-28.78 (Lide 2003)

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

162.0 (Horvath 1982; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

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

1.6796 (Horvath 1982; Weast 1982–83)

1.6808, 1.6732 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

120 (calculated-density, Abernethy et al. 1988)

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

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

40.79, 36.941 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

11.34 (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):

345 (volumetric method, Wright & Schaffer 1932)

470 ( $20^{\circ}C$ , shake flask, Van Arkel & Vles 1936)

463 (Seidell 1940)

500 (data presented in graph, temp range  $0$ – $70^{\circ}C$ , McGovern 1943)

500\* (shake flask-GC, temp range  $10$ – $80^{\circ}C$ , Walraevens et al. 1974)

$\log [S/(mol\ dm^{-3})] = 2070/(T/K) - 16.412 + 0.0230 \cdot (T/K)$ ; temp range  $283$ – $353\ K$  (Walraevens et al. 1974)

480 (literature average, Dilling et al. 1975; Dilling 1977)

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

500\* (summary of literature data, temp range  $0$ – $80^{\circ}C$ , Horvath 1982)

500 (Dean 1985; Riddick et al. 1986)

470, 490 ( $20^{\circ}C$ ,  $25^{\circ}C$ , recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

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):

467\* ( $25.1^{\circ}C$ , static method, measured range  $25.1$ – $162.2^{\circ}C$ , Nelson 1930)

$\log (P/mmHg) = 7.80304 - 2129.6/(T/K)$ ; temp range  $25.1$ – $162.2^{\circ}C$  (static method, Nelson 1930)

596\* (Antoine eq. regression, temp range  $1.0$ – $160.5^{\circ}C$ , Stull 1947)

596 (calculated-Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 9800.1/(T/K)] + 7.832202$ ; temp range  $1.0$ – $160.6^{\circ}C$  (Antoine eq., Weast 1972–73)

465 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 6.74011 - 1378.096/(197.367 + t/^{\circ}C)$ ; temp range  $25.1$ – $162^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

600 (literature average, Dilling 1977)

453, 800 ( $20^{\circ}C$ ,  $30^{\circ}C$ , Verschueren 1983)

- 467 (calculated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 5.92765 - 1419.719/(202.285 + t/^{\circ}\text{C})$ ; temp range 25.1–162°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log(P/\text{mmHg}) = 6.740 - 1378/(197 + t/^{\circ}\text{C})$ , temp range: 25–162°C (Antoine eq., Dean 1985, 1992)  
 590 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 5.7199 - 1295.67/(188.96 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 625 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.69025 - 1982.65/(-10.577 + T/\text{K})$ ; temp range 274–434 K (Antoine eq., Stephenson & Malanowski 1987)  
 467, 453 (quoted, calculated-UNIFAC, Banerjee et al. 1990)  
 $\log(P/\text{mmHg}) = 72.1134 - 4.6522 \times 10^3/(T/\text{K}) - 23.777 \cdot \log(T/\text{K}) + 9.6908 \times 10^{-3} \cdot (T/\text{K}) - 3.3886 \times 10^{-13} \cdot (T/\text{K})^2$ ;  
 temp range 244–665 K (vapor pressure eq., Yaws 1994)

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

- 247.9 (exptl  $-1/K_{\text{AW}} = C_{\text{W}}/C_{\text{A}}$ , Hine & Mookerjee 1975)  
 247.9 (calculated-P/C, Dilling 1977)  
 96.44 (calculated-QSAR, Nirmalakhandan & Speece 1988)  
 196.5 (calculated-P/C, Howard 1990)  
 188.9, 53.73 (quoted, calculated-bond contribution method, Meylan & Howard 1991)  
 183.9 (computed value, Yaws et al. 1991)

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

- 2.89 (shake flask-LSC, Veith et al. 1980)  
 3.05 (HPLC-RT correlation, McDuffie 1981; quoted, Sangster 1993)  
 3.22 (recommended, Hansch et al. 1995)

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

- 1.826 (bluegill sunfish, Barrows et al. 1980)  
 1.83 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)  
 1.78 (fathead minnow, Veith & Kosian 1982)

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

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

Volatilization: estimated experimental  $t_{1/2} = 48$  min for 1 mg/L aqueous solution when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975)

Evaporation  $t_{1/2}(\text{exptl}) = 46.5$  min,  $t_{1/2}(\text{calc}) = 2.3$  min, 32 min from water (Dilling 1977)

#### 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 see reference:

$k_{\text{OH}}(\text{calc}) = 1.93 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{exptl}) = 2.33 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

#### Hydrolysis:

#### Biodegradation:

#### Biotransformation:

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

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4$ –24 h from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

estimated tropospheric lifetime of 0.58 h (Nimitz & Skaggs 1992).

#### Surface water:

#### Ground water:

#### Sediment:

#### Soil:

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

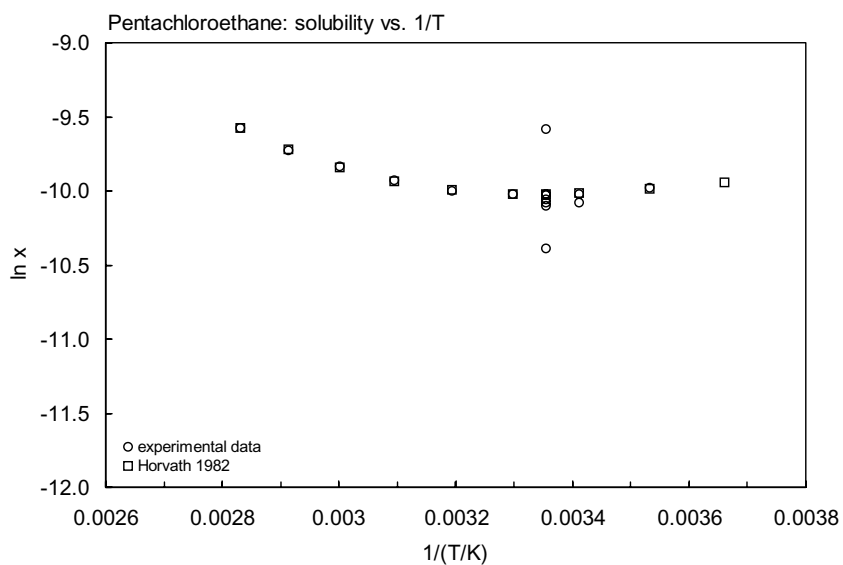
TABLE 5.1.1.12.1

Reported aqueous solubilities and vapor pressures of pentachloroethane at various temperatures

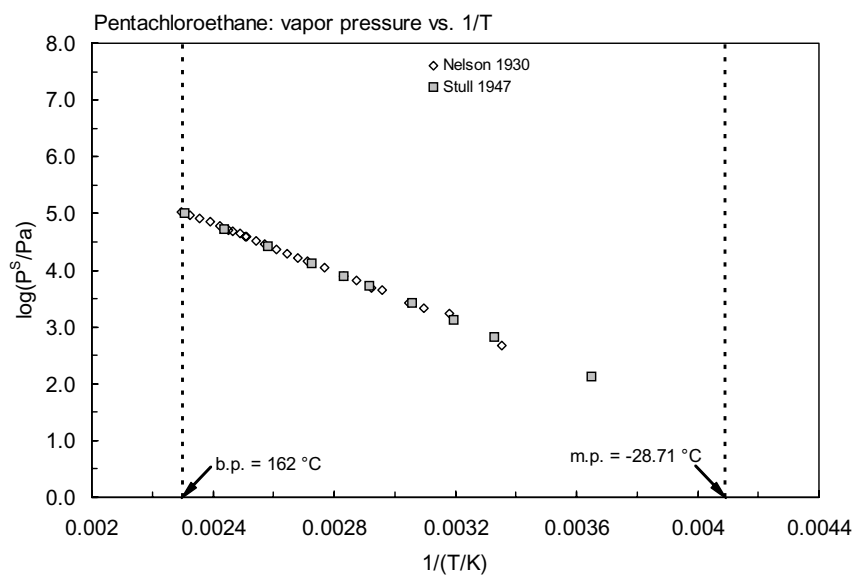
$$S/(\text{wt}\%) = 5.41068 \times 10^{-2} - 2.81268 \times 10^{-4} \cdot (t/^{\circ}\text{C}) + 3.41333 \times 10^{-6} \cdot (t/^{\circ}\text{C})^2 + 4.76167 \times 10^{-8} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$\log S = A/(T/K) - B + C \cdot (T/K) \quad (2)$$

Aqueous solubility				Vapor pressure			
Walraevens et al. 1974		Horvath 1982		Nelson 1930		Stull 1947	
shake flask-GC		summary of literature data		static method		summary of literature data	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	P/Pa
10	520	0	541.1	25.1	467	1.0	133.3
20	500	10	516.8	41.1	1733	27.2	666.6
25	500	20	502.3	50.0	2133	39.8	1333
30	500	25	499.5	55.0	2666	53.9	2666
40	510	30	500.3	65.0	4453	69.9	5333
50	550	40	513.6	69.0	4986	80.0	7999
60	600	50	545.3	75.0	6573	93.5	13332
70	670	60	598.0	80.0	7973	114.0	26664
80	780	70	674.8	88.2	10959	137.2	53329
		80	778.3	95.7	14212	160.5	101325
eq. 2	S/(mol/L)			100.2	16732		
A	2070	eq.1	S/wt%	105.0	19852	mp/°C	57
B	16.412			110.0	23771		
C	0.0230			115.6	28491		
				119.9	33064		
				124.9	39170		
				125.6	39957		
				128.7	43876		
				132.4	49049		
				134.6	50249		
				139.4	59555		
				145.3	70741		
				151.3	80660		
				157.3	94859		
				162.2	108137		



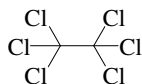
**FIGURE 5.1.1.12.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for pentachloroethane.



**FIGURE 5.1.1.12.2** Logarithm of vapor pressure versus reciprocal temperature for pentachloroethane.



## 5.1.1.13 Hexachloroethane



Common Name: Hexachloroethane

Synonym: carbon hexachloride, perchloroethane, phenohep, HCE

Chemical Name: hexachloroethane

CAS Registry No: 67-72-1

Molecular Formula:  $C_2Cl_6$ ,  $CCl_3CCl_3$

Molecular Weight: 236.739

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

186.8 (triple point) (Lide 2003)

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

184.7 (sublimation point) (Lide 2003)

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

2.091 (McGovern 1943; Horvath 1982; Weast 1982–83; Dean 1985)

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

113 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

177.2 (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  $25^{\circ}C$ , F:

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

50 ( $22.3^{\circ}C$ , shake flask, Van Arkel & Vles 1936)

50 ( $22.3^{\circ}C$ , McGovern 1943)

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

50 ( $22.3^{\circ}C$ , recommended, Horvath 1982)

77.1 ( $20^{\circ}C$ , EPICS-LSC, Munz & Roberts 1986)

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

42.7\* (gas saturation method, extrapolated, measured range  $31$ – $55^{\circ}C$ , Nelson 1930)

75.4\* (extrapolated-Antoine eq. regression, temp range  $32.7$ – $186.5^{\circ}C$ , Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11711.3/(T/K)] + 8.440623$ ; temp range  $32.7$ – $185.6^{\circ}C$  (Antoine eq., Weast 1972–73)

49.5 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 7.9015 - 3077/(T/K)$ ; temp range  $317$ – $345\ K$  (Antoine eq.-I, solid, rhombic, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 7.856 - 2677/(T/K)$ ; temp range  $345$ – $460\ K$  (Antoine eq.-II, solid, cubic, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.6075 - 2103.6/(T/K)$ ; temp range  $460$ – $513\ K$  (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -366.2243 + 6.67893 \times 10^3/(T/K) + 155.63 \cdot \log(T/K) - 0.15563 \cdot (T/K) + 5.56 \times 10^{-5} \cdot (T/K)^2$ ; temp range  $306$ – $698\ K$  (vapor pressure eq., Yaws 1994)

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

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

123.9 (calculated-P/C, Dilling 1977)

285\* ( $20^{\circ}C$ , EPICS-LSC, measured range  $10$ – $30^{\circ}C$ , Munz 1985)

$\log K_{AW} = 6.982 - 2320/(T/K)$ , temp range  $10$ – $30^{\circ}C$  (EPICS-LSC measurements, Munz & Roberts 1987)

846\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 3.744 - 2550/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 253.3 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 226.7 (computed value, Yaws et al. 1991)  
 285 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 6.982 - 2320/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

4.14 (20°C, shake flask-GC, both phases, Chiou et al. 1977)  
 3.82 (HPLC- $k'$  correlation, Könemann et al. 1979)  
 3.93 (shake flask-LSC, Veith et al. 1980)  
 4.05 (RP-HPLC-RT correlation, Veith et al. 1980)  
 4.04 (HPLC-RT correlation, McDuffie 1981)  
 4.14 (recommended, Sangster 1993)  
 4.14 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

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

Bioconcentration Factor,  $\log BCF$ :

0.92–3.23 (calculated- $K_{OW}$ , Veith et al. 1979, 1980)  
 2.143 (bluegill sunfish, Barrows et al. 1980)  
 2.14 (bluegill sunfish, Veith et al. 1980)  
 3.83 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 2.14 (bluegill sunfish, Veith & Kosian 1982)  
 2.85 (fathead minnow, Veith & Kosian 1982)  
 4.57 (calculated- $K_{OW}$ , Thomann 1989)

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

4.3 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)

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

Volatilization: estimated experimental  $t_{1/2} = 40\text{--}45$  min from dilute aqueous solution in open container of depth 65mm and stirring at 200 rpm (Dilling et al. 1975)

Evaporation  $t_{1/2}(\text{exptl}) = 28.0$  min,  $t_{1/2}(\text{calc}) = 4.5$  min, 24.5 min from water (Dilling 1977)

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:

$k_{OH} < 1.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , estimated residence time  $> 11600$  d, loss  $\approx 0.0\%$  in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} > 7.3\text{--}73$  yr, based on estimated maximum rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: not significant, based on hydrolysis studies after 13 d at 85°C and pH 3, 7, and 11 (Ellington et al. 1987; quoted, Howard et al. 1991)

Biodegradation:

$k = (5.0 \pm 0.34) \times 10^{-2} \text{ min}^{-1}$  in Bar-H sediment-water slurry,  $k = (2.0 \pm 0.17) \times 10^{-2} \text{ min}^{-1}$  in Beaver Dam sediment-water slurry,  $k = (2.6 \pm 0.2) \times 10^{-2} \text{ min}^{-1}$  in Hickory Hill sediment-water slurry,  $k = (1.9 \pm 0.16) \times 10^{-2} \text{ min}^{-1}$  in Memorial Park sediment-water slurry and  $k = (1.9 \pm 0.1) \times 10^{-2} \text{ min}^{-1}$  with  $t_{1/2} = 36$  min in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

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

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

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

Biotransformation: estimated rate constant of  $1 \times 10^{-10} \text{ ml cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

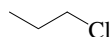
## Half-Lives in the Environment:

- Air: disappearance  $t_{1/2} > 10$  d for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);  
 $t_{1/2} > 7.3$ –73 yr, based on estimated maximum rate constant for reaction with hydroxyl radical (Singh et al. 1980; quoted, Howard et al. 1991);  
 residence time  $> 11600$  d, loss  $\approx 0.0$  in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical K for the reaction with OH radical (Singh et al. 1981)
- Surface water:  $t_{1/2} = 36$  min in anoxic sediment-water suspension (Jafvert & Wolfe 1987);  
 $t_{1/2} = 672$ –4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)  
 $t_{1/2}(\text{aerobic}) = 28$  d,  $t_{1/2}(\text{anaerobic}) = 110$  d in natural waters (Capel & Larson 1995).
- Ground water:  $t_{1/2} = 1344$ –8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Sediment: disappearance  $k = (5.0 \pm 0.34) \times 10^{-2} \text{ min}^{-1}$  in Bar-H sediment-water slurry,  $k = (2.0 \pm 0.17) \times 10^{-2} \text{ min}^{-1}$  in Beaver Dam sediment-water slurry,  $k = (2.6 \pm 0.2) \times 10^{-2} \text{ min}^{-1}$  in Hickory Hill sediment-water slurry,  $k = (1.9 \pm 0.16) \times 10^{-2} \text{ min}^{-1}$  in Memorial Park sediment-water slurry and  $k = (1.9 \pm 0.1) \times 10^{-2} \text{ min}^{-1}$  with  $t_{1/2} = 36$  min in Bar-H sediment-water suspension (Jafvert & Wolfe 1987)
- Soil:  $t_{1/2} = 672$ –4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Biota:  $t_{1/2} < 1$  d in tissues of bluegill sunfish (Barrows et al. 1980)

TABLE 5.1.1.13.1

Reported vapor pressures and Henry's law constant of hexachloroethane at various temperatures

Vapor pressure				Henry's law constant			
Nelson 1930		Stull 1947		Ashworth et al. 1988		Munz 1985	
gas saturation		summary of literature data		EPICS-GC		EPICS-LSC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
31	73.3	32.7	133.3	10	601	10	74.2
35	93.3	49.8	666.6	15	566.4	20	285
40	133.3	73.5	1333	20	598.8	30	537
45	198.7	87.6	2666	25	846.1		
50	282.6	102.3	5333	30	1044		
55	390.6	112.0	7999				
		124.2	13332	$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$			
		143.1	26664	A	3.744		
		163.8	53332	B	2550		
		185.6	101325				

5.1.1.14 1-Chloropropane (*n*-Propyl chloride)

Common Name: 1-Chloropropane

Synonym: *n*-Propyl chloride, propyl chloride

Chemical Name: 1-chloropropane, *n*-Propyl chloride, propyl chloride

CAS Registry No: 540-54-5

Molecular Formula: CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>Cl

Molecular Weight: 78.541

Melting Point (°C):

−122.9 (Lide 2003)

Boiling Point (°C):

46.5 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.8909 (Dreisbach 1961; Horvath 1982)

0.8899, 0.8830 (20°C, 25°C, Riddick et al. 1986)

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

88.3 (20°C, calculated-density)

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

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

28.48, 27.25 (25°C, normal bp, Dreisbach 1961)

28.50, 27.24 (25°C, bp, Riddick et al. 1986)

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

5.544 (Riddick et al. 1986)

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

2720\* (20°C, measured range 0–30°C, volumetric method, Rex 1906)

2500 (Wright & Schaffer 1932)

2772 (30°C, shake flask, Van Arkel & Vles 1936)

2334 (Seidell 1941)

2333 (20°C, Saracco & Spaccamela Marchetti 1958)

2700 (20°C, Verschueren 1983)

2651\* (summary of literature data, Horvath 1982)

2710 (20°C, quoted, Riddick et al. 1986)

2500\* (reported value of IUPAC-NIST Solubility Data Series, temp range 0–37°C, Horvath & Getzen 1999)

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):

37360, 55240 (20°C, 30°C, Rex 1906)

46500\* (interpolated-Antoine eq. regression, temp range −68.3 to 36.5°C, Stull 1947)

46000 (calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.93111 − 1121.123/(230.2 + t/°C); temp range −25 to 88°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.93111 − 1121.123/(230.20 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

40517\* (21.8°C, differential thermal analysis, measured range −25.1 to 47.1°C, Kemme & Kreps 1969)

log (P/mmHg) = [−0.2185 × 7485.7/(T/K)] + 8.028733; temp range −63.8 to 46.4°C (Antoine eq., Weast 1972–73)

log (P/kPa) = 6.07206 − 1120.381/(229.061 + t/°C); temp range −25.1 to 47.1°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

log (P/mmHg) = 6.92648 − 1110.19/(227.94 + t/°C); temp range −25 to 47°C (Antoine eq., Dean 1985, 1992)

45920 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.07655 - 1125.09/(229.86 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

46060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.09145 - 1126.383/(-43.78 + T/\text{K})$ ; temp range 248–320 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 32.3325 - 2.485 \times 10^3/(T/\text{K}) - 8.8052 \cdot \log(T/\text{K}) + 8.9119 \times 10^{-11} \cdot (T/\text{K}) + 3.6803 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 150–503 K (vapor pressure eq., Yaws 1994)

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

1341 (calculated-P/C, using Hine & Mookerjee 1975 data)

1600 (calculated-QSAR, Nirmalakhandan & Speece 1988)

1091 (computed value, Yaws et al. 1991)

1450 ( $\gamma^{\infty}$  from gas stripping-GC, Li et al. 1993)

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

2.04 (shake flask, Log P Database, Hansch & Leo 1987)

2.04 (recommended, Sangster 1989)

2.04 (recommended, Hansch et al. 1995)

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

2.24 (head-space GC, Abraham et al. 2001)

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

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

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

Half-Lives in the Environment:

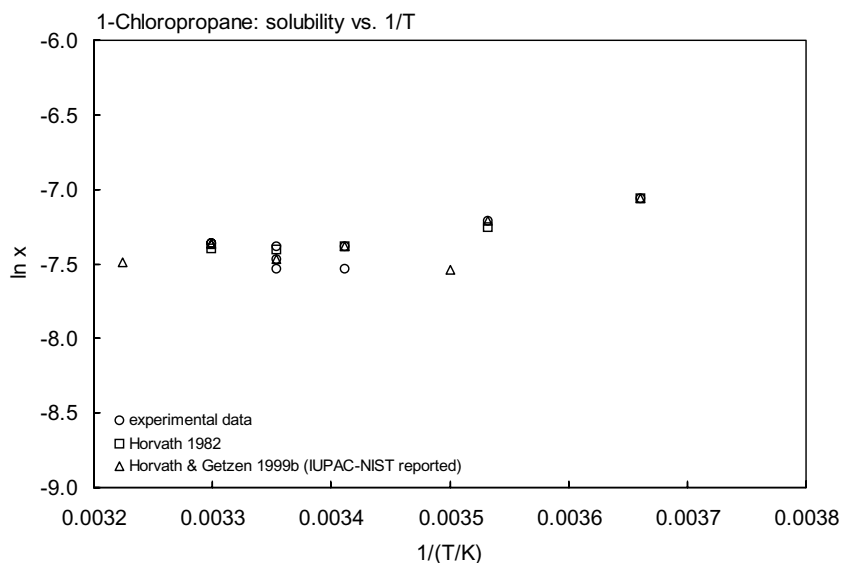
Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (Darnall et al. 1976).

**TABLE 5.1.1.14.1**

**Reported aqueous solubilities of 1-chloropropane at various temperatures**

$$S/(\text{wt}\%) = 0.3746 - 0.007725 \cdot (t/^{\circ}\text{C}) + 1.05001 \times 10^{-6} \cdot (t/^{\circ}\text{C})^2 + 1.14998 \times 10^{-6} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		reported, IUPAC-NIST	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	3760	0	3746	0	3750
10	3230	10	3090	10	3220
20	2720	20	2713	12.5	2320
30	2770	25	2651	20	2710
		30	2684	25	2500
				30	2760
		eq. 1	$S/\text{wt}\%$	30	2770
				37	2440



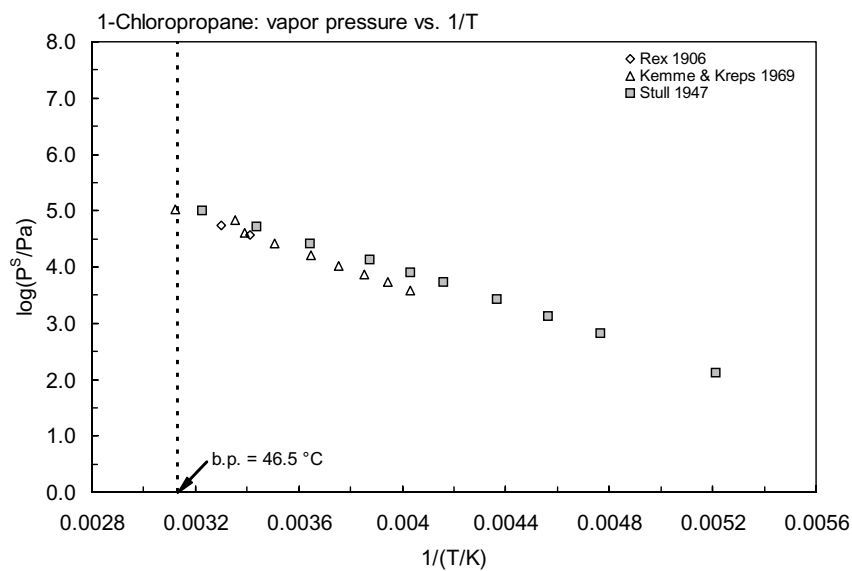
**FIGURE 5.1.1.14.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-chloropropane.

**TABLE 5.1.1.14.2**

**Reported vapor pressures of 1-chloropropane at various temperatures and the coefficients for the vapor pressure equations**

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

Stull 1947		Kempe & Kreps 1969	
summary of literature data		differential thermal analysis	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-63.8	133.3	-25.1	3840
-50.0	666.6	-19.6	5320
-41.0	1333	-13.7	7386
-31.0	2666	-6.90	10599
-19.5	5333	1.20	16065
-12.1	7999	12.1	26691
-2.50	13332	21.8	40517
12.1	26664	34.9	67194
29.4	53329	47.1	103458
46.4	101325		
mp/ $^{\circ}\text{C}$	-117	eq. 2	P/mmHg
		A	8.18894
		B	1690.864
		C	221.346



**FIGURE 5.1.14.2** Logarithm of vapor pressure versus reciprocal temperature for 1-chloropropane.

## 5.1.1.15 2-Chloropropane



Common Name: 2-Chloropropane

Synonym: isopropyl chloride

Chemical Name: 2-chloropropane, isopropyl chloride

CAS Registry No: 75-29-6

Molecular Formula:  $C_3H_7Cl$ ,  $CH_3CHClCH_3$

Molecular Weight: 78.541

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

-117.18 (Lide 2003)

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

35.7 (Lide 2003)

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

0.8626, 0.8560 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959)

0.8617, 0.8563 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961; Riddick et al. 1986)

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

91.2 ( $20^{\circ}C$ , calculated from density)

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

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

26.86, 26.26 ( $25^{\circ}C$ , normal bp, Dreisbach 1961)

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

7.39 (calculated, Dreisbach 1959)

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):

3050\* ( $20^{\circ}C$ , measured range  $0-30^{\circ}C$ , volumetric method, Rex 1906)

3444 (shake flask, Fühner 1924)

3056 (Seidell 1940)

3000 (Seidell 1941)

2950 (selected exptl., Horvath 1982)

3400 (Dean 1985)

3040\* ( $20^{\circ}C$ , tentative values, temp range  $0-30^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

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):

58050, 83940 ( $20^{\circ}C$ ,  $30^{\circ}C$ , Rex 1906)

53329\* ( $18.1^{\circ}C$ , summary of literature data, temp range  $-78.8$  to  $36.5^{\circ}C$ , Stull 1947)

70580 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.96540 - 1081.6/(230 + t/^{\circ}C)$ ; temp range  $-32$  to  $90^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

68700 (interpolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 6.91997 - 1081.4/(232 + t/^{\circ}C)$ ; temp range  $-33$  to  $68^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 6855.2/(T/K)] + 7.75768$ ; temp range  $-78.8$  to  $36.5^{\circ}C$  (Antoine eq., Weast 1972-73)

70000 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.91429 - 1593.593/(289.355 + t/^{\circ}C)$ ; temp range  $0-30^{\circ}C$  (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)

69440 (interpolated-Antoine eq., temp range  $0-30^{\circ}C$ , Dean 1985, 1992)

$\log(P/mmHg) = 7.771 - 1582.0/(288.0 + t/^{\circ}C)$ ; temp range  $0-30^{\circ}C$  (Antoine eq., Dean 1985, 1992)



68700 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 5.3643 - 779.7/(196.5 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

68800 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.54823 - 860.49/(-66.25 + T/\text{K})$ ; temp range 239–310 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 115.1259 - 4.6278 \times 10^3/(T/\text{K}) - 42.197 \cdot \log (T/\text{K}) + 2.526 \times 10^{-2} \cdot (T/\text{K}) - 9.8906 \times 10^{-14} \cdot (T/\text{K})^2$ ; temp range 156–589 K (vapor pressure eq., Yaws 1994)

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

1652 (calculated-P/C, using Hine & Mookerjee 1975 data)

1248 (calculated-QSAR, Nirmalakhandan & Speece 1988)

1468 (computed value, Yaws et al. 1991)

1836 ( $\gamma^{\infty}$  from gas stripping-GC, Li et al. 1993)

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

1.69 (calculated- $\pi$  const., Hansch et al. 1968)

1.90 (shake flask, Log P Database, Hansch & Leo 1987)

1.90 (recommended, Sangster 1989)

1.90 (recommended, Hansch et al. 1995)

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

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

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

Hydrolysis: rate constant  $k = 2.12 \times 10^7 \text{ s}^{-1}$  with  $t_{1/2} = 38 \text{ d}$  at  $25^{\circ}\text{C}$  and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

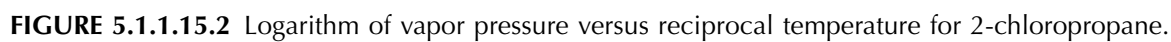
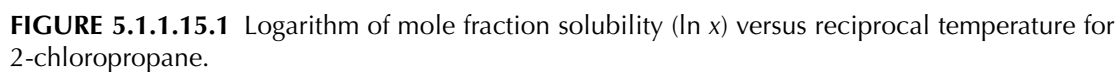
Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (Darnall et al. 1976).

Surface water:  $t_{1/2} = 38 \text{ d}$  at  $25^{\circ}\text{C}$  and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)

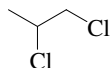
**TABLE 5.1.1.15.1**

**Reported aqueous solubilities and vapor pressures of 2-chloropropane at various temperatures**

Aqueous solubility				Vapor pressure			
Rex 1906		Horvath 1982		Rex 1906		Stull 1947	
volumetric method		summary of literature data				summary of literature data	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{P/Pa}$	$t/^{\circ}\text{C}$	$\text{P/Pa}$
0	440	0	4381	0	25558	−78.8	133.3
10	362	10	3607	10	38863	−61.1	666.6
20	305	20	3141	20	58062	−52.0	1333
30	304	25	2945	30	83953	−42.0	2666
		30	3031			−31.0	5333
						−23.5	7999
						−13.7	13332
						1.30	26664
						18.1	53329
						36.5	101325
						$\text{mp}/^{\circ}\text{C}$	−117



## 5.1.1.16 1,2-Dichloropropane



Common Name: 1,2-Dichloropropane

Synonym: propylene chloride, propylene dichloride,  $\alpha,\beta$ -propylene dichloride

Chemical Name: 1,2-dichloropropane

CAS Registry No: 78-87-5

Molecular Formula: 1,2-C<sub>3</sub>H<sub>6</sub>Cl<sub>2</sub>, CH<sub>3</sub>CHClCH<sub>2</sub>Cl

Molecular Weight: 112.986

Melting Point (°C):

−100.53 (Lide 2003)

Boiling Point (°C):

96.40 (McGovern 1943; Timmermans 1950; Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.1560 (Dreisbach 1959, 1961; Horvath 1982; Weast 1982–83; Riddick et al. 1986)

1.1494 (25°C, Dreisbach 1959, 1961)

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

98 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

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

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

36.33, 30.5 (25°C, normal bp, Dreisbach 1961)

36.40, 32.004 (25°C, bp, Riddick et al. 1986)

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

6.40 (calculated, Dreisbach 1959; quoted, Riddick et al. 1986)

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

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

2800 (shake flask-interferometer, Gross 1929; Stephen & Stephen 1963)

2773 (Seidell 1940)

2700 (20°C, McGovern 1943)

2750 (measured by Dow Chemical, Dreisbach 1955–1961)

2096 (shake flask-GC, Jones et al. 1977/1978)

3520 (shake flask-GC, Chiou et al. 1979)

2800\* (summary of literature data, Horvath 1982)

2420 (headspace-GC, McNally & Grob 1983)

2070 (30°C, headspace-GC, McNally & Grob 1984)

2600 (Dean 1985)

2740 (selected, Riddick et al. 1986; Howard 1990)

3000\*, 2900 (20°C, 29.7°C, shake flask-GC/TC, measured range 0–90.4°C, Stephenson 1992)

3005, 3129, 3261 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)

3287, 3706, 4152 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -UNIFAC, Tse et al. 1992)

2683, 2717, 3003 (20, 30, 40°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)

2650 (20°C, limiting activity coeff.  $\gamma^\infty$  by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

2740\* (recommended, temp range 278.15–313.15 K, IUPAC-NIST Series, Horvath & Getzen 1999)

$S/(wt\%) = 3.3285 - 0.021464 \cdot (T/K) + 3.7632 \times 10^{-5} \cdot (T/K)^2$ , temp range 275–313 K (Horvath & Getzen 1999)

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):

7200\* (isoteniscope method, measured range 15–99.7°C, Nelson & Young 1933)

$\log (P/\text{mmHg}) = 7.7085 - 1782.8/(T/K)$ ; temp range 15–100°C (isoteniscope, Nelson & Young 1933)

6930 (McGovern 1943)

- 6780\* (Antoine eq. regression, temp range -7 to 141.6°C, Stull 1947)  
 16500\* (44.78°C, ebulliometry, measured range 44.78–96.2°C, Dreisbach & Shrader 1949)  
 6620 (calculated-Antoine eq., Dreisbach 1959, 1961)  
 $\log(P/\text{mmHg}) = 6.96395 - 1295.9/(221.0 + t/^\circ\text{C})$ ; temp range 15–160°C (Antoine eq. for liquid state, Dreisbach 1959)  
 $\log(P/\text{mmHg}) = 6.96546 - 1296.4/(221.0 + t/^\circ\text{C})$ ; temp range 15–135°C (Antoine eq. for liquid state, Dreisbach 1961)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 8428.5/(T/K)] + 7.882416$ ; temp range -38.5 to 96.8°C (Antoine eq., Weast 1972–73)  
 6720 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log(P/\text{mmHg}) = 6.98047 - 1308.138/(222.845 + t/^\circ\text{C})$ ; temp range 44.8–96.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)  
 6720, 7120 (calculated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.10153 - 1305.689/(222.567 + t/^\circ\text{C})$ , temp range 55.78–96.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.73547 - 1717.264/(266.9 + t/^\circ\text{C})$ , temp range 15–99.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log(P/\text{mmHg}) = 6.9807 - 1308.1/(222.8 + t/^\circ\text{C})$ ; temp range 45–96°C (Antoine eq., Dean 1985, 1992)  
 6622 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 6.08885 - 1295.9/(221.0 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 6620 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_1/\text{kPa}) = 6.08324 - 1292.64/(-52.52 + T/K)$ ; temp range 239–373 K (Antoine eq., Stephenson & Malanowski 1987)  
 5410, 8790, 13790 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)  
 $\log(P/\text{mmHg}) = 5.4819 - 2.1918 \times 10^3/(T/K) + 2.6014 \cdot \log(T/K) - 1.1751 \times 10^{-2} \cdot (T/K) + 7.3435 \times 10^{-6} \cdot (T/K)^2$ ; temp range 173–572 K (vapor pressure eq., Yaws 1994)

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):

- 298 (calculated- $1/K_{\text{AW}}$ ,  $C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)  
 31.21, 2261 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)  
 280\* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)  
 $\ln(k_{\text{H}}/\text{atm}) = 19.60 - 4333/(T/K)$ ; temp range: 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 210 (calculated-P/C, Mackay & Yuen 1983)  
 286 (gas stripping-GC, Warner et al. 1987)  
 362\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 9.843 - 4708/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 233 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 150 (computed value, Yaws et al. 1991)  
 213, 324, 486 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)  
 216, 347, 497 (20, 35, 50°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 3.37, 5.93 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 222 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 226.8 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 232 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 4.878 - 1730/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)  
 227.6\* (EPICS-SPME, measured range 2–70°C, Görgényi et al. 2002)  
 $\ln K_{\text{AW}} = 9.49 - 3494.7/(T/K)$ ; temp range 2–70°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:

- 2.00 (Hansch & Leo 1979)  
 1.98 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)  
 1.99\* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)

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

2.96 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

< 1.0 (fish, Kawasaki 1980; quoted, Howard 1990)

1.29 (calculated- $K_{OW}$ , Howard 1990)

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

1.43 (soil, equilibrium sorption isotherm, Chiou et al. 1979)

1.67 (silt loam soil, quoted from Chiou et al. 1979; Howard 1990)

1.70 (calculated-MCI  $\chi$ , Sabljic 1984)

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

Volatilization:  $t_{1/2} < 50$  min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Mills et al. 1982);

$t_{1/2} = 8$  min from a stirred solution 1.6 cm deep (Chiou et al. 1980; quoted, Howard 1990);

$t_{1/2} = 1.7$ – $10$  d, estimated from an EXAMS model of the fate of 1,2-dichloropropane in a pond, river, and two lakes (Burns 1981; quoted, Howard 1990);

$t_{1/2} = 8.3$  h at 1 m depth of stirred aqueous solution (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} \sim 5.5$  h for the removal from a stream of 1 m depth with 1 m/s current, based on laboratory-determined relative transfer coefficients (Cadena et al. 1984; quoted, Howard 1990).

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:

photooxidation  $t_{1/2} = 65$ – $646$  h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{O_3}(aq.) \leq 0.004 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $22^\circ\text{C}$ , with a half-life of 100 d at pH 7 (Yao & Haag 1991).

Hydrolysis:  $k = 5.0 \times 10^{-6} \text{ h}^{-1}$  at pH 7 to 9 and  $25^\circ\text{C}$  with a calculated  $t_{1/2} = 15.8$  yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biodegradation: aerobic  $t_{1/2}(aq.) = 4008$ – $30936$  h, based on acclimated aerobic soil grab sample data (Roberts & Stoydin 1976; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2}(aq.) = 16032$ – $123744$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4$ – $24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 65$ – $646$  h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

$t_{1/2} > 23$  d, reaction with photochemically produced OH radical (Howard 1990).

Surface water:  $t_{1/2} = 4008$ – $30936$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); measured rate constant  $k \leq 0.004 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $22^\circ\text{C}$ , with  $t_{1/2} \geq 100$  d at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 8016$ – $61872$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 4008$ – $30936$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.1.16.1

Reported aqueous solubilities of 1,2-dichloropropane at various temperatures

$$S/(\text{wt}\%) = 0.1300 + 1.43332 \times 10^{-2} \cdot (t/^{\circ}\text{C}) - 4.99992 \times 10^{-4} \cdot (t/^{\circ}\text{C})^2 + 6.66654 \times 10^{-6} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 3.3285 - 0.021464 \cdot (T/\text{K}) + 3.7632 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

Horvath 1982		Stephenson 1992		Tse et al. 1992		Horvath & Getzen 1999	
summary of literature data		shake flask-GC		activity coefficient		recommended IUPAC-NIST	
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	2300	0	2900	20	3005	5	2799
20	2700	9.5	2800	30	3129	10	2680
25	2800	20	3000	40	3261	15	268-
30	2900	29.7	2900			20	2700
		40.3	3000			25	2740
eq.1	S/wt%	49.8	3200	Wright et al. 1992		30	2800
		60	3500	activity coefficient		35	2880
		70.5	3900	t/°C	S/g·m <sup>-3</sup>	40	2970
		80.2	4700				
		90.4		20	2583	eq. 2	S/wt%
				30	2717	temp range 275–313 K	
				40	3003		

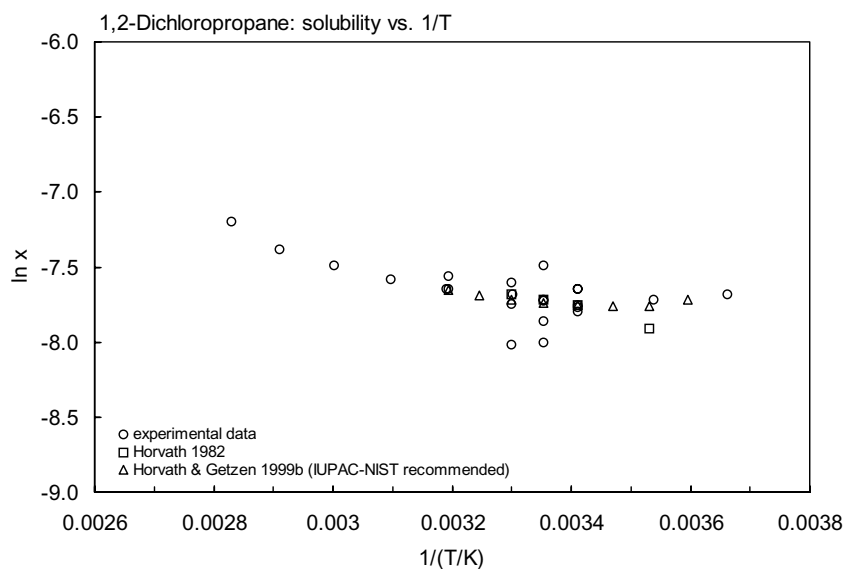


FIGURE 5.1.1.16.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.16.2

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

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

Nelson & Young 1933		Stull 1947		Dreisbach & Shrader 1949	
static method		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
15.0	4400	-7.0	133.3	44.78	16500
20.0	5600	17.3	666.6	69.0	42066
25.0	7199	29.4	1333	83.18	67661
30.0	8999	42.3	2666	96.2	101325
35.0	11199	57.2	5333		
40.0	13799	66.4	7999		
45.0	16839	75.7	13332		
50.0	20625	97.8	26664		
55.0	24065	118.5	53329		
60.0	30317	141.6	101325		
65.0	36397				
70.0	43570	mp/°C	-34.4		
75.0	51729				
80.0	61235				
85.0	71874				
90.0	84059				
95.0	97792				
96.0	100525				
96.4	101325				
99.7	112937				

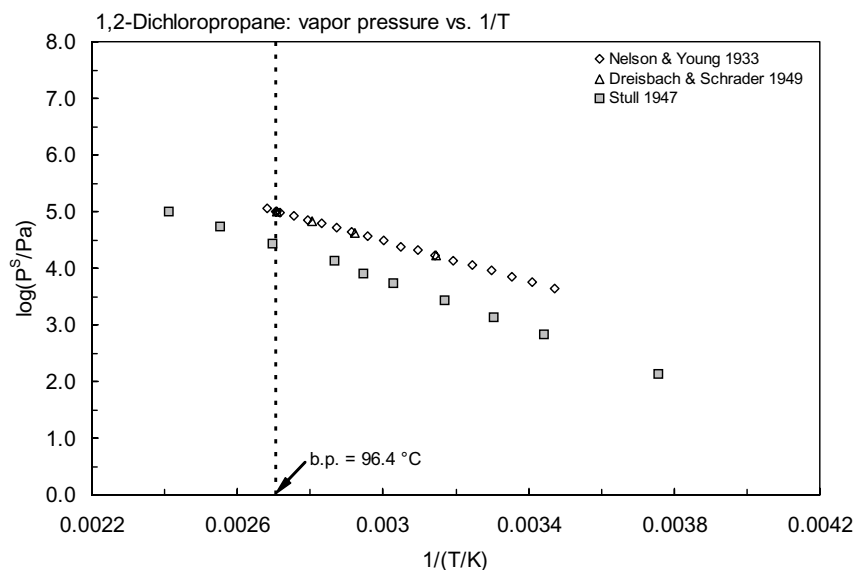


FIGURE 5.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloropropane.

TABLE 5.1.1.16.3

Reported Henry's law constants of 1,2-dichloropropane 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)				
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)						
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)				
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)						
<b>Leighton &amp; Calo 1981</b>	<b>Ashworth et al. 1988</b>	<b>Tse et al. 1992</b>	<b>Görgényi et al. 2002</b>				
<b>equilibrium cell-GC</b>	<b>EPICS-GC</b>	<b>activity coefficient</b>	<b>EPICS-SPME method</b>				
<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>
1.90	83.5	10	123.6	20	213	2	82.35
13.5	164.5	15	127.7	30	324	6	109
15.7	185.3	20	192.5	40	486	10	134.2
17.1	239.7	25	361.7			18	203.3
22.0	239.7	30	289.8			25	227.6
24.9	280.0					30	341.8
				<b>Wright et al. 1992</b>			
				<b>activity coefficient</b>		40	524.9
eq. 3	k <sub>H</sub> /atm	eq. 4	H/(atm m³/mol)	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	50	759.8
A	19.6	A	9.843			60	1014
B	4333	B	4708			70	1226
				20	216		
				35	347		
				50	497	eq. 1	K <sub>AW</sub>
						A	9.49
						B	3494.7

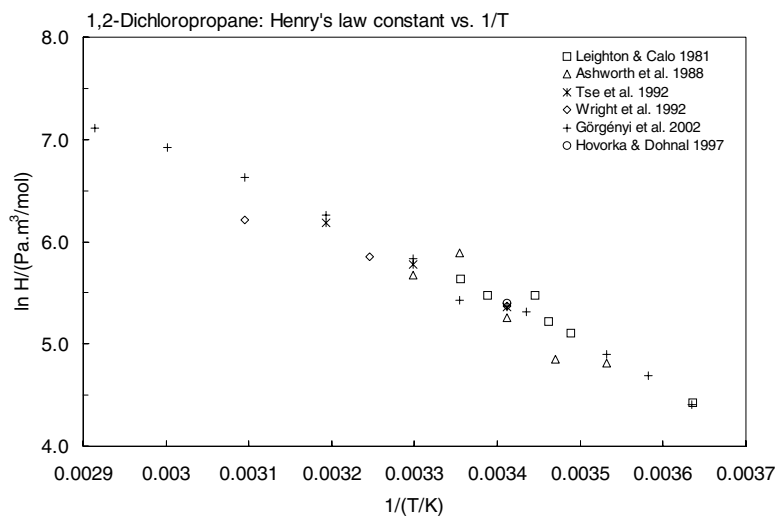
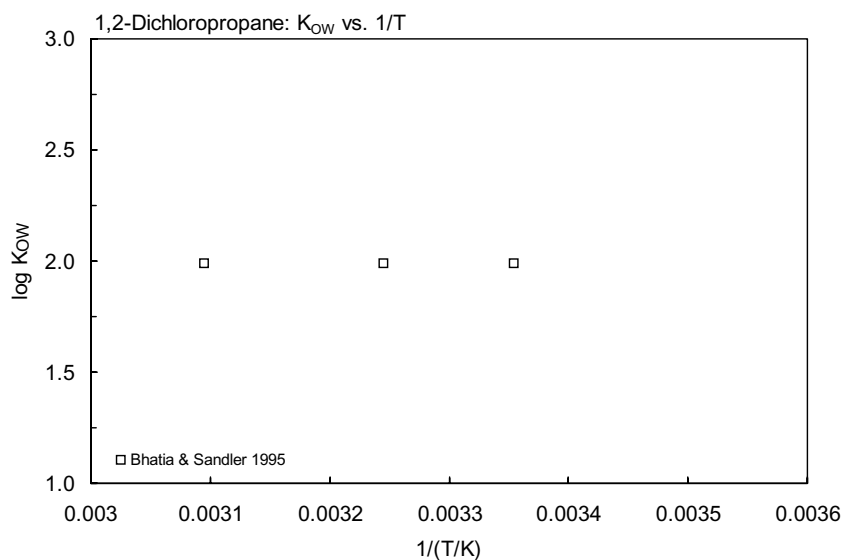


FIGURE 5.1.1.16.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dichloropropane.



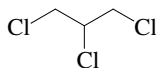
**TABLE 5.1.1.16.4**  
**Reported octanol-water partition coefficient of**  
**1,2-dichloropropane at various temperatures**

Bhatia & Sandler 1995	
relative GC-RT technique	
t/°C	log K <sub>OW</sub>
25	1.99
35	1.99
50	1.99
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$	
$\log K_{OW} = A - \Delta H/2.303RT$	
A	1.0195
$\Delta H$	-20.2



**FIGURE 5.1.1.16.4** Logarithm of K<sub>OW</sub> versus reciprocal temperature for 1,2-dichloropropane.

## 5.1.1.17 1,2,3-Trichloropropane



Common Name: 1,2,3-Trichloropropane

Synonym:

Chemical Name: 1,2,3-trichloropropane

CAS Registry No: 96-18-4

Molecular Formula: 1,2,3-C<sub>3</sub>H<sub>3</sub>Cl<sub>3</sub>, CH<sub>2</sub>ClCHClCH<sub>2</sub>Cl

Molecular Weight: 147.431

Melting Point (°C):

-14.7 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

157 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.3888 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

1.3832 (25°C, Dreisbach 1961; Riddick et al. 1986)

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

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

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

46.93, 37.12 (25°C, normal bp, Dreisbach 1961; Riddick et al. 1986)

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 or as indicated):

1900 (20°C, literature average, Dilling 1977)

1896 (recommended, Horvath 1982)

1900 (selected, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

492 (extrapolated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.98716 – 1502.3/(209.0 + t/°C); temp range 64–204°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = [–0.2185 × 10714.3/(T/K)] + 8.326893; temp range 9.0–158°C (Antoine eq., Weast 1972–73)

266.6, 533.2 (20°C, 30°C, Verschuereen 1983)

492.0 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P<sub>L</sub>/kPa) = 6.11206 – 1502.3/(–64.15 + T/K); temp range 337–477 K (Antoine eq., Stephenson & Malanowski 1987)

413, 960 (quoted, calculated-solvatochromic parameters. and UNIFAC, Banerjee et al. 1990)

log (P/mmHg) = –3.9501 – 2.4501 × 10<sup>3</sup>/(T/K) + 6.6887 · log (T/K) – 1.4991 × 10<sup>–2</sup> · (T/K) + 7.3403 × 10<sup>–6</sup> · (T/K)<sup>2</sup>; temp range 258–652 K (vapor pressure eq., Yaws 1994)

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):

32.22 (calculated-C<sub>A</sub>/C<sub>w</sub>, Dilling 1977)

36.1\* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)

ln (k<sub>H</sub>/atm) = 14.61 – 3477/(T/K); temp range: 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

24.91\* (25.6°C, EPICS-GC, tap water, measured range 25.6–45°C, Tancredi & Yanagisawa 1990)

log K<sub>AW</sub> = 3.351 – 1606/(T/K); temp range 26.5–45°C (EPICS measurements, Tancredi & Yanagisawa 1990)

34.4 (computed value, Yaws et al. 1991)

22.31 (interpolated from Tancredi & Yanagisawa 1990, Tancredi et al. 1992)

23.71 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 22.74 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{AW} = 3.073 - 1496/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

2.63 (estimated, Abernethy et al. 1988)  
 1.98 (quoted, Van Leeuwen et al. 1992; Verhaar et al. 1992)  
 2.25, 2.36 (quoted, calculated-molar volume, Wang et al. 1992)

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

Bioconcentration Factor,  $\log BCF$ :

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

1.98; 1.89; 1.92 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)

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

Volatilization: evaporation  $t_{1/2} = 51$  min from dilute aqueous solution (Dilling 1975)

Evaporation  $t_{1/2}(\text{exptl}) = 56.1$  min,  $t_{1/2}(\text{calc}) = 18$  min, 44.7 min from water (Dilling 1977)

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 61\text{--}613$  h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:  $k = 1.8 \times 10^{-6} \text{ h}^{-1}$  at pH 7 to 9 at 25°C with a calculated  $t_{1/2} = 44$  yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biodegradation: aerobic  $t_{1/2}(\text{aq.}) = 4320\text{--}8640$  h, based on acclimated aerobic grab sample test data for 1,3-dichloropropane (Roberts & Stoydin 1976; quoted, Howard et al. 1991); anaerobic  $t_{1/2}(\text{aq.}) = 17280\text{--}34560$  h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 61\text{--}613$  h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 4320\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water:  $t_{1/2} = 8640\text{--}17280$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

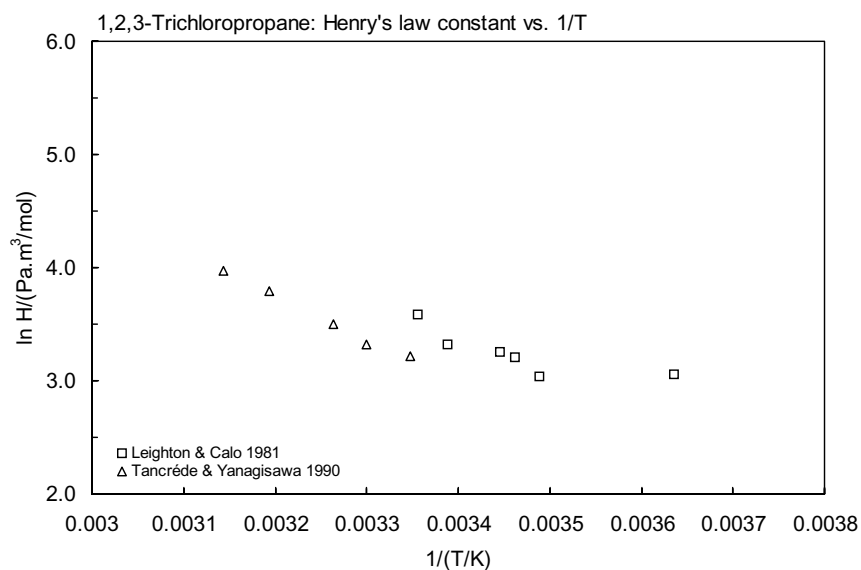
Soil: disappearance  $t_{1/2} = 2.7$  d was calculated from first-order kinetic for volatilization loss of mixtures in soils (Anderson et al. 1991);

$t_{1/2} = 4320\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

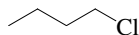
Biota:

**TABLE 5.1.1.17.1**  
**Reported Henry's law constants of 1,2,3-trichloropropane at various temperatures**

Leighton & Calo 1981	
equilibrium cell-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)
1.90	21.27
13.5	20.90
15.7	24.71
17.1	25.86
22.0	27.58
24.9	36.13
$\ln (k_H/\text{atm}) = A - B/(T/K)$	
A	14.61
B	3477



**FIGURE 5.1.1.17.1** Logarithm of Henry's law constant versus reciprocal temperature for 1,2,3-trichloropropane.

5.1.1.18 1-Chlorobutane (*n*-Butyl chloride)

Common Name: 1-Chlorobutane

Synonym: *n*-butyl chloride, butyl chlorideChemical Name: 1-chlorobutane, *n*-butyl chloride

CAS Registry No: 109-69-3

Molecular Formula:  $C_4H_9Cl$ ,  $CH_3CH_2CH_2CH_2Cl$ 

Molecular Weight: 92.567

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

-123.1 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

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

78.44 (Dreisbach 1959, 1961; Horvath 1982; Dean 1985)

78.4 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):0.8862, 0.8808 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959, 1961; Horvath 1982)0.8857, 0.8810 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)Molar Volume ( $cm^3/mol$ ):

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

104.5 ( $20^{\circ}C$ , calculated-density)Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):30.02, 33.32 (normal bp,  $25^{\circ}C$ , Dreisbach 1961)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):

666 ( $12.5^{\circ}C$ , shake flask, Fühner 1924)

640 (Seidell 1940)

741 (Kakovsky 1957)

667 ( $17.5^{\circ}C$ , Saracco & Spaccamela Marchetti 1958)671 ( $20^{\circ}C$ , exptl., Korenman et al. 1971; Horvath 1982)

614.7\* (summary of literature data, Horvath 1982)

872 (generator column-HPLC, Tewari et al. 1982)

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):

4173\* ( $20^{\circ}C$ , static method-manometer, measured range  $20$ – $70^{\circ}C$ , Smyth & Engel 1929)14170\* (interpolated compiled data, temp range  $-49$  to  $77.8^{\circ}C$ , Stull 1947)

13650 (calculated-Antoine eq., Dreisbach 1959)

 $\log(P/\text{mmHg}) = 6.93790 - 1227.43/(224.1 + t/^{\circ}C)$ ; temp range  $0$ – $123^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

 $\log(P/\text{mmHg}) = 6.93790 - 1227.433/(224.1 + t/^{\circ}C)$ ; temp range  $1$ – $116^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

 $\log(P/\text{mmHg}) = 6.93790 - 1227.433/(224.10 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
10639\* ( $19.7^{\circ}C$ , differential thermal analysis, measured range  $-16.7$  to  $78.5^{\circ}C$ , Kemme & Kreps 1969)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8144.8/(T/K)] + 7.979366$ ; temp range  $-49$  to  $77.8^{\circ}C$  (Antoine eq., Weast 1972–73)
14719\* ( $26.85^{\circ}C$ , differential thermal analysis, measured range  $26.85$ – $80.0^{\circ}C$ , Gutsche & Knapp 1982)
 $\log(P/\text{mmHg}) = 6.83694 - 1173.79/(218.13 + t/^{\circ}C)$ , temp range:  $-17$  to  $78.6^{\circ}C$  (Antoine eq., Dean 1985, 1992)
13300 ( $24.47^{\circ}C$ , selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.0514 - 1216.82/(222.33 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

13660 (interpolated-Antoine eq., Stephenson &amp; Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.0628 - 1227.433/(-49.05 + T/\text{K})$ ; temp range 257–389 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 35.7808 - 2.8632 \times 10^3/(T/\text{K}) - 8.8957 \cdot \log (T/\text{K}) + 5.1598 \times 10^{-11} \cdot (T/\text{K}) + 3.5488 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
temp range 150–537 K (vapor pressure eq., Yaws 1994)

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):

1970 (exptl- $1/K_{AW} = C_W/C_A$ , Hine & Mookerjee 1975)

1800, 8600 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1530\* (23°C, equilibrium cell-concn ratio-GC/FID, measured range 1–23°C, Leighton & Calo 1981)

$\ln (k_H/\text{atm}) = 18.51 - 3482/(T/\text{K})$ ; temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

1708 (computed value, Yaws et al. 1991)

1878 ( $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)

1485 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

1384 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.488 - 1388/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

2.39 (shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)

2.64 (shake flask, Hansch & Leo 1979; 1987)

2.55 (generator column-GC, DeVoe et al. 1981)

2.55 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)

2.64 (recommended, Sangster 1989, 1993)

2.64 (recommended, Hansch et al. 1995)

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

2.72 (head-space GC, Abraham et al. 2001)

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

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

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (Darnall et al. 1976).

**TABLE 5.1.1.18.1**

**Reported aqueous solubilities and Henry's law constants of 1-chlorobutane at various temperatures**

$$S/(\text{wt}\%) = 0.07703 - 6.75497 \times 10^{-4} \cdot (t/^\circ\text{C}) - 1.00170 \times 10^{-10} \cdot (t/^\circ\text{C})^2 + 8.50030 \times 10^{-8} \cdot (t/^\circ\text{C})^3 \quad (1)$$

Aqueous solubility		Henry's law constant	
Horvath 1982		Leighton & Calo 1981	
summary of literature data		equilibrium cell-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
0	770.3	1.0	593.7
10	703.6	3.0	684.5
20	642.0	12.4	979.2
25	614.7	12.5	1038
30	590.6	17.9	1265

TABLE 5.1.1.18.1 (Continued)

Aqueous solubility		Henry's law constant	
Horvath 1982		Leighton & Calo 1981	
summary of literature data		equilibrium cell-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	H/(Pa m <sup>3</sup> /mol)
eq. 1	S/wt%	22.7	1251
		23.0	1530
		ln (k <sub>H</sub> /atm) = A – B/(T/K)	
		A	18.51
		B	3482

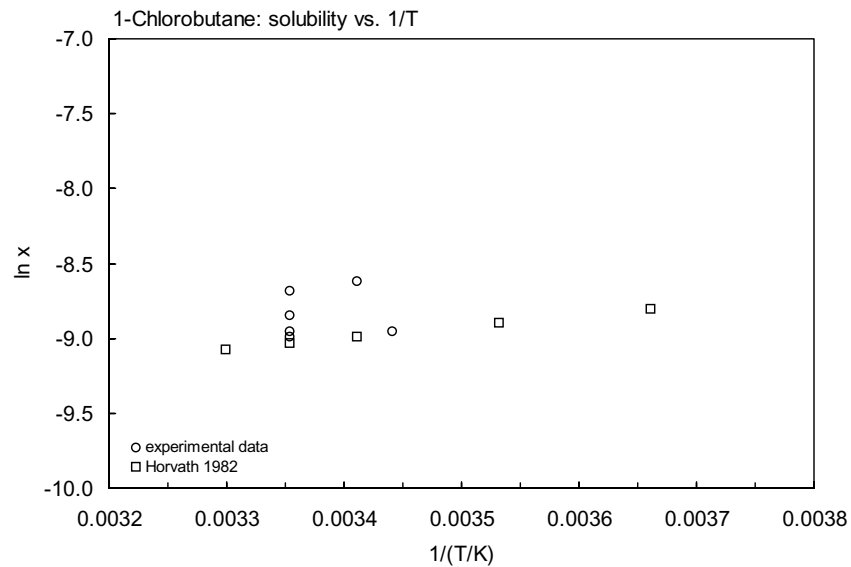


FIGURE 5.1.1.18.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-chlorobutane.

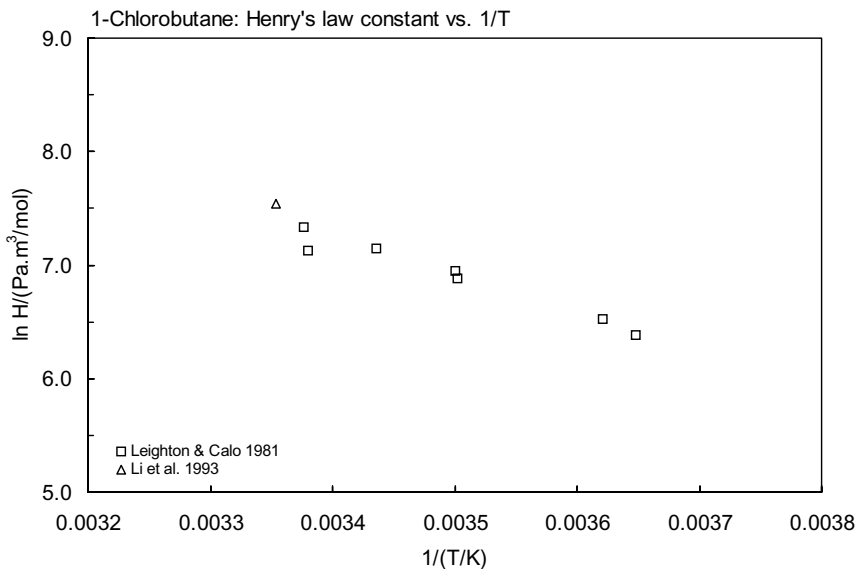


FIGURE 5.1.1.18.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorobutane.

TABLE 5.1.1.18.2

Reported vapor pressures of 1-chlorobutane at various temperatures and the coefficients for the vapor pressure equations

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

Smyth & Engel 1929		Stull 1947		Kemme & Kreps 1969		Gutsche & Knapp 1982	
static-manometry		summary of literature data		static method-DTA*		Vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20.0	4173	-49.0	133.3	-16.7	1347	26.85	14719
30.0	6799	-28.9	666.6	-10.5	2026	30.0	17001
40.0	10959	-18.6	1333	-6.20	2640	50.0	38434
50.0	16892	-7.40	2666	0.80	3946	51.85	41397
60.0	25278	5.0	5333	6.20	5360	78.85	96925
70.0	36170	13.0	7999	12.0	7306	80.0	106255
		24.0	13332	19.7	10639		
		40.0	26664	28.8	16212		
		55.8	53329	41.1	27078		
		77.8	101325	51.3	40263		
				65.5	66541		
		mp/°C	-123.1	78.5	101165		
				eq. 2	P/mmHg		
				A	6.87098		
				B	1182.903		
				C	218.285		

\*DTA—differential thermal analyzer

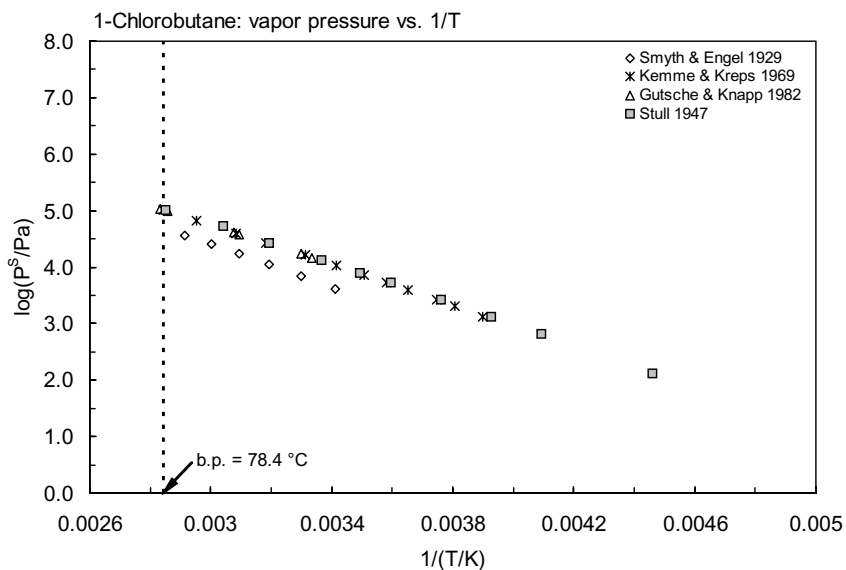


FIGURE 5.1.1.18.3 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorobutane.



## 5.1.1.19 2-Chlorobutane



Common Name: 2-Chlorobutane

Synonym: methylethylchloromethane, *sec*-butyl chloride

Chemical Name: 2-chlorobutane, methylethylchloromethane, *sec*-butyl chloride

CAS Registry No: 78-86-4

Molecular Formula:  $C_4H_9Cl$ ,  $CH_3CH_2CHClCH_3$

Molecular Weight: 92.567

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

−131.3 (Dreisbach 1961; Horvath 1982; Lide 2003)

−113.3, −140.5 (racemic, active, Riddick et al. 1986)

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

68.25 (Dreisbach 1961; Horvath 1982; Riddick et al. 1986)

68.2 (Lide 2003)

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

0.8732, 0.8677 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961; Horvath 1982; Dean 1985)

0.8732 (racemic, Riddick et al. 1986)

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

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

106.0 ( $20^{\circ}C$ , calculated-density)

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

31.81, 29.20 ( $25^{\circ}C$ , bp, Dreisbach 1961)

31.56, 29.20 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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 and reported temperature dependence equations):

1000 (volumetric method, Wright & Schaffer 1932)

1000 (Dean 1985; Riddick et al. 1986)

1070, 930, 850, 820, 840, 920 (0, 5, 10, 15, 20,  $35^{\circ}C$ , tentative values, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

$S/(wt\%) = 8.9653 - 0.061598 \cdot (T/K) + 1.0678 \times 10^{-4} \cdot (T/K)^2$ , temp range 273–298 K (equation derived from reported solubility data, Horvath & Getzen 1999)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

20210 (interpolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 6.94469 - 1195.8/(226.0 + t/^{\circ}C)$ ; temp range  $-7$  to  $104^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 7407.9/(T/K)] + 7.625620$ ; temp range  $-60.2$  to  $68^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = 6.79923 - 1149.12/(224.68 + t/^{\circ}C)$ ; temp range  $0$ – $40^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P/kPa) = 6.1222 - 1145.2/(234.4 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

20200 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.06958 - 1195.8/(-47.15 + T/K)$ ; temp range  $266$ – $377$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 28.2992 - 2.4355 \times 10^3/(T/K) - 7.359 \cdot \log(T/K) - 1.3048 \times 10^{-11} \cdot (T/K) + 3.0834 \times 10^{-6} \cdot (T/K)^2$ ; temp range  $142$ – $521$  K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa  $m^3/mol$  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):

2268\* ( $24.9^{\circ}C$ , equilibrium cell-concn ratio-GC/FID, measured range  $1.9$ – $24.9^{\circ}C$ , Leighton & Calo 1981)

$\ln(k_H/atm) = 22.29 - 4499/(T/K)$ ; temp range  $1.9$ – $24.9^{\circ}C$  (equilibrium cell-concn ratio, Leighton & Calo 1981)

1869 (computed value, Yaws et al. 1991)

1886 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.129 - 1829/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

1.51 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

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

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

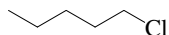
Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radicals (Darnall et al. 1976).

**TABLE 5.1.1.19.1**  
**Reported Henry's law constants of 2-chlorobutane at various temperatures**

Leighton & Calo 1981

equilibrium cell-GC	
$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
1.90	653.3
13.5	1411
15.7	1545
17.1	1625
22.0	2023
24.9	2268
$\ln (k_H/\text{atm}) = A - B/(T/K)$	
A	22.29
B	4499

5.1.1.20 1-Chloropentane (*n*-Amyl chloride)

Common Name: 1-Chloropentane

Synonym: *n*-amyl chloride, monochloropentane, pentyl chloride

Chemical Name: *n*-amyl chloride, 1-chloropentane, pentyl chloride

CAS Registry No: 543-59-9

Molecular Formula:  $C_5H_{11}Cl$ ,  $CH_3CH_2CH_2CH_2CH_2Cl$

Molecular Weight: 106.594

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

−99.0 (Dreisbach 1961; Horvath 1982; Riddick et al. 1982; Dean 1985; Lide 2003)

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

108.4 (Lide 2003)

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

0.8818 ( $20^{\circ}C$ , Weast 198–83; Horvath 1982)

0.8820, 0.8770 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

120.9 ( $20^{\circ}C$ , calculated-density)

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

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

38.24, 32.77 ( $25^{\circ}C$ , bp, Dreisbach 1961; Riddick et al. 1986)

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 and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

200 (volumetric method, Wright & Schaffer 1932)

789 (shake flask-residue volume method, Booth & Everson 1948)

190.6\* ( $24.3^{\circ}C$ , converted-distribution coeff., temp range  $2.5$ – $26.1^{\circ}C$ , Leighton & Calo 1981)

198.2\* (summary of literature data, Horvath 1982)

200 (Dean 1985; Riddick et al. 1986)

201\* (tentative values, measured range  $5$ – $35^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

$S/(wt\%) = 0.55726 - 3.7269 \times 10^{-3} \cdot (T/K) + 6.457 \times 10^{-6} \cdot (T/K)^2$ , temp range  $276$ – $310 K$  (equation derived from reported solubility data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

4142 (calculated-Antoine eq, Dreisbach 1961)

$\log (P/mmHg) = 6.96617 - 1332.890/(218.5 + t/^{\circ}C)$ ; temp range  $24$ – $148^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.96617 - 1332.890/(218.50 + t/^{\circ}C)$ ; pressure range 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

4142 (selected, Riddick et al. 1986)

$\log (P/kPa) = 5.93641 - 1271.15/(215.0 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

4148 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.09107 - 1332.89/(T/K - 54.65)$ ; temp range  $289$ – $409 K$  (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = -4.4886 - 2.2604 \times 10^3/(T/K) + 7.8088 \cdot \log (T/K) - 2.3675 \times 10^{-2} \cdot (T/K) + 1.4884 \times 10^{-5} \cdot (T/K)^2$ ; temp range  $174$ – $568 K$  (vapor pressure eq., Yaws 1994)

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

2209 (exptl.-  $1/K_{\text{AW}} = C_{\text{W}}/C_{\text{A}}$ , Hine & Mookerjee 1975)

2480, 13010 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2376\* ( $24.3^\circ\text{C}$ , equilibrium cell-concn ratio-GC/FID, measured range  $2.5$ – $26.1^\circ\text{C}$ , Leighton & Calo 1981)

$\ln(k_{\text{H}}/\text{atm}) = 23.04 - 4727/(T/\text{K})$ ; temp range  $2.5$ – $26.1^\circ\text{C}$  (equilibrium cell-concn ratio, Leighton & Calo 1981)

4942 (computed value, Yaws et al. 1991)

2407 (activity coefficient  $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)

1835 ( $20^\circ\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.455 - 1928/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

2.41 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

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

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

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4$ – $24$  h from air for the reaction with OH radical (Darnall et al. 1976).

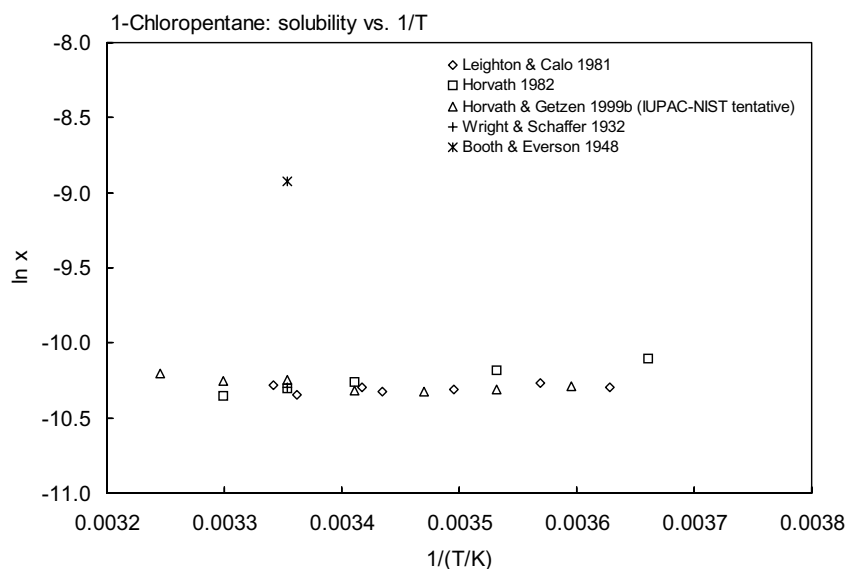
**TABLE 5.1.1.20.1**

**Reported aqueous solubilities and Henry's law constant of 1-chloropentane at various temperatures**

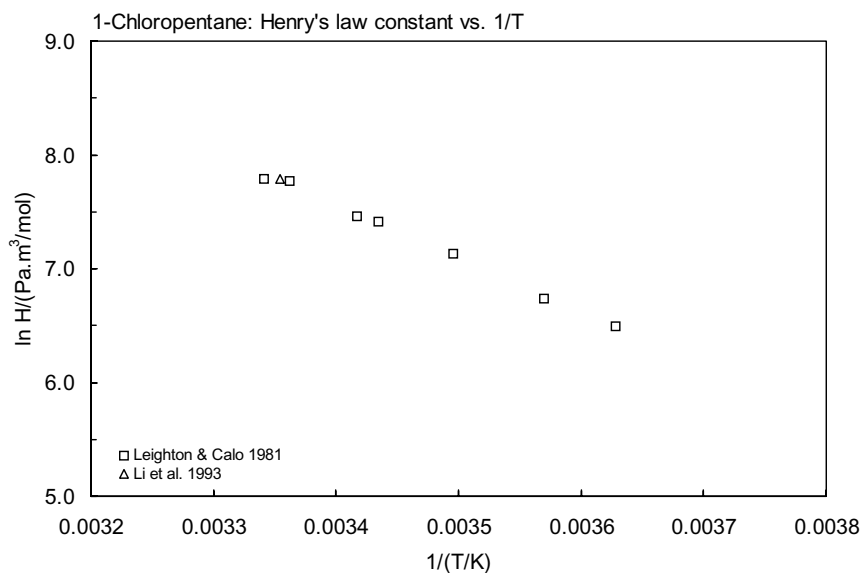
$$S/(\text{wt}\%) = 0.02426 - 1.79166 \times 10^{-4} \cdot (t/^\circ\text{C}) + 1.49999 \times 10^{-7} \cdot (t/^\circ\text{C})^2 - 3.33355 \times 10^{-9} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 0.55726 - 3.7269 \times 10^{-3} \cdot (T/\text{K}) + 6.457 \times 10^{-6} \cdot (T/\text{K})^2 \quad (2)$$

Aqueous solubility						Henry's law constant	
Leighton & Calo 1981		Horvath 1982		Horvath & Getzen 1999b		Leighton & Calo 1981	
converted-distribution coeff.		summary of literature data		summary of literature data		equilibrium cell-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
2.5	200.6	0	242.6	5	202	2.5	661
7.0	205.2	10	224.8	10	197	7.0	846.6
12.9	196.8	20	207.1	15	195	12.9	1246
18.0	195.0	25	198.2	20	196	18.0	1654
19.5	200.5	30	189.3	25	210	19.5	1742
24.3	190.6			30	209	24.3	2376
26.1	203.2	eq. 1	$S/\text{wt}\%$	35	220	26.1	2404
				eq. 2	$S/\text{wt}\%$	$\ln k_{\text{H}}/\text{atm} = A - B/(T/\text{K})$	
				temp range 276–310 K		A	23.04
						B	4727

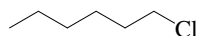


**FIGURE 5.1.1.20.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-chloropentane.



**FIGURE 5.1.1.20.2** Logarithm of Henry's law constant versus reciprocal temperature for 1-chloropentane.

## 5.1.1.21 1-Chlorohexane



Common Name: 1-Chlorohexane

Synonym: *n*-hexyl chloride

Chemical Name: 1-chlorohexane

CAS Registry No: 544-10-5

Molecular Formula: C<sub>6</sub>H<sub>13</sub>Cl

Molecular Weight: 120.620

Melting Point (°C):

−94 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

135.1 (Lide 2003)

Density (g/cm<sup>3</sup>):

0.8785; 0.8739 (20°C, 25°C, Dreisbach 1961)

0.8785 (20°C, Weast 1982–83)

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

137.7 (20°C, calculated-density, Stephenson & Malanowski 1987)

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

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

43.22, 35.39 (25°C, bp, Dreisbach 1961)

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 or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

83.6 (volumetric method, Wright & Schaffer 1932)

57.93\* (23.0°C, converted-distribution coeff., temp range 1.0–23.0°C, Leighton & Calo 1981)

91.01\* (summary of literature data, Horvath 1982)

54.3\* (tentative values, measured range 5–25°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

$S/(\text{wt}\%) = -0.019959 + 8.852 \times 10^{-5} \cdot (T/K)$ , temp range 274–296 K (equation derived from reported solubility data, Horvath & Getzen 1999b)

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):

1284 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.0115 - 1437.05/(213.4 + t/^\circ\text{C})$ ; temp range 46–178°C (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.0115 - 1437.05/(213.4 + t/^\circ\text{C})$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

1387\* (26.7°C, differential thermal analysis, measured range 15–135.6°C, Kemme & Kreps 1969)

$\log(P/\text{mmHg}) = 6.76886 - 1304.968/(t/^\circ\text{C} + 200.058)$ ; temp range 15–135.6°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

1230 (interpolated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 7.05136 - 1461.72/(t/^\circ\text{C} + 136.92)$ ; temp range 15–136°C (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1973)

1246 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_t/\text{kPa}) = 5.89376 - 1304.968/(T/K - 73.092)$ ; temp range: 288–409 K (Antoine eq., Stephenson & Malanowski 1987)

1260 (interpolated-Antoine eq., Dean 1992)

$\log(P/\text{mmHg}) = 7.05136 - 1461.72/(t/^\circ\text{C} + 215.57)$ ; temp range 15–136°C (Antoine eq., Dean 1992)

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

2312\* ( $23^\circ\text{C}$ , equilibrium cell-concn ratio-GC/FID, measured range  $1\text{--}23^\circ\text{C}$ , Leighton & Calo 1981)  
 $\ln(k_{\text{H}}/\text{atm}) = 22.16 - 4469/(T/\text{K})$ ; temp range  $1.0\text{--}23.0^\circ\text{C}$  (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 1899 ( $20^\circ\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 6.073 - 1812/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

3.68 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

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:

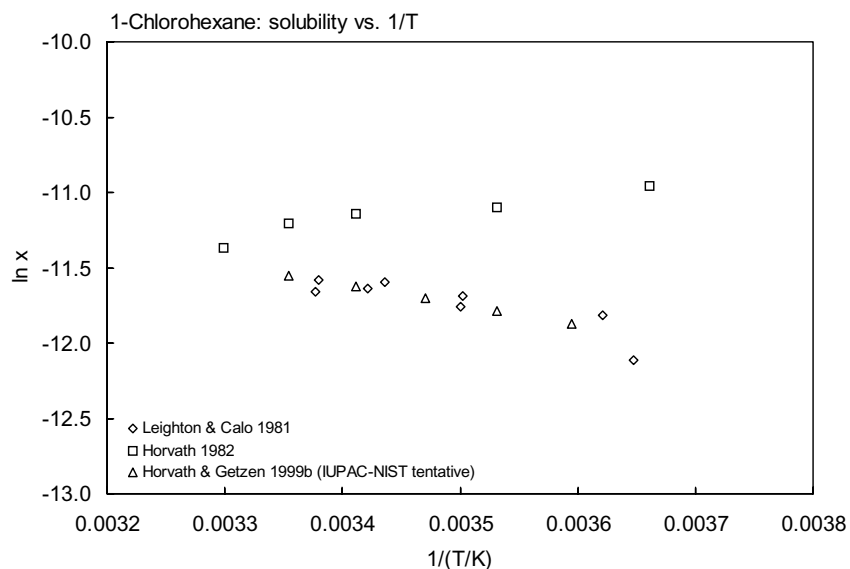
**TABLE 5.1.1.21.1**

**Reported aqueous solubilities and Henry's law constant of 1-chlorohexane at various temperatures**

$$S/(\text{wt}\%) = 0.01172 - 0.000313(t/^\circ\text{C}) - 1.078 \times 10^{-5} \cdot (t/^\circ\text{C})^2 - 4.58 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = -0.019959 + 8.852 \times 10^{-5} \cdot (T/\text{K}) \quad (2)$$

Aqueous solubility						Henry's law constant	
Leighton & Calo 1981		Horvath 1982		Horvath & Getzen 1999b		Leighton & Calo 1981	
converted-distribution coeff.		summary of literature data		summary of literature data		equilibrium cell-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
1.0	36.87	0	117.2	5	46.7	1.0	728.6
3.0	49.46	10	101.1	10	51.1	3.0	666.6
12.4	56.45	20	97.08	15	55.5	12.4	1219
12.5	52.48	25	91.01	20	59.9	12.5	1328
17.9	61.87	30	77.66	25	64.3	17.9	1593
19.1	59.29			30	209	22.7	2118
22.7	62.37	eq. 1	$S/\text{wt}\%$	35	220	23.0	2312
23.0	57.93			eq. 2	$S/\text{wt}\%$	$\ln k_{\text{H}}/\text{atm} = A - B/(T/\text{K})$	
				temp range 274–296 K		A	22.16
						B	4459



**FIGURE 5.1.1.21.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-chlorohexane.

**TABLE 5.1.1.21.2**

**Reported vapor pressures of 1-chlorohexane at various temperatures**

**Kemme & Kreps 1969**

**Static method-DTA\***

t/°C	P/Pa	t/°C	P/Pa
15.0	667	104.6	40757
26.7	1387	120.3	66781
33.1	2000	135.6	103191
38.6	2680		
46.7	4013	$\log P = A - B/(C + t/^{\circ}\text{C})$ P/mmHg	
52.6	5320		
59.7	7333		
68.4	10639		
79.5	16745		
92.6	27091		

\*DTA—differential thermal analyzer



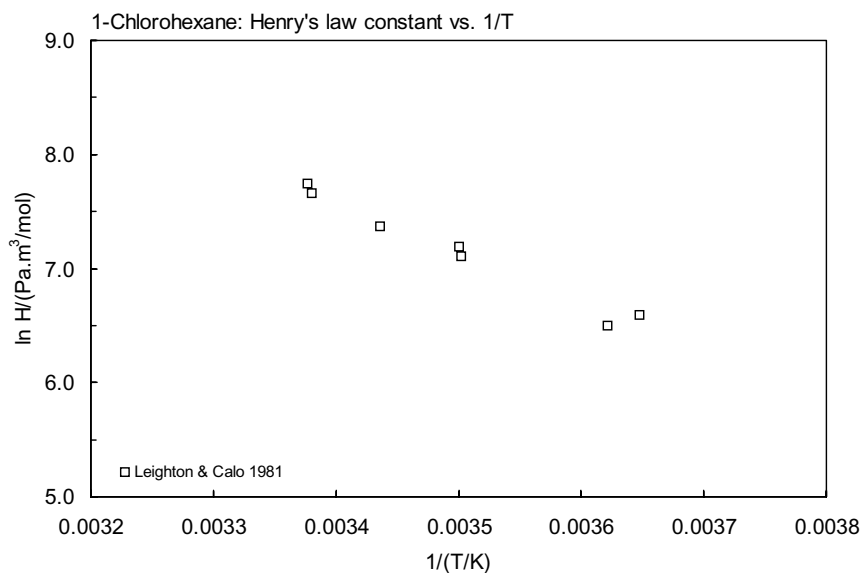


FIGURE 5.1.1.21.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorohexane.

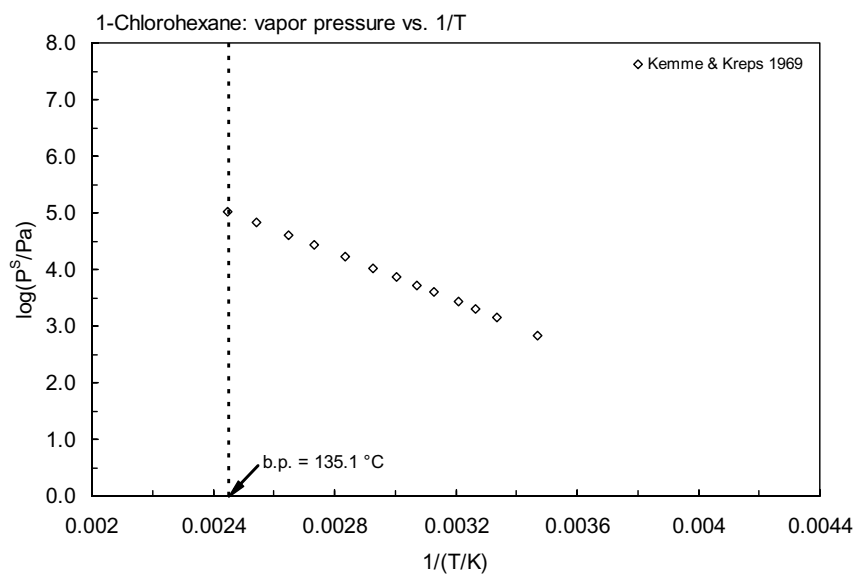
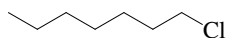


FIGURE 5.1.1.21.3 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorohexane.

## 5.1.1.22 1-Chloroheptane



Common Name: 1-Chloroheptane

Synonym: heptyl chloride

Chemical Name: 1-chloroheptane

CAS Registry No: 629-06-1

Molecular Formula:  $C_7H_{15}Cl$

Molecular Weight: 134.647

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

-69.5 (Dreisbach 1961; Weast 1982–83; Lide 2003)

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

160.4 (Lide 2003)

Density ( $g/cm^3$ ):

0.8758, 0.8715 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

0.8758 ( $20^{\circ}C$ , Weast 1982–83)

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

153.7 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

48.19, 37.95 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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  $25^{\circ}C$ ):

13.6 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)

13.6 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

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):

404 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.0650 - 1539.35/(208.8 + t/^{\circ}C)$ ; temp range  $67$ – $206^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.0650 - 1539.35/(208.8 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

680\* ( $34.4^{\circ}C$ , differential thermal analysis, measured range  $34.4$ – $160^{\circ}C$ , Kemme & Kreps 1969)

$\log(P/mmHg) = 6.83820 - 1410.064/(t/^{\circ}C + 195.639)$ ; temp range  $34.4$ – $160.1^{\circ}C$  (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

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

$\log(P/kPa) = 6.05057 - 1459.652/(t/^{\circ}C + 160.428)$ ; temp range  $34.4$ – $160^{\circ}C$  (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P_L/kPa) = 6.9631 - 1410.064/(T/K - 77.511)$ ; temp range 307–434 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 6.91670 - 1453.96/(t/^{\circ}C + 199.83)$ ; temp range  $36$ – $160^{\circ}C$  (Antoine eq., Dean 1992)

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

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

4.08 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

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

Bioconcentration Factor, log BCF or log  $K_B$ :

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

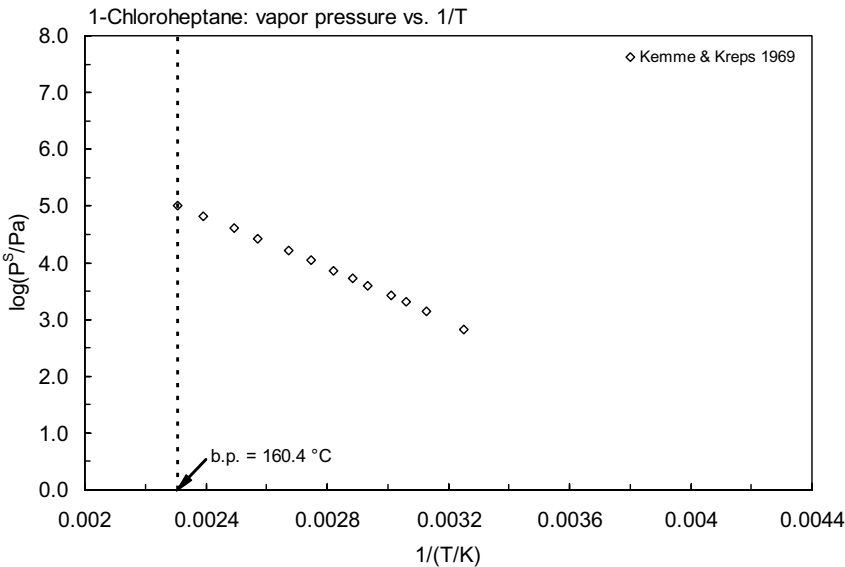
Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 5.1.1.22.1**  
**Reported vapor pressures of 1-chloroheptane at various temperatures**

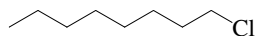
Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
34.4	679.9	127.9	40343
46.6	1400	145.1	66994
53.5	2027	160.1	100445
59.1	2680		
67.5	4013	log P = A – B/(C + t/°C)	
73.6	5306		P/mmHg
81.1	7333	A	6.83820
90.9	10919	B	1410.064
101.1	16212	C	195.639
115.6	27064		

\*DTA—differential thermal analyzer



**FIGURE 5.1.1.22.1** Logarithm of vapor pressure versus reciprocal temperature for 1-chloroheptane.

## 5.1.1.23 1-Chlorooctane



Common Name: 1-Chlorooctane

Synonym: octyl chloride

Chemical Name: 1-chlorooctane

CAS Registry No: 111-85-3

Molecular Formula:  $C_8H_{17}Cl$

Molecular Weight: 148.674

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

-57.8 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

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

183.5 (Lide 2003)

Density ( $g/cm^3$ ):

0.8738, 0.8695 (20 $^{\circ}C$ , 25 $^{\circ}C$ , Dreisbach 1961; Weast 1982–83)

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

170.2 (15 $^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

53.25, 41.09 (25 $^{\circ}C$ , bp, Dreisbach 1961)

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):

3.67\* (generator column-GC, measured range 5–40 $^{\circ}C$ , Sarraute et al. 2004)

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):

127 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.1231 - 1639.2/(204.2 + t/^{\circ}C)$ ; temp range 86–231 $^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.1231 - 1369.20/(204.4 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

747\* (54.1 $^{\circ}C$ , differential thermal analysis, measured range 54.1–184.1 $^{\circ}C$ , Kemme & Kreps 1969)

$\log(P/mmHg) = 6.84310 - 1469.829/(t/^{\circ}C + 187.157)$ ; temp range 54.1–184.1 $^{\circ}C$  (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

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

$\log(P/kPa) = 6.17348 - 1598.257/(t/^{\circ}C + 200.076)$  (Antoine eq. based on exptl. data of Kemme & Kreps 1969, temp range 54–184 $^{\circ}C$ , Boublik et al. 1984)

$\log(P_L/kPa) = 5.968 - 1469.829/(T/K - 85.993)$ ; temp range 327–457 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.05152 - 1600.24/(t/^{\circ}C + 200.28)$ ; temp range 64–184 $^{\circ}C$  (Antoine eq., Dean 1992)

126.6\* (calculated-Antoine eq. of Li & Rossini 1961, temp range 5–40 $^{\circ}C$ , Saraute et al. 2004)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at 25 $^{\circ}C$ . Additional data at other temperatures designated \* are compiled at the end of this section):

4437\* (calculated-P/C, temp range 5–40 $^{\circ}C$ , Sarraute et al. 2004)

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

4.48 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

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,  $t_{1/2}$ :

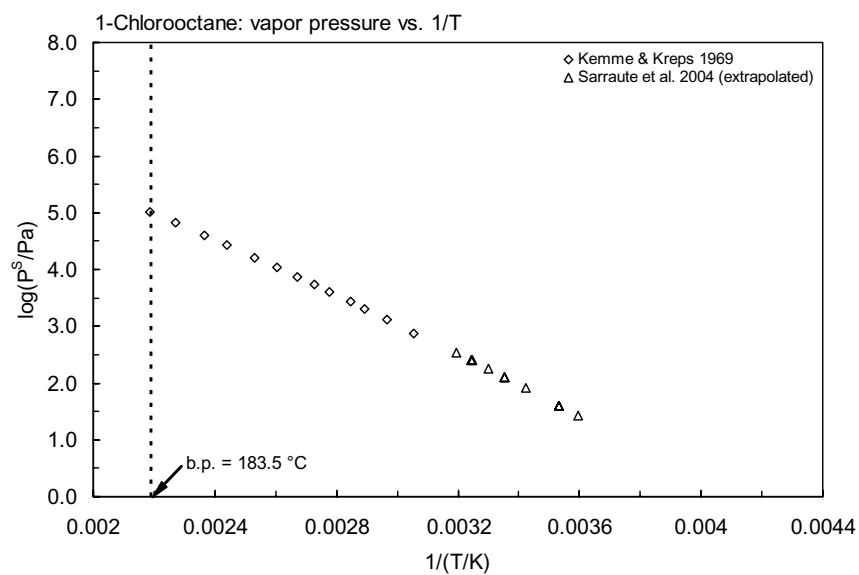
Half-Lives in the Environment:

**TABLE 5.1.1.23.1**

**Reported aqueous solubilities, vapor pressures and Henry's law constants of 1-chlorooctane at various temperatures and the coefficients for the vapor pressure equations**

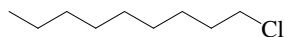
$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Aqueous solubility		Vapor pressure				Henry's law constant	
Sarraute et al. 2004		Kemme & Kreps 1969		Sarraute et al. 2004		Sarraute et al. 2004	
generator column-GC		static method-DTA*		extrapolated -Antoine eq.#		calculated-P/C	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
5.0	3.38	54.1	746.6	5.0	26.30	5.0	925
9.9	3.52	63.9	1307	9.9	39.55	9.9	1365
9.9	3.49	72.4	2040	9.9	39.71	9.9	1365
9.9	3.36	78.2	2706	9.9	39.71	9.9	1435
10.0	3.29	87.1	4040	10.0	40.04	10.0	1460
19.1	3.78	93.4	5346	19.1	81.99	19.1	2721
25.0	3.67	101.1	7359	25.0	126.6	25.0	4437
25.1	3.90	110.7	10732	25.1	127.1	25.1	4215
25.2	3.84	121.8	16159	25.2	128.0	25.2	4291
30.0	4.03	136.7	27798	30.0	179.8	30.0	5847
34.8	4.01	149.8	40210	34.8	248.4	34.8	8103
35.1	4.0	167.4	66795	35.1	252.5	35.1	8406
35.1	4.16	184.1	103085	35.1	252.5	35.1	8073
40.0	4.09			40.0	347.5	40.0	11429
		eq. 2	P/mmHg				
		A	6.84310	Antoine eq.			
		B	1469.829	#see Li & Rossini 1961			
		C	187.157	eq. 2			
				P/mmHg			
				A			
				7.1231			
				B			
				1369.20			
				C			
				204.4			
pressure range 10–1500 torr mmHg							

\*DTA—differential thermal analyzer



**FIGURE 5.1.1.23.1** Logarithm of vapor pressure versus reciprocal temperature for 1-chlorooctane.

## 5.1.1.24 1-Chlorononane



Common Name: 1-Chlorononane

Synonym: nonyl chloride

Chemical Name: 1-chlorononane

CAS Registry No: 2473-01-0

Molecular Formula:  $C_9H_{19}Cl$

Molecular Weight: 162.700

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

-39.4 (Dreisbach 1961; Weast 1982–83; Lide 2003)

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

205.2 (Lide 2003)

Density ( $g/cm^3$ ):

0.7886 ( $20^{\circ}C$ , Weast 1982–83)

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

206.3 ( $20^{\circ}C$ , calculated-density)

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

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

58.27, 42.89 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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):

40.0 (extrapolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.1802 - 1736.11/(200.4 + t/^{\circ}C)$ ; temp range  $104\text{--}255^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.1802 - 1736.11/(200.4 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

680\* ( $69.1^{\circ}C$ , differential thermal analysis, measured range  $69.1\text{--}204.8^{\circ}C$ , Kemme & Kreps 1969)

$\log(P/mmHg) = 6.90463 - 1586.937/(t/^{\circ}C + 185.505)$ ; temp range  $69.1\text{--}204.8^{\circ}C$  (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

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

$\log(P/kPa) = 6.17172 - 1655.007/(t/^{\circ}C + 205.166)$ ; temp range  $69.1\text{--}204.8^{\circ}C$  (Antoine eq., based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P_L/kPa) = 6.09107 - 1332.89/(T/K - 54.65)$ ; temp range 289–409 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.04654 - 1665.57/(t/^{\circ}C + 192.26)$ ; temp range  $69\text{--}205^{\circ}C$  (Antoine eq., Dean 1992)

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

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

4.88 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

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 5.1.1.24.1

Reported vapor pressures of 1-chlorononane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
69.1	679.9	156.7	26731
70.8	733.3	170.3	40317
80.6	1280	188.6	66901
89.9	2013	204.8	100365
95.4	2613		
104.5	3933	$\log P = A - B/(C + t/^{\circ}\text{C})$	
111.5	5280		P/mmHg
119.8	7333	A	6.94063
129.5	10626	B	1586.937
141.3	16159	C	185.505

\*DTA—differential thermal analyzer

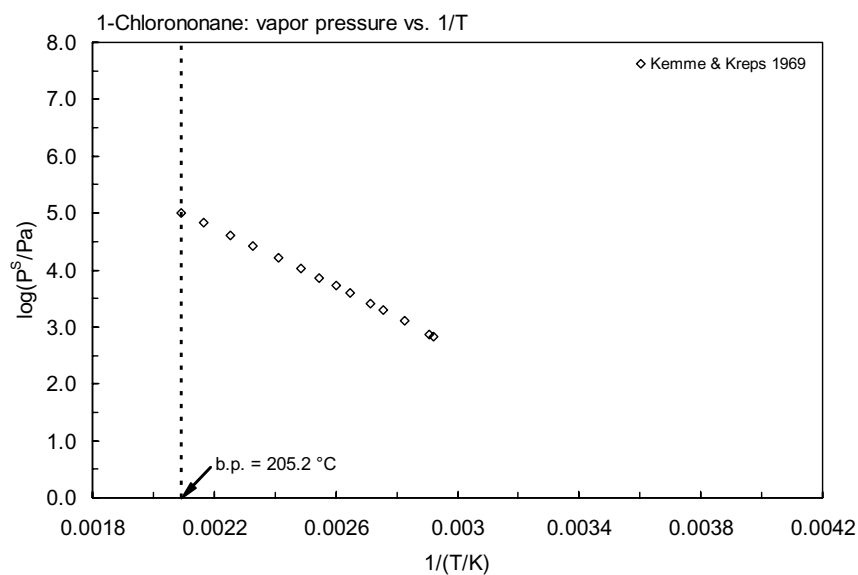
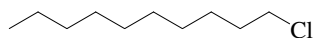


FIGURE 5.1.1.24.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorononane.



## 5.1.1.25 1-Chlorodecane



Common Name: 1-Chlorodecane

Synonym: decyl chloride

Chemical Name: 1-chlorodecane

CAS Registry No: 1002-69-3

Molecular Formula:  $C_{10}H_{21}Cl$

Molecular Weight: 176.727

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

-31.3 (Dreisbach 1961; Stephenson & Malanowski 1987; Lide 2003)

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

225.9 (Lide 2003)

Density ( $g/cm^3$ ):

0.8705, 0.8666 (20 $^{\circ}C$ , 25 $^{\circ}C$ , Dreisbach 1961)

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

203.0 (20 $^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

63.35, 45.2 (25 $^{\circ}C$ , bp, Dreisbach 1961)

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):

13.3 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.2372 - 1829.68/(196.6 + t/^{\circ}C)$ ; temp range 121–278 $^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.2372 - 1829.68/(196.6 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

733\* (86.2 $^{\circ}C$ , differential thermal analysis, measured range 86.2–225.6 $^{\circ}C$ , Kemme & Kreps 1969)

$\log(P/mmHg) = 6.99172 - 1676.793/(t/^{\circ}C + 182.017)$ ; temp range 86.2–225.6 $^{\circ}C$  (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

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

$\log(P/kPa) = 6.07379 - 1645.521/(t/^{\circ}C + 178.639)$ ; temp range 86.2–225.6 $^{\circ}C$  (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P_L/kPa) = 6.11662 - 1676.793/(T/K - 91.133)$ ; temp range 359–499 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 6.93986 - 1639.06/(t/^{\circ}C + 177.04)$ ; temp range 86–225.9 $^{\circ}C$  (Antoine eq., Dean 1992)

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25 $^{\circ}C$ ):

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

5.29 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

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 5.1.1.25.1

Reported vapor pressures of 1-chlorodecane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
86.2	733.3	189.5	40183
98.9	1400	208.6	66861
106.2	2000	225.6	100618
112.8	2693		
122.7	4106	$\log P = A - B/(C + t/^{\circ}\text{C})$	
129.2	5346		P/mmHg
137.1	7293	A	6.99172
147.7	10666	B	1676.793
159.3	16065	C	182.017
175.7	26878		

\*DTA—differential thermal analyzer

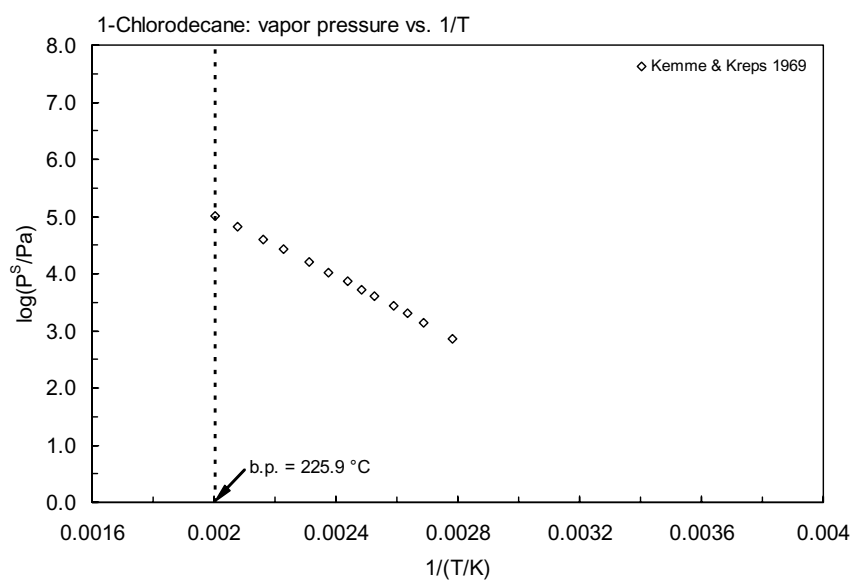


FIGURE 5.1.1.25.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorodecane.

## 5.1.1.26 Chloroethene (Vinyl chloride)



Common Name: Vinyl Chloride

Synonym: chloroethene, chloroethylene, monochloroethylene, monovinylchloride, MVC

Chemical Name: chloroethylene, vinyl chloride, chloroethene

CAS Registry No: 75-01-4

Molecular Formula:  $C_2H_3Cl$ ,  $H_2C = CHCl$

Molecular Weight: 62.498

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

−153.84 (Lide 2003)

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

−13.8 (Lide 2003)

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

0.9106 (Riddick et al. 1986)

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

68.5 ( $20^{\circ}C$ , Stephenson & Malanowski 1987)

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

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

18.636, 20.799 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

4.745 (Dreisbach 1959; 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):

8720, 9000 (15,  $30^{\circ}C$ , shake flask-interferometry, Gross & Saylor 1931)

2700\* (continuous solvent flow system at 1 atmospheric pressure, measured range  $0.2$ – $75^{\circ}C$ , Hayduk & Laudie 1974)

60 ( $10^{\circ}C$ , Pearson & Connell 1975)

60, 2700 (10,  $25^{\circ}C$ , selected, Dilling 1977)

1100 (Verschuereen 1977, 1983)

6800 ( $20^{\circ}C$ , selected, Nathan 1978)

8700\* (restatement of Hayduk & Laudie 1974, temp range  $0.2$ – $75^{\circ}C$  at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)

8800\* ( $26^{\circ}C$ , solubility bomb-headspace GC, measured range  $15$ – $85^{\circ}C$  at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)

2763\* (recommended, temp range  $0$ – $175^{\circ}C$ , Horvath 1982)

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):

538000\* (Antoine eq. regression, temp range  $-105.6$  to  $-13.8^{\circ}C$ , Stull 1947)

354600 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.49712 - 783.4/(230.0 + t/^{\circ}C)$ , temp range  $-100$  to  $50^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

104698\* ( $-13.00^{\circ}C$ , ebulliometry, measured range  $-64.9$  to  $-13.00^{\circ}C$ , McDonald et al. 1959)

381600 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 6.88054 - 912.5/(242.0 + t/^{\circ}C)$ ; temp range  $-73$  to  $46^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 6.86108 - 892.757/(238.099 + t/^{\circ}C)$ ; temp range  $-64.9$  to  $13.0^{\circ}C$  (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)

- 172719\* (0°C, temp range -59.4 to 0°C, Huccura & Mathieu 1967)  
 546800 (calculated-Antoine eq., Weast 1972-73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 6263.0/(T/K)] + 8.202782$ ; temp range -105.1 to -13.8°C (Antoine eq., Weast 1972-73)  
 392800 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log (P/\text{mmHg}) = 6.89117 - 905.008/(239.475 + t/^{\circ}\text{C})$ ; temp range -64.9 to -13.0°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 309300 (Pearson & McConnell 1975)  
 $\log (P/\text{mmHg}) = 6.89117 - 905.01/(239.48 + t/^{\circ}\text{C})$ ; temp range -657 to -13°C (Antoine eq., Dean 1985, 1992)  
 $\log (P/\text{kPa}) = 5.98598 - 892.757/(238.099 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 387000 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 5.98598 - 892.757/(-35.051 + T/K)$ ; temp range 208-260 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 5.20198 - 556.26/(-85.385 + T/K)$ ; temp range 259-328 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P/\text{mmHg}) = 52.9654 - 2.5016 \times 10^3/(T/K) - 17.914 \cdot \log (T/K) + 1.0821 \times 10^{-2} \cdot (T/K) - 4.531 \times 10^{-14} \cdot (T/K)^2$ ; temp range 119-432 K (vapor pressure eq., Yaws 1994)

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):

- 5680 (exptl.- $1/K_{AW} = C_W/C_A$ , Hine & Mookerjee 1975)  
 4723 (calculated-bond contribution method, Hine & Mookerjee 1975)  
 117705 (10°C, Pearson & McConnell 1975)  
 39660 (calculated-P/C, Neely 1976)  
 106590 (calculated-P/C, Dilling 1977)  
 2350 (calculated-P/C, Mackay & Shiu 1981)  
 2817\* (24.8°C, EPICS-GC/FID, measured range 10.3-34.6°C, Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 7.385 - 3286/(T/K)$ ; temp range 10.3-34.6°C (EPICS measurements, Gossett 1987)  
 2685\* (EPICS-GC/FID, measured range 10-30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 6.138 - 2931/(T/K)$ ; temp range 10-30°C (EPICS measurements, Ashworth et al. 1988)  
 2271 (computed value, Yaws et al. 1991)  
 2172 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 4.119 - 1223/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

- 1.39 (calculated- $\pi$  substituent const., Hansch et al. 1968)  
 0.60 (Callahan et al. 1979; Mills et al. 1982)  
 1.23 (calculated-fragment const., Mabey et al. 1982)  
 2.79 (Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

- 0.845 (estimated-S, Lyman et al. 1982)  
 0.756 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 3.04, 1.60, < 1.0 (activated sludge, *Chlorella fusca*, golden ide, Freitag et al. 1984)  
 0.068 (from USEPA 86, Yeh & Kastenbergs 1991)

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

- 0.9138 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)  
 1.748 (estimated-S, Lyman et al. 1982)  
 0.477 (soil, selected, Jury et al. 1990)  
 1.756 (quoted from USEPA 1986, Yeh & Kastenbergs 1991)

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

Volatilization:  $t_{1/2} = 25$  min from water, by rapidly stirring aqueous solutions in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

$t_{1/2}(\text{exptl}) = 27.6$  min,  $t_{1/2}(\text{calc}) = 0.0054$  min, 16.1 min from water at 10°C (Dilling 1977)

$t_{1/2} \sim 0.805$  h for volatilization from a river of 1-m deep with a current of 3 m/s and wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

estimated  $t_{1/2} \sim 2.5$  h from water (Thomas 1982);

volatilization  $t_{1/2} = 0.2$  to 0.5 d from soil at 1 and 10 cm incorporation (Jury et al. 1984);

$t_{1/2} = 30$  d, estimated volatilization from soil (Jury et al. 1990).

Photolysis: degrade rapidly in air by reaction with photochemically produced hydroxyl radicals with an estimated  $t_{1/2} = 1.5$  d (Perry et al. 1977; quoted, Howard 1989).

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:

$k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 26°C (Perry et al. 1977)

photooxidation  $t_{1/2}$  was reported to be a few hours in the troposphere (Callahan et al. 1979)

$k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson et al. 1979, 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{\text{O}_3} = 6.5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K (Sanhueza et al. 1976; quoted, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Gay et al. 1976; quoted, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson et al. 1979, 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 1.8 d, loss of 42.6% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}}(\text{calc}) = 3.9 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , and  $k_{\text{O}_3} = 1.2 \times 10^6 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at 300 K (Lyman 1982)

$k < 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $3.0 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)

$k_{\text{O}_3} = (2.45 \pm 0.45) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Zhang et al. 1983; quoted, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Tuazon et al. 1984)

$k_{\text{NO}_3} = (1.4 \pm 0.9) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 1$  K (Andersson & Ljungström 1989)

photooxidation  $t_{1/2} = 9.7\text{--}97$  h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{\text{NO}_3} = (2.3 \pm 1.1) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  relative to ethene at  $298 \pm 2$  K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{\text{NO}_3} = 2.30 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculate atmospheric lifetime  $\tau = 42$  d, and  $k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $\tau(\text{calc}) = 3.5$  d and  $k_{\text{O}_3} = 2.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $\tau(\text{calc}) = 66$  d at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = (3.30 \pm 1.66) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 1$  K (quoted from Anderson & Ljungström 1989, Atkinson 1991)

$k_{\text{NO}_3} = 4.45 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Sabljic & Güsten 1990)

$k_{\text{NO}_3} = 4.3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 5.25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (as per Atkinson 1987 and 1988, Müller & Klein 1991)

Hydrolysis:  $t_{1/2} < 10$  yr (Callahan et al. 1979);

estimated acid-catalyzed rate constant of  $3.30 \times 10^{-12} \text{ mol}^{-1} \text{ s}^{-1}$  at pH 5 with calculated  $t_{1/2} = 2 \times 10^{11}$  d (Wolfe 1980; quoted, Ma et al. 1990)

abiotic hydrolysis or dehydrohalogenation  $t_{1/2} < 120$  months (Olsen & Davis 1990).

Biodegradation: abiotic degradation rate constant of  $k = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 26°C determined in laboratory experiments for the vapor phase reaction with hydroxyl radicals (Perry et al. 1977; quoted, Howard 1989)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320$  h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991)

greater than 99% degraded after 108 d under aerobic conditions and approximately 65% being mineralized to  $^{14}\text{CO}_2$  under aerobic conditions (Davis & Carpenter 1990);

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

$t_{1/2} > 60$  d (Olsen & Davis 1990)

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

Biotransformation:

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

#### Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 11$  wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} = 0.24\text{--}2.4$  h from air for the reaction with OH radical (Darnall et al. 1976);

photodecomposition  $t_{1/2} = 4.3$  h with NO under simulated atmospheric conditions (Dilling et al. 1976);  
estimated  $t_{1/2} = 1.5$  d, based on its photochemical reaction with OH radical in air (Perry et al. 1977; quoted, Howard 1989);

residence time of 1.8 d, loss of 42.6% in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

$t_{1/2} = 9.7\text{--}97$  h, based on measured rate for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetimes  $\tau = 42$  d for the reaction with  $\text{NO}_3$  radical for a 12-h nighttime, average concn. of  $2.4 \times 10^9$  molecule/ $\text{cm}^3$ ,  $\tau = 3.5$  d for the reaction with OH radical for a 12-h average concn. of  $1.0 \times 10^6$  molecule/ $\text{cm}^3$ , and  $\tau = 66$  d for the reaction with  $\text{O}_3$  for a 24-h, average concn. of  $7 \times 10^{11}$  molecule/ $\text{cm}^3$  (Atkinson et al. 1987).

Surface water: estimated  $t_{1/2} = 0.805$  h for volatilization from a river of 1 m deep with a current of 3 m/s and a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} = 672\text{--}4320$  h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 1344\text{--}69000$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life and an estimated half-life for anaerobic biodegradation from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

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

$t_{1/2} = 0.2$  to  $0.5$  d for volatilization from soil at 1 and 10 cm incorporation (Jury et al. 1984; quoted, Howard 1989);

$t_{1/2} = 30$  d, estimated volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 30\text{--}180$  d (Howard et al. 1991; quoted, Jury et al. 1992);

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

Biota:  $t_{1/2} < 10$  d, subject to plant uptake via volatilization (Ryan et al. 1988; quoted, Jury et al. 1992).

TABLE 5.1.1.26.1  
Reported aqueous solubilities of chloroethene (vinyl chloride) at various temperatures

Hayduk & Laudie 1974		DeLassus & Schmidt 1981		DeLassus & Schmidt 1981		Horvath 1982	
compressibility apparatus		“restatement” data#		solubility bomb-GC/FID		summary of literature data	
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>
at 1.0 atm							
0.2	7537	0.2	9000	15	9500	0	5460.
25	2700	25	8700	16	9950	25	2764
50	1278	50	10100	20.5	9150	50	1421
75	507	75	12800	26	8800	75	780
at 1.36 atm				29.5	8900	100	538
0.2	8438	# “restatement” data		35	9400	150	337
at 3.06 atm		from Hayduk & Laudie 1974		41	8900	175	320
25	7153			46.5	8800		
50	3993			55	9500		
75	2125			65	9200		
at 6.12 atm				72.5	9800		
50	7674			80	10000		
75	4965			85	11200		
ΔH <sub>sol</sub> /(kJ mol <sup>-1</sup> )							
25°C							

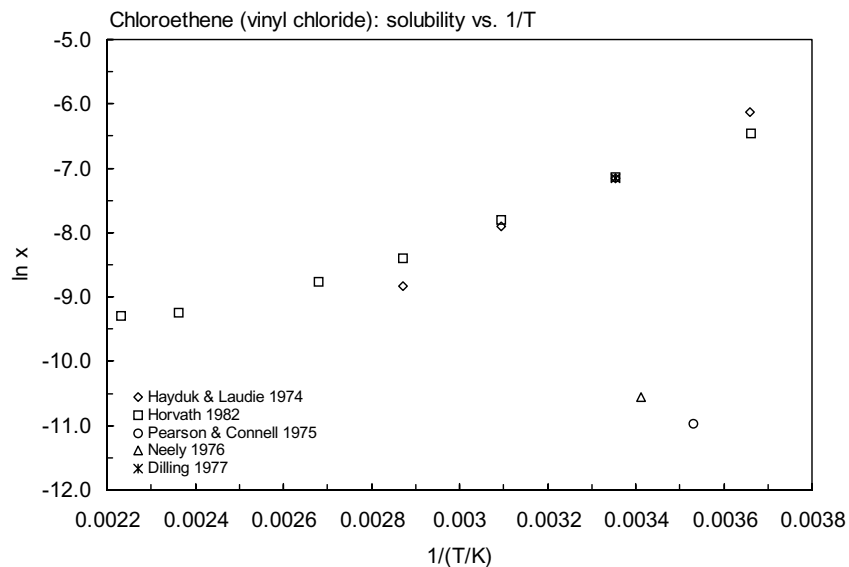


FIGURE 5.1.1.26.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chloroethene.

TABLE 5.1.1.26.2

Reported vapor pressures of chloroethene (vinyl chloride) 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)		
$\log P = A - B/(T/K) - C \cdot (T/K) + D \cdot (T/K)^2$	(5)		

Stull 1947		Huccura & Mathieu 1967		McDonald et al. 1959	
summary of literature data				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-103.6	133.3	-59.4	9870	-64.9	6769
-90.8	666.6	-54.3	13566	-56.4	12147
-83.7	1333	-49.4	18032	-43.37	25114
-75.7	2666	-44.5	23713	-29.09	51852
-66.8	5333	-39.5	31881	-14.83	97132
-61.1	7999	-34.5	39695	-13.64	102045
-53.2	13332	-29.65	50510	-13.00	104698
-41.3	26664	-24.9	63349		
-28.0	53329	-20.1	78440		
-13.8	101325	0.0	172719		
mp/°C	-153.7				

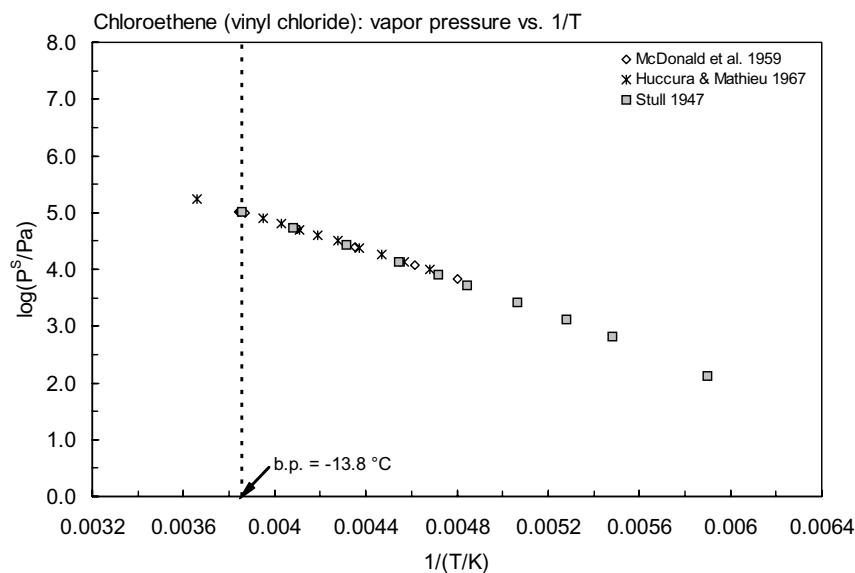


FIGURE 5.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for chloroethene.



TABLE 5.1.1.26.3

Reported Henry's law constants of chloroethene (vinyl chloride) at various temperatures and temperature dependence equations

$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) & (4a) \\ K_{AW} &= A - B\cdot(T/K) + C\cdot(T/K)^2 & (5) & & \end{aligned}$$

Hayduk & Laudie 1974		Gossett 1987		Ashworth et al. 1988	
compressibility measurement		EPICS-GC		EPICS-GC	
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)
at 1 atm					
0.2	834	10.3	1489	10	1520
25	2342	17.5	1956	15	1702
50	4348	24.8	2819	20	2199
75	7751	34.6	3627	25	2685
at 1.36 atm					
0.2	1018	eq. 4a	H/(atm m <sup>3</sup> /mol)	30	3850
at 3.06 atm					
		A	7.385	eq. 4a	H/(atm m <sup>3</sup> /mol)
25	2685	B	3286	A	6.138
50	4669			B	2931
75	7988				

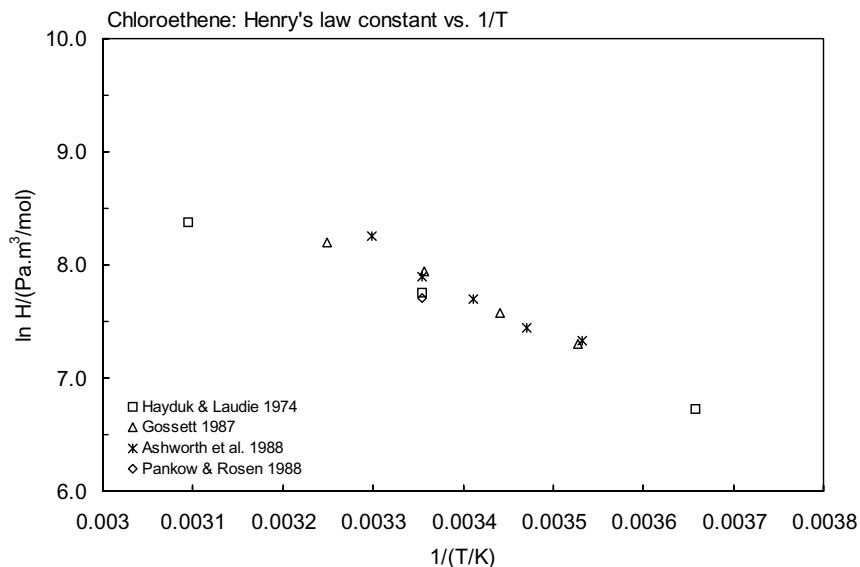


FIGURE 5.1.1.26.3 Logarithm of Henry's law constant versus reciprocal temperature for chloroethene.

## 5.1.1.27 1,1-Dichloroethene



Common Name: 1,1-Dichloroethene

Synonym: 1,1-dichloroethylene, vinylidene chloride, vinylidine chloride, 1,1-DCE

Chemical Name: 1,1-dichloroethene, 1,1-dichloroethylene

CAS Registry No: 75-35-4

Molecular Formula:  $C_2H_2Cl_2$ ,  $CH_2 = CCl_2$

Molecular Weight: 96.943

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

-122.56 (Lide 2003)

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

31.6 (Lide 2003)

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

1.2180 (Horvath 1982; Weast 1982-83; Verschuereen 1983)

1.2132 (Riddick et al. 1986)

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

79.9 ( $20^{\circ}C$ , calculated-density)

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

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

26.49, 28.18 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

6.514 (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):

400 ( $20^{\circ}C$ , shake flask-GC, McConnell et al. 1975; Pearson & McConnell 1975)

400 ( $20^{\circ}C$ , literature average, Dilling 1977)

2250\* (solubility bomb-headspace GC, measured range  $15-90.5^{\circ}C$ , DeLassus & Schmidt 1981)

210\* (summary of literature data, Horvath 1982)

2640, 3675 ( $20^{\circ}C$ ,  $30^{\circ}C$ , saturation concn., Verschuereen 1983)

2232 ( $30^{\circ}C$ , headspace-GC, McNally & Grob 1984)

210 (Dean 1985; Riddick et al. 1986)

2843, 2790, 2782 ( $20$ ,  $30$ ,  $40^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

2420\* (recommended, temp range  $0-90^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 6.27413 - 3.8257 \times 10^{-2} \cdot (T/K) + 6.04607 \times 10^{-5} \cdot (T/K)^2$ , temp range  $288-363 K$  (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

86430\* (Antoine eq. regression, temp range  $-77.2$  to  $31.7^{\circ}C$ , Stull 1947)

97241\* ( $30.39^{\circ}C$ , ebulliometry, measured range  $-28.36$  to  $32.50^{\circ}C$ , Hildebrand et al. 1959)

84500 (calculated-Antoine eq., Weast 1972-73)

$\log (P/mmHg) = [-0.2185 \times 7211.8/(T/K)] + 8.087140$ ; temp range  $-77.2$  to  $31.7^{\circ}C$  (Antoine eq., Weast 1972-73)

80040 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 6.97215 - 1099.446/(237.184 + t/^{\circ}C)$ ; temp range  $-28$  to  $32.5^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

79710 (literature average, Dilling 1977)

78780 (Verschuereen 1977, 1983)

- 80040 (interpolated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.09904 - 1100.431/(237.274 + t/^{\circ}\text{C})$ ; temp range  $-28$  to  $32.5^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log(P/\text{mmHg}) = 6.9722 - 1099.4/(237.2 + t/^{\circ}\text{C})$ ; temp range  $-28$  to  $32^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)  
 79860 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 6.10690 - 1104.29/(237.697 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 80060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.10046 - 1100.67/(-35.9 + T/\text{K})$ ; temp range  $244$ – $306$  K (Antoine eq., Stephenson & Malanowski 1987)  
 66190, 95740, 134520 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , quoted from DIPPR, Tse et al. 1992)  
 $\log(P/\text{mmHg}) = -16.5419 - 1.6655 \times 10^3/(T/\text{K}) + 13.923 \cdot \log(T/\text{K}) - 4.0958 \times 10^{-2} \cdot (T/\text{K}) + 2.9995 \times 10^{-5} \cdot (T/\text{K})^2$ ; temp range  $151$ – $482$  K (vapor pressure eq., Yaws 1994)

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

- 3729 ( $20^{\circ}\text{C}$ , batch stripping, Mackay et al. 1979)  
 3127\* ( $24.3^{\circ}\text{C}$ , equilibrium cell-concn ratio, measured range  $2.5$ – $26.1^{\circ}\text{C}$ , Leighton & Calo 1981)  
 $\ln(k_H/\text{atm}) = 23.12 - 4618/(T/\text{K})$ ; temp range  $2.5$ – $26.1^{\circ}\text{C}$  (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 2649 ( $20^{\circ}\text{C}$ , EPICS-GC, Linoff & Gossett 1983; Gossett 1985)  
 2645 ( $24.8^{\circ}\text{C}$ , EPICS-GC, measured range  $10$ – $34.6^{\circ}\text{C}$ , Gossett 1987)  
 $\ln[H/(\text{atm m}^3/\text{mol})] = 8.845 - 3729/(T/\text{K})$ ; temp range  $10.0$ – $34.6^{\circ}\text{C}$  (EPICS measurements, Gossett 1987)  
 1520 (gas stripping-GC, Warner et al. 1987)  
 7529 ( $20^{\circ}\text{C}$ , EPICS-GC, Yurteri et al. 1987)  
 2624\* (EPICS-GC/FID, measured range  $10$ – $30^{\circ}\text{C}$ , Ashworth et al. 1988)  
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 6.123 - 2907/(T/\text{K})$ ; temp range  $10$ – $30^{\circ}\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 19249 ( $20$ – $25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 2316 (computed value, Yaws et al. 1991)  
 2320, 3415, 4813 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)  
 2376 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 5.397 - 1586/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

- 2.13 (shake flask, Log P Database, Hansch & Leo 1987)  
 2.13 (recommended, Sangster 1993)  
 2.13 (recommended, Hansch et al. 1995)

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

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

- 1.72 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)

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

- 2.176 (calculated- $K_{OW}$ , Kenaga & Goring 1980)  
 1.813 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)

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

- Volatilization:  $t_{1/2}(\text{exptl}) \sim 22$  min at  $25^{\circ}\text{C}$  for volatilization of  $1$  mg/L in water in an open container of  $65$ -mm in depth stirring at  $200$  rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)  
 Evaporation  $t_{1/2}(\text{exptl}) = 27.2$  min,  $t_{1/2}(\text{calc}) = 0.029$  min,  $20.1$  min from water (Dilling 1977)  
 $t_{1/2}(\text{calc}) = 5.9, 1.2$ , and  $4.7$  d from a pond, river, and lake, respectively, using data for the oxygen reaeration rate of typical bodies of water (Mill et al. 1982; quoted, Howard 1989).

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:

$k_{O_3} = (3.7 \pm 1.0) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Hull et al. 1973; quoted, Atkinson & Carter 1984)  
 Photooxidation  $t_{1/2} \sim 50$  min reaction with  $\text{NO}_2$  under UV irradiation (Gay, Jr. et al. 1976)  
 $k < 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $3.0 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at  $25^\circ\text{C}$  (Mabey et al. 1982)  
 $k_{OH} \sim 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 2.9 d, loss of 29.2% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)  
 $k \sim 10^3 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 1.5 mM *t*-BuOH as scavenger at pH 2 and  $20\text{--}23^\circ\text{C}$  (Hoigné & Bader 1983)  
 $k_{O_3} = 3.7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Tuazon et al. 1984)  
 $k_{OH} = (14.9 \pm 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with reference to *n*-butane at  $22.3 \pm 1.2^\circ\text{C}$  with a lifetime of 0.75 d and  $k_{OH} = 15.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with reference to *n*-pentane at  $24.4 \pm 0.4^\circ\text{C}$  (relative rate method, Edney et al 1986)  
 photooxidation  $t_{1/2} = 11$  h in relatively clean air or under 2 h in polluted air (Howard 1989)  
 photooxidation  $t_{1/2} = 9.9\text{--}98.7$  h, based on measured rate data for the vapor phase reaction with OH radical in air (Goodman et al. 1986; quoted, Howard et al. 1991)  
 $k_{NO_3} = (6.60 \pm 3.10) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  relative to ethene at  $298 \pm 2$  K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)  
 $k_{NO_3} = 6.6 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated atmospheric lifetime of 15 d,  $k_{OH} = 8.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a lifetime of 3.4 d and  $k_{O_3} = 3.7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a lifetime of 12 yr at room temp. (Atkinson et al. 1987; quoted, Sabljic & Güsten 1990)  
 $k_{OH}(\text{calc}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs.}) = 8.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)  
 $k_{NO_3} = 1.28 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)  
 $k_{NO_3} = 1.23 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2$  K (Atkinson 1991)  
 $k_{OH}(\text{calc}) = 2.04 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (as per Atkinson 1987 and 1988, Müller & Klein 1991)  
 $k_{OH}(\text{calc}) = 2.67 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{exptl}) = 10.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis: estimated acid-catalyzed rate constant  $k = 1.4 \times 10^{-13} \text{ mol}^{-1} \text{ s}^{-1}$  at pH 5 with  $t_{1/2}(\text{calc}) = 6 \times 10^{12}$  d at pH 5 (Wolfe 1980);

estimated  $t_{1/2} \sim 2.0$  yr at pH 7.0 (Schmidt-Bleek et al. 1982; quoted, Howard 1989);

$t_{1/2} = 6\text{--}9$  months has been observed with no significant difference in hydrolysis rate between pH 4.5 and 8.5 (Cline & Delfino 1987; quoted, Howard 1989);

abiotic hydrolysis or dehydrohalogenation half-life of 12 months (Olsen & Davis 1990).

Biodegradation: aerobic  $t_{1/2}(\text{aq.}) = 672\text{--}4320$  h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic  $t_{1/2}(\text{aq.}) = 1944\text{--}4152$  h, based on anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard 1989; Olsen & Davis 1990; Howard et al. 1991).

Biotransformation:

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

#### Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 8.0$  wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} = 0.24\text{--}2.4$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition  $t_{1/2} = 2.1$  h with NO under simulated atmospheric conditions (Dilling et al. 1976);

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photooxidation  $t_{1/2} = 11$  h in relatively clean air (Edney et al. 1983; quoted, Howard 1989) or under 2 h in polluted air (Gay et al. 1976; quoted, Howard 1989);

lifetime of 0.75 d, based on measured rate data for the vapor phase reaction with OH radical in air at  $(22.3 \pm 1.2)^\circ\text{C}$  (Edney et al. 1986);

$t_{1/2} = 9.9\text{--}98.7$  h, based on measured rate data for the vapor phase reaction with OH radical in air (Goodman et al. 1986; quoted, Howard et al. 1991);

atmospheric lifetimes: 15 d for the reaction with  $\text{NO}_3$  radical for a 12-h nighttime average concn. of  $2.4 \times 10^9 \text{ molecule cm}^{-3}$ , 3.4 d for the reaction with OH radical for a 12-h average concentration

of  $1.0 \times 10^6$  molecule  $\text{cm}^{-3}$ , and 12 yr for the reaction with  $\text{O}_3$  for a 24-h average concentration of  $7 \times 10^{11}$  molecule  $\text{cm}^{-3}$  at room temp. (Atkinson et al. 1987).

Surface water:  $t_{1/2} = 672\text{--}4320$  h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 1344\text{--}3168$  h, based on estimated aqueous aerobic biodegradation half-life and anaerobic grab sample data for soil from ground water aquifer receiving landfill leachate (Wilson et al. 1986; quoted, Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 672\text{--}4320$  h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

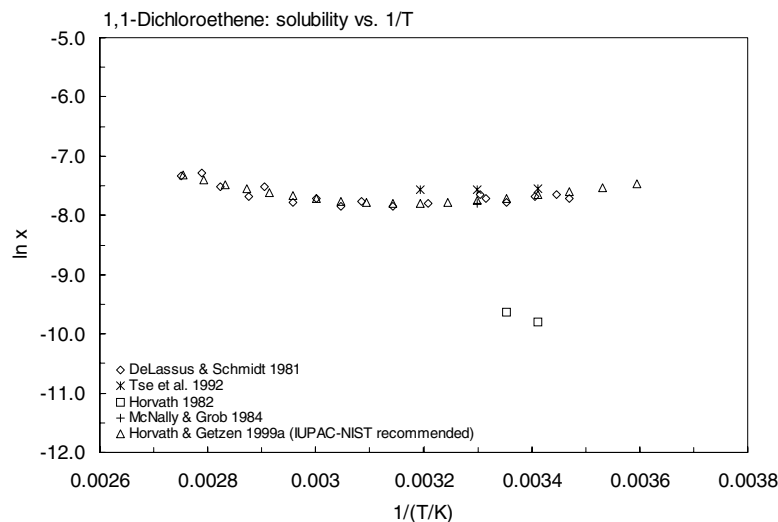
$t_{1/2} < 10$  d (Ryan et al. 1988).

Biota:  $t_{1/2} < 10$  d, subject to plant uptake via volatilization (Ryan et al. 1988).

**TABLE 5.1.1.27.1**

**Reported aqueous solubilities of 1,1-dichloroethene at various temperatures**

DeLassus & Schmidt 1981		Horvath 1982		Tse et al. 1992		Horvath & Getzen 1999a	
solubility bomb-GC/FID		summary of literature data		activity coefficient $\gamma^\infty$ -GC		recommended, IUPAC-NIST	
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>
15	2400	20	300	20	2843	5	3100
17	2550	25	350	30	2790	10	2890
20.5	2500			40	2782	15	2700
25	2250					20	2550
28.5	2400					25	2420
29.5	2550					30	2330
38.5	2200					35	2260
45	2100					40	2230
51	2300					45	2220
55	2100					50	2250
60	2400					55	2300
65	2250					60	2390
71	2950					65	2510
74.5	2500					70	2650
81	2950					75	2830
85.5	3700					80	3040
90.5	3500					85	3280
						90	3550
						eq. 1	S/wt%
						temp range 288–363 K	



**FIGURE 5.1.1.27.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,1-dichloroethene.

**TABLE 5.1.1.27.2**

**Reported vapor pressures of 1,1-dichloroethene 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)		
$\log P = A - B/(T/K) - C \cdot (T/K) + D \cdot (T/K)^2$	(5)		

Stull 1947		Hildenbrand et al. 1959	
summary of literature data		ebulliometry	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
-77.2	133.3	-28.36	6793
-60.0	666.6	-17.72	12204
-51.2	1333	-2.96	25279
-41.7	2666	13.75	51913
-31.1	5333	30.39	97241
-24.0	7999	31.56	101325
-15.0	13332	31.73	101986
-1.0	26664	32.50	104626
14.8	53329		
31.7	101325		
mp/ $^{\circ}\text{C}$	-122.5		

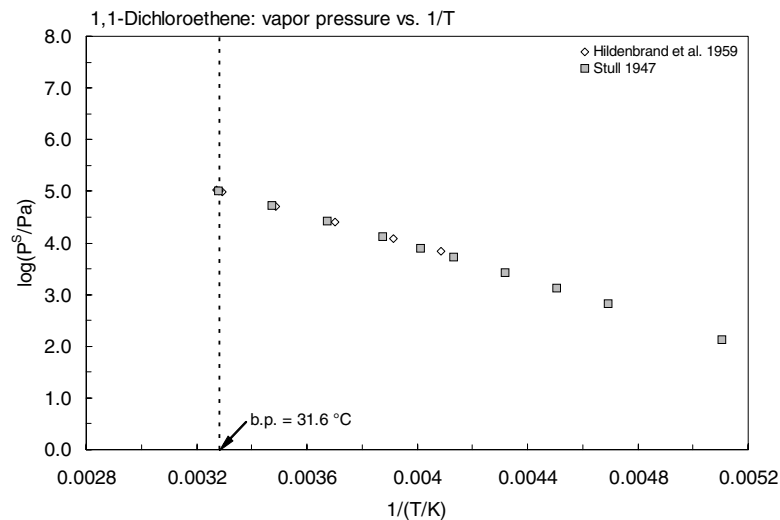


FIGURE 5.1.1.27.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethene.

TABLE 5.1.1.27.3  
Reported Henry’s law constants of 1,1-dichloroethene at various temperatures and temperature dependence equations

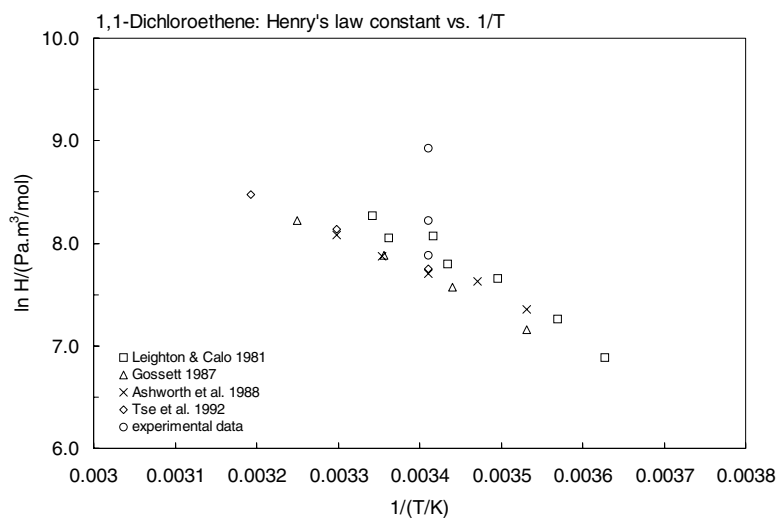
$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/\text{atm}) = A - B/(T/K)$$
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$
$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

$$(1)$$
$$(2)$$
$$(3)$$
$$(4)$$
$$(5)$$

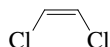
$$(1a)$$
$$(2a)$$
$$(4a)$$

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tse et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		activity coefficient $\gamma^\infty$ -GC	
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)
2.5	973	10.0	1287	10	1560	20	2320
7.0	1423	17.5	1935	15	2057	30	3415
12.9	2119	24.8	2645	20	2209	40	4813
18.0	2437	34.6	3708	25	2624		
19.5	3195			30	3222		
24.3	3127	eq. 4a	H/(atm m <sup>3</sup> /mol)				
26.1	3914	A	8.845	eq. 4a	H/(atm m <sup>3</sup> /mol)		
		B	3729	A	6.123		
eq. 3	H/atm			B	2907		
A	23.12						
B	4618						



**FIGURE 5.1.1.27.3** Logarithm of Henry's law constant versus reciprocal temperature for 1,1-dichloroethene.



5.1.1.28 *cis*-1,2-Dichloroethene

Common Name: *cis*-1,2-Dichloroethylene

Synonym: *cis*-acetylene dichloride, *cis*-1,2-dichloroethene, *cis*-1,2-dichloroethylene, (Z)-1,2-dichloroethene

Chemical Name: *cis*-1,2-dichloroethene, *cis*-1,2-dichloroethylene

CAS Registry No: 156-59-2

Molecular Formula: C<sub>2</sub>H<sub>2</sub>Cl<sub>2</sub>, CHCl=CHCl

Molecular Weight: 96.943

Melting Point (°C):

−80.0 (Lide 2003)

Boiling Point (°C):

60.1 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.2837 (Horvath 1982; Weast 1982–83; Riddick et al. 1986)

1.2818 (Dean 1985)

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

75.52 (20°C, calculated-density)

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

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

31.57, 30.23 (25°C, bp, Dreisbach 1961)

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

7.205 (Riddick et al. 1986)

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 or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

3520 (Seidell 1940)

3500 (selected from literature or measured in DuPont laboratories, McGovern 1943)

5560 (37°C, shake flask-GC, Sato & Nakijima 1979)

3500 (summary of literature data, Horvath 1982)

7700 (Dean 1985)

6575, 6707, 6674 (20, 30, 40°C, infinite dilution activity coeff. γ<sup>∞</sup>-GC, Tse et al. 1992)

6292, 6092, 6220 (20, 30, 40°C, activity coeff. γ<sup>∞</sup>-differential pressure transducer, Wright et al. 1992)

6608 (20°C, limiting activity coeff. γ<sup>∞</sup> by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

6410\* (tentative values, measured range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

S/(wt%) = 27.7353 − 0.178316·(T/K) + 2.93282 × 10<sup>−4</sup>·(T/K)<sup>2</sup>, temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

25571\* (23.74°C, temp range 0.76–83.63°C, Ketelaar et al. 1947)

27260\* (interpolated-Antoine eq. regression, temp range −58.4 to 59°C, Stull 1947)

28984\* (dynamic-ebulliometry, measured range 19.2–62°C, Flom et al. 1951)

23540 (calculated-Antoine eq., Weast 1972–73)

log (P/mmHg) = [−0.2185 × 7420.6/(T/K)] + 7.685137; temp range −58.4 to 260°C (Antoine eq., Weast 1972–73)

27010 (calculated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 7.0233 − 1105.436/(230.62 + t/°C); temp range 0.76–83°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

27010, 26740 (interpolated-Antoine equations; Boublik et al. 1984)

log (P/kPa) = 6.14603 − 1204.804/(230.55 + t/°C); temp range 0.76–83.63°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.03144 - 1153.738/(222.905 + t/^{\circ}\text{C})$ ; temp range 19.2–62°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{mmHg}) = 7.0223 - 1205.4/(230.6 + t/^{\circ}\text{C})$ ; temp range 0–84°C (Antoine eq., Dean 1985, 1992)  
 26700 (selected, Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 6.9771 - 1651.52/(T/\text{K})$ , temp range not specified (Antoine eq., Riddick et al. 1986)  
 26980 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.30025 - 1293.95/(-32.41 + T/\text{K})$ ; temp range 273–334 K, (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.22178 - 1271.55/(-30.557 + T/\text{K})$ ; temp range 332–495 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 21710, 33305, 49350 (20, 30, 40°C, estimated, Tse et al. 1992)  
 $\log (P/\text{mmHg}) = 55.9403 - 3.1677 \times 10^3/(T/\text{K}) - 18.572 \cdot \log (T/\text{K}) + 9.8828 \times 10^{-3} \cdot (T/\text{K}) + 5.7644 \times 10^{-14} \cdot (T/\text{K})^2$ ;  
 temp range 193–527 K (vapor pressure eq., Yaws 1994)

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):

342.2 (exptl.- $1/K_{\text{AW}} = C_{\text{W}}/C_{\text{A}}$ , Hine & Mookerjee 1975;)  
 1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)  
 444 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)  
 413.4\* (EPICS-GC, measured range 10.3–34.6°C, Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 8.479 - 4192/(T/\text{K})$ ; temp range 10.3–34.6°C (EPICS measurements, Gossett 1987)  
 441.1 (20°C, EPICS, Yurteri et al. 1987)  
 460\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.164 - 3143/(T/\text{K})$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 745.5 (computed value, Yaws et al. 1991)  
 324, 496, 740 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)  
 331, 518, 751 (20, 30, 40°C, activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)  
 319 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 674.5 (modified EPICS method-GC, Ryu & Park 1999)  
 341 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 4.464 - 1559/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

1.86 (shake flask, Hansch & Leo 1985, 1987)  
 1.86 (recommended, Sangster 1993)  
 1.85 (infinite dilution activity coefficient-GC, Tse & Sandler 1994)

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

2.56 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

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

1.176 (calculated- $K_{\text{OW}}$ , Lyman et al. 1982; quoted, Howard 1990)

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

1.69 (calculated- $K_{\text{OW}}$ , Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: evaporation  $t_{1/2} = 18$  min from dilute aqueous solution (Dilling 1975);  
 Evaporation  $t_{1/2}(\text{exptl}) = 19.4$  min,  $t_{1/2}(\text{calc}) = 0.75$  min, 20.7 min from water (Dilling 1977);  
 $t_{1/2} = 19.4$  min from a slowly stirred beaker 6.5 cm deep equivalent to  $t_{1/2} = 5.0$  h in a body of water 1 m deep (Dilling 1977; quoted, Verschueren 1983; Howard 1990)  
 $t_{1/2} = 3.1$  h was estimated from Henry's law constant for a model river 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

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 see reference:

$k_{\text{O}_3} = 6.2 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{\text{OH}} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} < 5.0 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{O}_3} = 3.7 \times 10^{-14} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , was estimated at 300 K (Lyman 1982)

$k < 800 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{O}_3} = 6.2 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Tuazon et al. 1984)

photooxidation  $t_{1/2} = 286 \text{ h}$ , based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{\text{NO}_3} = (7.5 \pm 3.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , relative to ethene at  $298 \pm 2 \text{ K}$  (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{\text{NO}_3} = 7.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated atmospheric lifetime of 130 d,  $k_{\text{OH}} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a lifetime of 12 d, and  $k_{\text{O}_3} < 5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a lifetime of > 9 yr at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 2.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 2.38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 1.46 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2 \text{ K}$  (relative rate method, Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{\text{OH}} = (2.38 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2 \text{ K}$  (relative rate method, Tuazon et al. 1988)

$k_{\text{NO}_3} = (1.39 \pm 0.13) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2 \text{ K}$  (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 2.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (as per Atkinson 1987 and 1988, Müller & Klein 1991)

$k_{\text{O}_3}(\text{aq.}) = (310 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2, with  $t_{1/2} = 1.8 \text{ min}$  at pH 7 and 25°C (Yao & Haag 1991).

#### Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 672\text{--}4320 \text{ h}$ , based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic  $t_{1/2} = 2688\text{--}17280 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} > 60 \text{ d}$  (Wood et al. 1985; quoted, Olsen & Davis 1990);

$k = 0.74 \text{ yr}^{-1}$  with  $t_{1/2} = 88\text{--}339 \text{ d}$  (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

#### Biotransformation:

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

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

Photooxidation  $t_{1/2} \sim 100 \text{ min}$  for reaction with  $\text{NO}_2$  under UV irradiation, isomer not specified (Gay, Jr., et al. 1976)

photodecomposition  $t_{1/2} = 3.0 \text{ h}$  with NO and 3.0 h with  $\text{NO}_2$  under simulated atmospheric conditions (Dilling et al. 1976);

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 129 \text{ d}$  resulting from the ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

$t_{1/2} = 8.0 \text{ d}$  in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

$t_{1/2} = 286 \text{ h}$ , based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes: 130 d for the reaction with  $\text{NO}_3$  radical for a 12-h nighttime average concn. of  $2.4 \times 10^9 \text{ molecule cm}^{-3}$ , 12 d for the reaction with OH radical for a 12-h average concn. of  $1.0 \times 10^6 \text{ molecule cm}^{-3}$ , and > 9.0 yr for the reaction with  $\text{O}_3$  for a 24-h average concn. of  $7 \times 10^{11} \text{ molecule cm}^{-3}$ , (Atkinson et al. 1987).

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

$k(\text{exptl}) = (310 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $25^\circ\text{C}$ , with  $t_{1/2} = 1.80$  min at pH 7 (Yao & Haag 1991).

Ground water:  $1344\text{--}69000$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation from a ground water field studies of chlorinated ethylenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

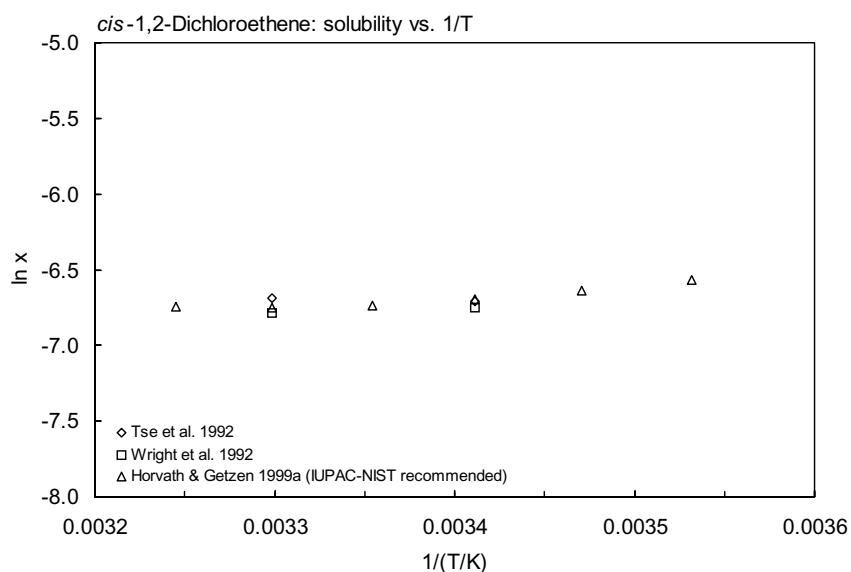
Soil:  $t_{1/2} = 672\text{--}4320$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

**TABLE 5.1.1.28.1**

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

Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999	
activity coefficient $\gamma^\infty$		activity coefficient $\gamma^\infty$		IUPAC-NIST recommended	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	6575	20	6292	10	7550
30	6707	30	6092	15	7050
40	6674	40	6220	20	6670
				25	6410
				30	6310
				35	6360
				40	6560



**FIGURE 5.1.1.28.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *cis*-1,2-dichloroethene.

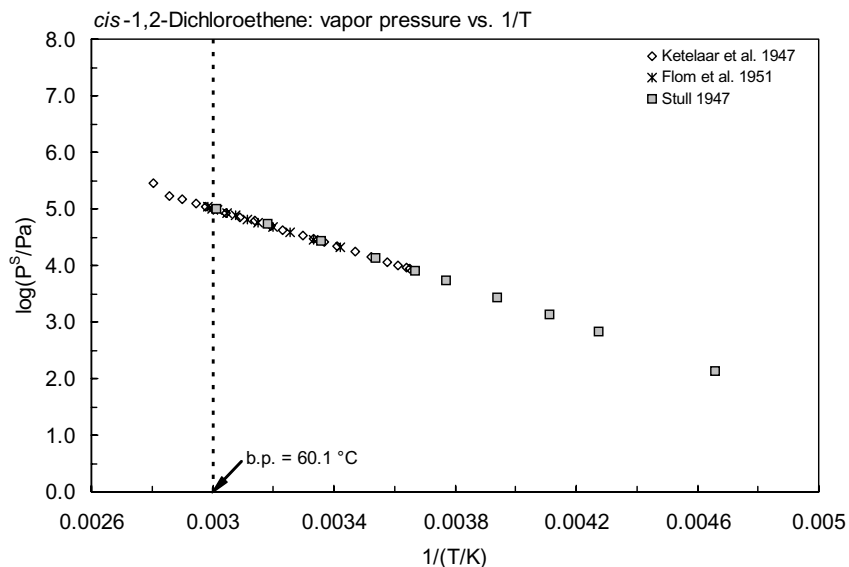
TABLE 5.1.1.28.2

Reported vapor pressures of *cis*-1,2-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947		Ketelaar et al. 1947*163		Flom et al. 1951	
summary of literature data				static method-manometer	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-58.4	133.3	0.76	8626	19.2	20732
-39.2	666.6	1.68	9066	26.9	28984
-29.9	1333	3.85	10186	34.1	38957
-19.4	2666	6.45	11572	39.3	48143
-7.90	5333	10.73	14172	44.4	58035
-0.50	7999	15.03	17425	47.8	66048
9.50	13332	20.19	21865	52.1	76833
24.6	26664	23.74	25571	55.0	85206
41.0	53329	26.73	29051	58.4	954-5
59.0	101325	30.11	33344	60.4	101578
		36.35	42823	62.0	107924
mp/ $^{\circ}\text{C}$	-80.5	40.02	49316		
		45.52	60728		
		50.34	71980		
		55.28	85193		
		59.97	98992		
		62.85	109631		
		66.56	123149		
		71.84	145094		
		76.76	168039		
		83.63	283929		

\*for a complete data set, see [references](#).



**FIGURE 5.1.1.28.2** Logarithm of vapor pressure versus reciprocal temperature for *cis*-1,2-dichloroethene.

**TABLE 5.1.1.28.3**

**Reported Henry's law constants of *cis*-1,2-dichloroethene at various temperatures and temperature dependence equations**

$$\ln K_{AW} = A - B/(T/K) \quad (1)$$

$$\log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2)$$

$$\log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4)$$

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

Gossett 1987		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
EPICS-GC		EPICS-GC		activity coefficient $\gamma_\infty$		activity coefficient $\gamma_\infty$	
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)
10.3	174	10	273.6	20	324	20	331
17.5	268.5	15	330.3	30	496	30	518
24.8	413.4	20	364.8	40	740	40	751
34.6	552	25	460.0				
		30	582.6				
eq. 4a	H/(atm m <sup>3</sup> /mol)	eq. 4a	H/(atm m <sup>3</sup> /mol)				
A	8.479	A	5.164				
B	4192	B	3143				

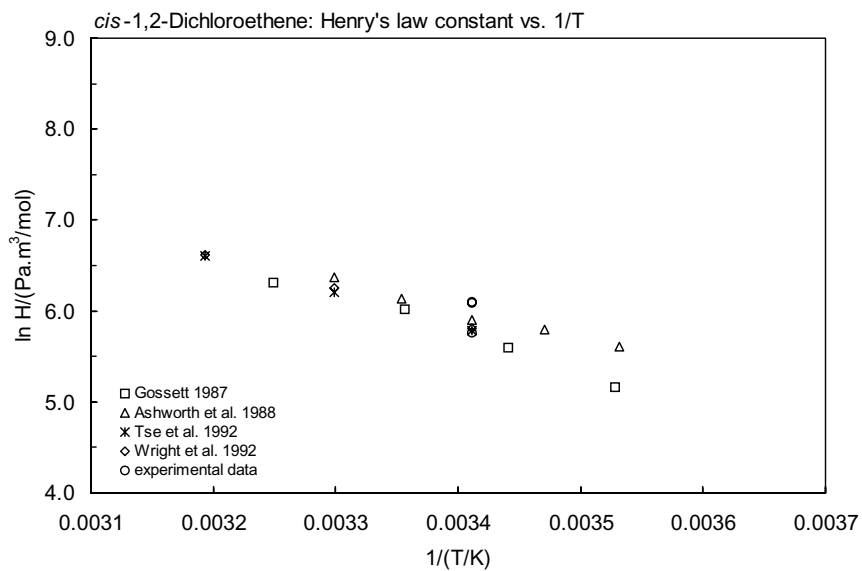
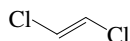


FIGURE 5.1.1.28.3 Logarithm of Henry's law constant versus reciprocal temperature for *cis*-1,2-dichloroethene.

5.1.1.29 *trans*-1,2-Dichloroethene

Common Name: *trans*-1,2-Dichloroethylene

Synonym: *trans*-1,2-dichloroethene, *trans*-1,2-dichloroethylene, *trans*-acetylene dichloride, Dioform, (E)-1,2-dichloroethene

Chemical Name: *trans*-1,2-dichloroethylene, *trans*-1,2-dichloroethene

CAS Registry No: 156-60-5

Molecular Formula: ClCH=CHCl

Molecular Weight: 96.943

Melting Point (°C):

−49.8 (Lide 2003)

Boiling Point (°C):

48.7 (Weast 1977, 1982–83)

Density (g/cm<sup>3</sup> at 20°C):

1.2565 (Horvath 1982; Weast 1982–83)

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

77.2 (20°C, calculated-density)

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

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

36.04, 28.89 (25°C, bp, Riddick et al. 1986)

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

11.98 (Riddick et al. 1986)

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

6260 (Seidell 1940)

6300 (selected from literature of measured in DuPont laboratories, McGovern 1943; Dilling 1977)

6260 (recommended, Horvath 1982)

4480, 4480, 4333 (20, 30, 40°C, infinite dilution activity coeff. γ<sup>∞</sup>-GC, Tse et al. 1992)

4488, 4111, 3931 (20, 30, 40°C, activity coeff. γ<sup>∞</sup>-differential pressure transducer, Wright et al. 1992)

4488 (20°C, limiting activity coeff. γ<sup>∞</sup> by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

4520\* (tentative values, temp range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

S/(wt%) = 7.803906 − 4.5457 × 10<sup>−2</sup> · (T/K) + 6.96755 × 10<sup>−4</sup> · (T/K)<sup>2</sup>, temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

44649\* (25.32°C, temp range −38.19 to 84.84°C, Ketelaar et al. 1947)

43180\* (interpolated-Antoine eq. regression, temp range −65.4 to 47.8°C, Stull 1947)

42970\* (25.2°C, dynamic-ebullimetry, measured range 13.5–51.6°C, Flom et al. 1951)

43470 (Hardie 1964)

36743 (calculated-Antoine eq., Weast 1972–73)

log (P/mmHg) = [−0.2185 × 7243.1/(T/K)] + 7.748400; temp range −65.4 to 236.5°C (Antoine eq., Weast 1972–73)

44190 (calculated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 6.96513 − 1141.984/(231.93 + t/°C); temp range −38 to 84°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

26660, 26660 (14, 20°C, Verschuereen 1977, 1983)

40792\* (23.138°C, temp range −0.68 to 46.721°C, Machat 1983; quoted, Boublik et al. 1984)

44190, 43960 (interpolated-Antoine equations, Boublik et al. 1984)



$\log (P/\text{kPa}) = 6.09105 - 1142.553/(231.998 + t/^{\circ}\text{C})$ ; temp range  $-38.2$  to  $84.84^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.04724 - 1112.321/(227.56 + t/^{\circ}\text{C})$ ; temp range  $-0.68$  to  $46.7^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{mmHg}) = 6.9651 - 1141.9/(231.9 + t/^{\circ}\text{C})$ ; temp range  $-38.2$  to  $85^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)  
 45300 (selected, Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 6.68147 - 1498.42/(T/\text{K})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 44400 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 5.93307 - 1059.93/(-50.83 + T/\text{K})$ ; temp range  $263$ – $323$  K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.27465 - 1226.69/(-33.653 + T/\text{K})$ ; temp range  $321$ – $473$  K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 36250, 53970, 78100 (20, 30,  $40^{\circ}\text{C}$ , quoted from DIPPR, Tse et al. 1992)  
 $\log (P/\text{mmHg}) = 48.4574 - 3.0496 \times 10^3/(T/\text{K}) - 14.694 \cdot \log (T/\text{K}) - 2.1262 \times 10^{-9} \cdot (T/\text{K}) + 7.3465 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
 temp range  $223$ – $508$  K (vapor pressure eq., Yaws 1994)

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

682.7 (calculated as  $1/K_{\text{AW}}$ ,  $C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)  
 1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)  
 669 (calculated-P/C, Dilling 1977)  
 669 (calculated-P/C, Mackay & Shiu 1981)  
 950.5 ( $20^{\circ}\text{C}$ , EPICS, Lincoff & Gossett 1983; Gossett 1985)  
 950\* (EPICS-GC/FID, measured range  $10$ – $34.6^{\circ}\text{C}$ , Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.341 - 4182/(T/\text{K})$ ; temp range  $10.0$ – $34.6^{\circ}\text{C}$  (EPICS measurements, Gossett 1987)  
 914 ( $20^{\circ}\text{C}$ , EPICS-GC, Yurteri et al. 1987)  
 539 (gas stripping-GC, Warner et al. 1987)  
 958\* (EPICS-GC/FID, measured range  $10$ – $30^{\circ}\text{C}$ , Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.333 - 2964/(T/\text{K})$ ; temp range  $10$ – $30^{\circ}\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 729 ( $20$ – $25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 676 (computed value, Yaws et al. 1991)  
 800, 1196, 1793 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)  
 768.7\* ( $20^{\circ}\text{C}$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, measured range  $20$ – $40^{\circ}\text{C}$ , Wright et al. 1992)  
 1023\* ( $26.2^{\circ}\text{C}$ , EPICS-GC, measured range  $26.2$ – $46.1^{\circ}\text{C}$ , Hansen et al. 1993)  
 773 ( $20^{\circ}\text{C}$ , equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 634.8 (modified EPICS method-GC, Ryu & Park 1999)  
 875 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 5.247 - 1669/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

2.06 (Hansch & Leo 1985)  
 2.09 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)  
 2.09 (recommended, Sangster 1993)

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

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

1.34 (calculated- $K_{\text{OW}}$ , Lyman et al. 1982; quoted, Howard 1990)  
 1.68 (microorganisms-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)

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

1.56 (calculated- $K_{\text{OW}}$ , Lyman et al. 1982; quoted, Howard 1990)  
 1.77 (sediment-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)

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

Volatilization: experimental  $t_{1/2}(\text{exptl}) = 24$  min for 1 mg/L from water when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation  $t_{1/2}(\text{exptl}) = 24$  min,  $t_{1/2}(\text{calc}) = 0.85$  min, 20.8 min from water (Dilling 1977)

Volatilization  $t_{1/2} = 3.0$  h from a model river 1 m deep with 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

## 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 see reference:

$k_{\text{O}_3} = 3.8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984)

$k_{\text{OH}} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} = (1.8 \pm 0.29) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Zhang et al. 1983)

$k_{\text{O}_3} = 1.2 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

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

$k_{\text{O}_3} = 2.3 \times 10^5 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , estimated at 300 K (Lyman 1982)

$k < 10^5 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $6.0 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radicals at 25°C (Mabey et al. 1982)

$k = (5.7 \pm 1.0) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{O}_3} = 1.8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Tuazon et al. 1984)

$k_{\text{OH}} = 1.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson 1986; quoted, Atkinson et al. 1987; Sabljic & Güsten 1990)

$k_{\text{NO}_3} = (5.7 \pm 2.7)5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2$  K (relative rate method, Atkinson et al. 1987)

$k_{\text{NO}_3} = 5.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated atmospheric lifetime of 179 d,  $k_{\text{OH}} = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a lifetime of 5.1 d and  $k_{\text{O}_3} = 1.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a lifetime of 110 d at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

photooxidation  $t_{1/2} = 25.2$  h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{\text{NO}_3} = 1.11 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{\text{NO}_3} = (1.07 \pm 0.11) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  relative to ethene at  $298 \pm 2$  K (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 2.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (as per Atkinson 1987 and 1988, Müller & Klein 1991)

## Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 672$ –4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2688$ –17280 h, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991);

$k = 0.1 \text{ yr}^{-1}$  with  $t_{1/2} = 53$  d (Wood et al. 1985; quoted, Olsen & Davis 1990);

rate constant  $k = 0.12$ –0.35  $\text{mini}^{-1}$  in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989);

$k = 1.8 \text{ yr}^{-1}$  with  $t_{1/2} = 132$ –147 d (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

## Biotransformation:

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

## Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 0.24$ –2.4 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition  $t_{1/2} = 2.9$  h with NO and  $t_{1/2} = 2.8$  h with  $\text{NO}_2$  under simulated atmospheric conditions (Dilling et al. 1976);

Photooxidation  $t_{1/2} \sim 100$  min for reaction with  $\text{NO}_2$  under UV irradiation, isomer not specified (Gay, Jr., et al. 1976)

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 44$  d resulting from ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

$t_{1/2} = 3.6$  d in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

$t_{1/2} = 25.2$  h, based on estimated rate constant for reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes,  $\tau = 170$  d for the reaction with  $\text{NO}_3$  radical for a 12-h nighttime average concn. of  $2.4 \times 10^9$  molecule  $\text{cm}^{-3}$ ,  $\tau = 5.1$  d for the reaction with OH radical for a 12-h average concn. of  $1.0 \times 10^6$  molecule  $\cdot \text{cm}^{-3}$ , and  $\tau = 110$  d for the reaction with  $\text{O}_3$  for a 24-h average concentration of  $7 \times 10^{11}$  molecule  $\cdot \text{cm}^{-3}$  (Atkinson et al. 1987).

Surface water:  $t_{1/2} = 672\text{--}4320$  h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 1344\text{--}69000$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life and estimated half-life for anaerobic biodegradation of chlorinated ethylenes from a ground water field study (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 672\text{--}4320$  h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

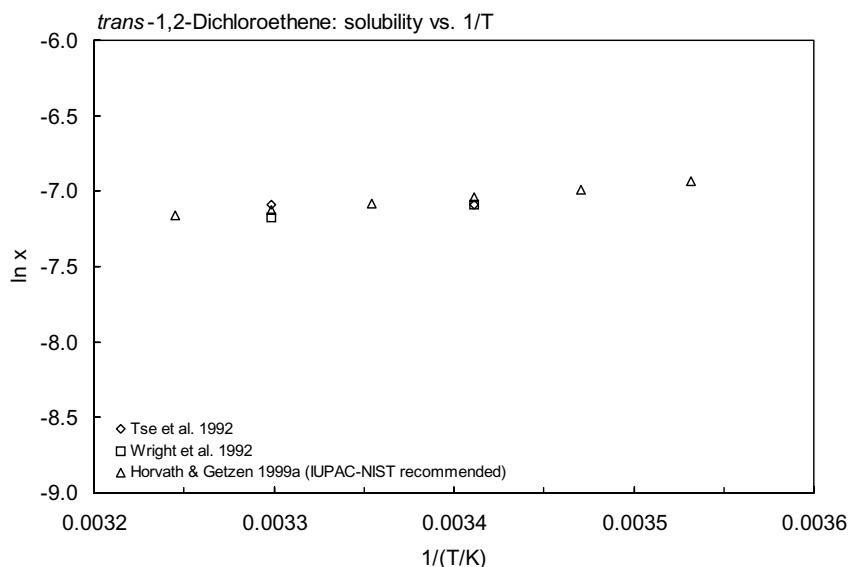
$t_{1/2} < 10$  d (Ryan et al. 1988).

Biota:  $t_{1/2} < 10$  d, subject to plant uptake via volatilization (Ryan et al. 1988).

**TABLE 5.1.1.29.1**

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

Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999	
activity coefficient $\gamma^\infty$		activity coefficient $\gamma^\infty$		IUPAC-NIST recommended	
$t/^\circ\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$
20	4480	20	4488	10	5250
30	4480	30	4111	15	4970
40	4333	40	3931	20	4720
				25	4520
				30	4330
				35	4190
				40	4080



**FIGURE 5.1.1.29.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *trans*-1,2-dichloroethene.

**TABLE 5.1.1.29.2**

Reported vapor pressures of *trans*-1,2-dichloroethene 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)		

Stull 1947		Ketelaar et al. 1947*		Flom et al. 1951		Machet 1983, Thesis	
summary of literature data		in Boublik et al. 1984		static method-manometer		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-65.4	133.3	-38.19	1387	13.5	26131	-0.68	13944
-47.4	666.6	-28.3	3000	20.5	35210	3.154	16825
-38.0	1333	-15.12	6733	25.3	42956	7.12	20300
-28.0	2666	-7.29	10092	29.7	50836	11.306	24599
-17.0	5333	0.52	15086	34.7	61835	15.344	29372
-10.0	7999	5.98	19438	38.6	71581	19.302	34777
-0.20	13332	11.12	24718	41.6	79300	23.138	40792
14.3	26664	16.91	31651	44.1	86513	27.017	47616
30.8	53329	19.06	34757	46.8	95099	33.103	60215
47.8	101325	25.32	44649	49.1	102165	38.951	74768
		28.23	50329	51.6	111151	45.27	93376

TABLE 5.1.1.29.2 (Continued)

Stull 1947		Ketelaar et al. 1947*		Flom et al. 1951		Machat 1983, Thesis	
summary of literature data				static method-manometer		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
mp/°C	-122.5	32.15	38448	$\Delta H_v/(\text{kJ mol}^{-1}) = 29.62$		46.721	98149
		35.84	66888				
		43.72	88272			bp/°C	47.655
		47.17	99365			Antoine eq	
		48.83	105591			eq. 2	P/kPa
		50.82	112737			A	6.04724
		56.12	133389			B	1112.321
		63.58	167812			C	227.560
		68.19	192917				
		77.16	248619				
		84.84	304561				

\*for a complete data set, see [references](#).

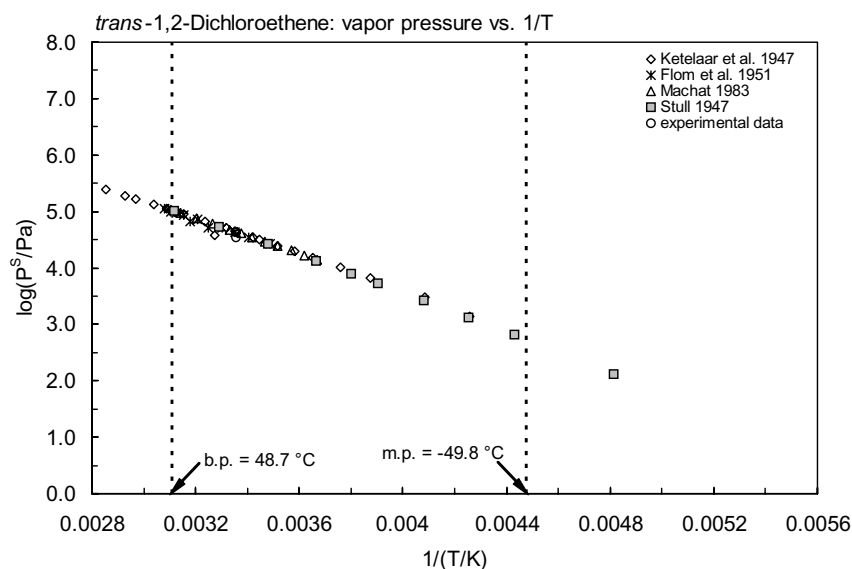


FIGURE 5.1.1.29.2 Logarithm of vapor pressure versus reciprocal temperature for *trans*-1,2-dichloroethene.

TABLE 5.1.1.29.3

Reported Henry's law constants of *trans*-1,2-dichloroethene 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)				
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)						
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)				
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)						
<b>Gossett 1987</b>	<b>Ashworth et al. 1988</b>	<b>Tse et al. 1992</b>	<b>Hansen et al. 1993</b>				
<b>EPICS-GC</b>	<b>EPICS-GC</b>	<b>activity coeff. <math>\gamma^\infty</math>-GC</b>	<b>EPICS-GC</b>				
<b>t/°C</b>	<b>H/(Pa m<sup>3</sup>/mol)</b>	<b>t/°C</b>	<b>H/(Pa m<sup>3</sup>/mol)</b>	<b>t/°C</b>	<b>H/(Pa m<sup>3</sup>/mol)</b>	<b>t/°C</b>	<b>H/(Pa m<sup>3</sup>/mol)</b>
10.0	425.6	10	597.8	20	800	26.2	1023
17.5	668.7	15	714.3	30	1196	35.0	1591
24.8	950.4	20	868.4	40	1793	46.1	2087
34.6	1398.3	25	957.5				
		30	1226.0				
eq. 4a	H/(atm m <sup>3</sup> /mol)			<b>Wright et al. 1992</b>		eq. 4a	H/(kPa m <sup>3</sup> /mol)
A	9.341	eq. 4a	H/(atm m <sup>3</sup> /mol)	<b>activity coeff. <math>\gamma^\infty</math></b>		A	11 ± 1.96
B	4182	A	10.65	<b>t/°C</b>		B	3396 ± 602
		B	4368	<b>H/(Pa m<sup>3</sup>/mol)</b>			
				20	768.7		
				30	1238		
				40	1854		

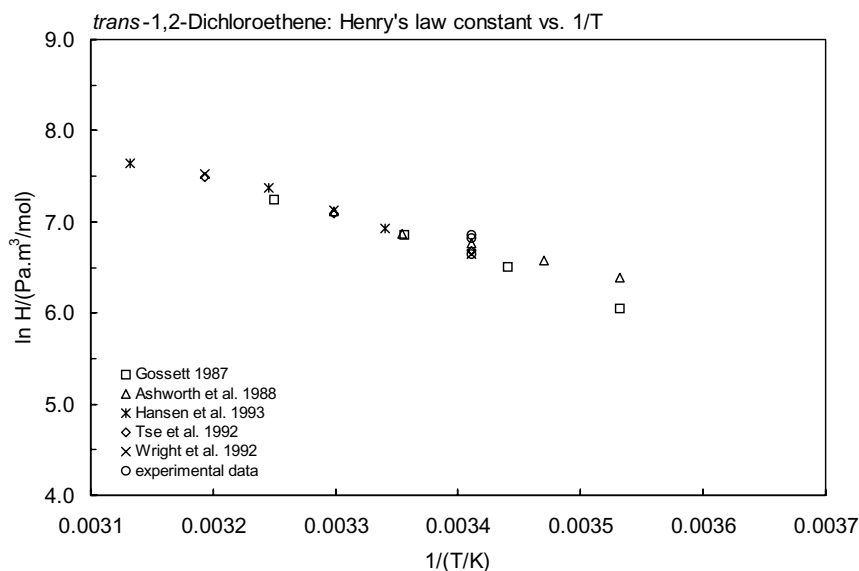
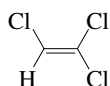


FIGURE 5.1.1.29.3 Logarithm of Henry's law constant versus reciprocal temperature for *trans*-1,2-dichloroethene.

## 5.1.1.30 Trichloroethylene



Common Name: Trichloroethylene

Synonym: TCE, acetylene trichloride, ethylene trichloride

Chemical Name: 1,1,2-trichloroethylene

CAS Registry No: 79-01-6

Molecular Formula:  $C_2HCl_3$ ,  $CHCl=CCl_2$

Molecular Weight: 131.388

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

-84.7 (Lide 2003)

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

87.21 (Lide 2003)

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

1.4642 (Dreisbach 1959; Horvath 1982; Weast 1982-83)

1.4554 ( $25^{\circ}C$ , Dreisbach 1959)

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

89.02 (calculated-density, Miller et al. 1985)

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

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

34.27, 31.47 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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 (Suntio et al. 1988)

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):

1818 (volumetric method, Wright & Schaffer 1932;)

1100 (data presented in graph, temp range  $0-80^{\circ}C$ , McGovern 1943)

1288\* (temp range  $10-50^{\circ}C$ , Vallaud et al. 1957)

1100 ( $20^{\circ}C$ , McConnell et al. 1975; Pearson & McConnell 1975)

1780, 1500, 1470 (3, 20,  $34^{\circ}C$ , shake flask-GC/ECD, Chiou & Freed 1977)

1000, 1100, 1100 (1.5, 20,  $25^{\circ}C$ , literature average, Dilling 1977)

1000 (shake flask-titration/turbidity, Coca et al. 1980)

1472 (shake flask-LSC, Banerjee et al. 1980)

1474 (shake flask-LSC, Veith et al. 1980)

1100\* (summary of literature data, temp range  $0-80^{\circ}C$ , Horvath 1982)

1366 (generator column-HPLC, Tewari et al. 1982)

743.1 ( $30^{\circ}C$ , headspace-GC, McNally & Grob 1984)

1370 (selected, Riddick et al. 1986)

1421 ( $23-24^{\circ}C$ , shake flask-GC, Broholm et al. 1992)

1350 ( $20^{\circ}C$ , calculated-activity coefficients, Wright et al. 1992)

1483, 1450, 1468 (20, 30,  $40^{\circ}C$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

1349, 1409, 1308 (20, 30,  $40^{\circ}C$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

1300-1500 ( $9-71^{\circ}C$ , generator column-GC, data presented in graph, Heron et al. 1998)

1330 ( $20^{\circ}C$ , limiting activity coeff.  $\gamma^{\infty}$  by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

1280\* (recommended, temp range  $0-60^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 1.4049 - 8.2223 \times 10^{-3} \cdot (T/K) + 1.3218 \times 10^{-5} \cdot (T/K)^2$ , temp range 273-333 K (equation derived from literature solubility data, Horvath & Getzen 1999a)

1417\* ( $21^{\circ}C$ , batch equilibrium-GC, sample prepared at 1.0 MPa, measure range  $21-117^{\circ}C$ , Knauss et al. 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):

- 19733\* (temp range 25–87.15°C, Hertz & Rathmann 1912)  
 9331 (extrapolated, data presented in graph, McGovern 1943)  
 9645\* (25.5°C, ebulliometry, measured range 18–86°C, McDonald 1944)  
 $\log (P/\text{cmHg}) = 30.482609 - 2936.227/(T/K) - 7.999975 \cdot \log (T/K)$ ; temp range 18–86°C (ebulliometry, McDonald 1944)  
 9735\* (interpolated-Antoine eq. regression, temp range 25–87.2°C, Stull 1947)  
 9906 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)  
 $\log (P/\text{mmHg}) = 7.02808 - 1315.0/(230.0 + t/^{\circ}\text{C})$ ; temp range 7–155°C (Antoine eq. for liquid state, Dreisbach 1959)  
 9723 (calculated-Antoine eq., Weast 1972–73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 8314.7/(T/K)] + 7.956342$ ; temp range –43.8 to 86.7°C (Antoine eq., Weast 1972–73)  
 9224 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log (P/\text{mmHg}) = 6.51827 - 1018.603/(192.731 + t/^{\circ}\text{C})$ ; temp range 17–86°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 8000 (20°C, Perry & Chilton 1973)  
 7700 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)  
 3066, 7866, 9866 (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)  
 7998, 12660 (20°C, 30°C, Verschuereen 1983; Hewitt et al. 1992)  
 9200, 9690 (interpolated-Antoine equations., Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 5.59553 - 994.46/(189.705 + t/^{\circ}\text{C})$ ; temp range 17.8–86.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 4.70615 - 614.104/(140.089 + t/^{\circ}\text{C})$ ; temp range 25–87.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{mmHg}) = 6.5183 - 1018.6/(192.7 + t/^{\circ}\text{C})$ ; temp range 18–86°C (Antoine eq., Dean 1985, 1992)  
 6307 (selected, Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 6.15298 - 1315.04/(230.0 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 9911 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.15298 - 1315.0/(-43.15 + T/K)$ ; temp range 280–428 K (Antoine eq., Stephenson & Malanowski 1987)  
 9691 (resistance measurement-Antoine eq., Foco et al. 1992)  
 7753, 12350, 19080 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)  
 $\log (P/\text{mmHg}) = 23.6735 - 2.3763 \times 10^3/(T/K) - 5.8275 \cdot \log (T/K) + 1.9586 \times 10^{-3} \cdot (T/K) + 2.8882 \times 10^{-14} \cdot (T/K)^2$ ; temp range 188–571 K (vapor pressure eq., Yaws 1994)

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):

- 1186 (calculated as  $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)  
 248, 1186 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)  
 967 (calculated-P/C, Neely 1976)  
 388.2, 1215 (1.5, 25°C, calculated-P/C, Dilling 1977)  
 890, 975 (20°C, exptl., calculated-P/C, Dilling 1977)  
 1103 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)  
 $\log (H/\text{atm}) = 8.59 - 1716.16/(T/K)$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)  
 985 (20°C, batch stripping-GC, Mackay et al. 1979)  
 985\* (25.2°C, equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)  
 $\ln (k_H/\text{atm}) = 21.89 - 4647/(T/K)$ ; temp range 1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 999 (20°C, batch stripping-GC, Munz & Roberts 1987)  
 970 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)  
 774; 683 (20°C, EPICS-GC; batch air stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 11.94 - 4929/(T/K)$ ; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.703 - 4308/(T/K)$ ; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)



- 452, 795, 1348 (10, 20, 30°C, multiple equilibrium technique-GC, Munz 1985)  
 1185 (adsorption isotherm, Urano & Murata 1985)  
 970.7\* (24.8°C, EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 11.37 - 4780/(T/K)$ ; temp range 9.6–34.6°C (EPICS-GC, Gossett 1987)  
 816 (20°C, EPICS-GC, Munz & Roberts 1987)  
 $\log K_{AW} = 6.026 - 1909/(T/K)$ ; temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)  
 1185 (gas stripping-P/C, Warner et al. 1987)  
 1048 (20°C, EPICS, Yurteri et al. 1987)  
 1034\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 7.845 - 3702/(T/K)$ ; temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)  
 922 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 768.4 (purge and trap method, Tancrède & Yanagisawa 1990)  
 768\* (tap water, EPICS-GC, measured range 25–47.2°C, Tancrède & Yanagisawa 1990)  
 $\log K_{AW} = 6.664 - 2141/(T/K)$ ; temp range 25–47.2°C (EPICS-GC, Tancrède & Yanagisawa 1990)  
 1182 (computed value, Yaws et al. 1991)  
 709, 1155, 1753 (20, 30, 40°C, determined from measured infinite dilution activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)  
 756, 1152, 1908 (20, 30, 40°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 996 (activity coefficient  $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)  
 1043\* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)  
 794 (23°C, batch air stripping-IR, Nielsen et al. 1994)  
 870\* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)  
 381, 1073 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)  
 $\ln K_{AW} = -3648/(T/K) + 0.00813 \cdot Z + 11.121$ ; with Z salinity 0–35.5‰, temp range 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)  
 775 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 1180 (vapor-liquid equilibrium-GC, Turner et al. 1996)  
 $K_{AW} = 0.151 - 0.00597 \cdot (T/K) + 0.000680 \cdot (T/K)^2$ ; temp range 0–45°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)  
 751 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 885\* (headspace equilibrium-GC, measured range 15–45°C, Peng & Wan 1997)  
 $\ln (k_H/\text{atm}) = 8.19 - 1642/(T/K)$ ; temp range 15–45°C (headspace-GC measurements, Peng & Wan 1997)  
 709\* (20°C, headspace equilibrium-GC, Peng & Wan 1998)  
 1195 (sea water 36‰, headspace-GC, measured range 15–45°C, Peng & Wan 1998)  
 $\log (k_H/\text{atm}) = 8.62 - 1736/(T/K)$ ; sea water 36‰ NaCl, temp range: 15–45°C (headspace-GC measurements, Peng & Wan 1998)  
 1055 (modified EPICS method-GC, Ryu & Park 1999)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 7.99 - 3736/(T/K)$ ; temp range 10–95°C (EPICS measurements, Heron et al. 1998)  
 1006; 981; 352 (EPICS-GC; quoted lit.; calculated-P/C, David et al. 2000)  
 703.4\* (calculated from P and exptl measured solubility, temp range 21–117°C, Knauss et al. 2000)  
 823\* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)  
 $\ln K_{AW} = 9.9697 - 3287.5/(T/K)$ ; measured range 15–4 0°C (SPME-GC, Bierwagen & Keller 2001)  
 765 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{AW} = 5.874 - 1871/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)  
 995\* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)  
 $\ln K_{AW} = 12.13 - 3908.2/(T/K)$ ; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

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:

- 2.37 (Hansch & Elkins 1971)  
 2.29 (Leo et al. 1971; Hansch & Leo 1979; 1987)  
 2.61 (shake flask-GC/ECD, Chiou & Freed 1977)  
 2.42 (shake flask-LSC, Banerjee et al. 1980)  
 2.42 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982; Veith et al. 1983)  
 2.86 (HPLC- $k'$  correlation, McDuffie 1981)

- 2.53 (generator column-HPLC, Tewari et al. 1982)
- 2.71, 2.79, 3.49, 3.57 (values used for OECD Lab. comparison tests, Harnisch et al. 1983)
- 2.84 (HPLC-RT correlation, Eadsforth 1986)
- 2.42 (recommended, Sangster 1993)
- 2.67 (calculated-activity coefficients  $\gamma^\circ$ , Tse & Sandler 1994)
- 2.61 (recommended, Hansch et al. 1995)
- 2.27\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

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

- 2.99 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 1.59 (rainbow trout, Neely et al. 1974)
- 1.23–1.36 (calculated- $K_{OW}$ , Veith et al. 1979; Veith et al. 1980)
- 1.23 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
- 1.23–1.59 (bluegill sunfish & rainbow trout, Barrows et al. 1980; Lyman 1981)
- 1.59 (rainbow trout, quoted, Bysshe 1982)
- 1.987 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)
- 1.20 (calculated-MCI  $\chi$ , Koch 1983)
- 2.996 (activated sludge, Freitag et al. 1984)
- 3.06, 2.39 (*Chlorella fusca*, calculated- $K_{OW}$ , Geyer et al. 1984)
- 1.20, 1.05 (quoted, calculated, Sabljic 1987)
- 1.025 (quoted from USEPA 1986, Yeh & Kastenbergh 1991)
- 1.420 (calculated- $K_{OW}$ , McCarty et al. 1992)

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

- 2.10 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)
- 2.20 (Pavlou & Weston 1983, 1984)
- 1.76, 2.20 (ICN humic acid-coated  $Al_2O_3$ , ICN humic acid, Garbarini & Lion 1985)
- 1.66; 2.14, 2.40 (predicted-S, predicted- $K_{OW}$ , Garbarini & Lion 1985)
- 1.76; 0.616 (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, Garbarini & Lion 1986)
- 1.238, 2.079, 2.045, 0.30, 1.827 (tannic acid, lignin, zein, cellulose, Aldrich humic acid, Garbarini & Lion 1986)
- 2.025, 2.086 (Sapsucker Woods soil, Sapsucker Woods ether-extracted soil, Garbarini & Lion 1986)
- 2.161, 2.458 (humins, oxidized humins, Garbarini & Lion 1986)
- 2.663 (fats, waxes, resins, Garbarini & Lion 1986)
- 2.54, 1.72 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
- 2.00; 1.84 (quoted from Seip et al. 1986, calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 2.03 (soil, Chiou et al. 1988; quoted, Grathwohl 1990)
- 2.02, 2.11 (soil: quoted, HPLC-RT correlation, Hodson & Williams 1988)
- 1.79 (20°C, humic acid, Peterson et al. 1988; quoted, Grathwohl 1990)
- 1.53 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.61, 2.12 (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)
- 2.89, 2.50, 2.25 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.09; 2.56; 3.43 (20°C, soil, sand and loess; weathered shale and mudrock; unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 1.97, 2.15 (20°C, calculated- $K_{OW}$ , Grathwohl 1990)
- 0.30–3.64 (cellulose anthracite, quoted, Grathwohl 1990)
- 2.01 (calculated average, Olsen & Davis 1990)
- 2.20, 1.78 (humic acid, humic acid-coated  $Al_2O_3$ , Pavlostathis & Jaglal 1991)
- 2.03 (surface soil, Pavlostathis & Jaglal 1991)

- 3.39, 2.00 (organic carbon soil, Doust & Huang 1992)  
 1.60, 1.60, 2.15 (bentonite, green & tan clay, Doust & Huang 1992)  
 0.35, 1.40, 1.90, 2.20 (Barnwell, Congaree, McBean I & II sands, Doust & Huang 1992)  
 1.66, 2.64, 2.83 (calculated-equilibrium desorption data, Pavlostathis & Mathavan 1992)  
 2.23, 2.33, 2.35, 2.34, 2.34, 2.36, 2.41 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)  
 2.80; 2.00 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)  
 1.92, 2.00, 1.75 (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 $K_{OM}$ :

- 1.23 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.42, 1.89 (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)  
 2.78, 2.36 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil B<sub>t</sub> horizon OM 4.38%; Oshtemo soil B<sub>t</sub> horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 1.74 (Florida peat, OC 57.1%, batch equilibrium-sorption isotherm, Rutherford & Chiou 1992)

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

Volatilization: evaporation  $t_{1/2}$ (exptl.) = 21 min, calculated  $t_{1/2}$ (calc) = 0.48 min from dilute aqueous solution of 1 ppm initial concn. in a 250 mL beaker with constant stirring at room temp (Dilling et al. 1975); volatilization  $k = 2.79, 5.07 \text{ g cm}^{-2} \text{ s}^{-1}$  at  $23.7 \pm 0.5^\circ\text{C}$  into the atmosphere (Chiou & Freed 1977); Evaporation  $t_{1/2}$ (exptl.) = 17.7, 18.5, 23.5 min,  $t_{1/2}$ (calc) = : 0.47 min, 23.8 min at  $20\text{--}25^\circ\text{C}$  and  $t_{1/2}$ (exptl.) = 31.9 min at  $1.5^\circ\text{C}$  from water (Dilling 1977)  
 ratio of evaporation rate constant to that of oxygen reaeration rate constant: measured as 0.49 as compared to the predicted 0.44 (Smith et al. 1980);  
 $t_{1/2}$ (exptl.) =  $1.42 \times 10^4 \text{ s}$  and  $t_{1/2}$ (calc) =  $5.1 \times 10^3 \text{ s}$  for water body of depth of 22.5 m (Klöpffer et al. 1982)  
 estimated  $t_{1/2} = 3.4 \text{ h}$  from water (Thomas 1982);  
 $k = 0.025 \text{ d}^{-1}$ ,  $t_{1/2} = 28 \text{ d}$  in spring at  $8\text{--}16^\circ\text{C}$ ,  $k = 0.052 \text{ d}^{-1}$ ,  $t_{1/2} = 13 \text{ d}$  in summer at  $20\text{--}22^\circ\text{C}$ ,  $k = 0.045 \text{ d}^{-1}$ ,  $t_{1/2} = 15 \text{ d}$  in winter at  $3\text{--}7^\circ\text{C}$  for the periods when volatilization appears to dominate, and  $k = 0.064 \text{ d}^{-1}$ ,  $t_{1/2} = 10.7 \text{ d}$  with  $\text{HgCl}_2$ , and  $k = 0.081 \text{ d}^{-1}$ ,  $t_{1/2} = 9.6 \text{ d}$  without  $\text{HgCl}_2$  in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);  
 $k = 7.22 \times 10^{-3} \text{ h}^{-1}$  (Mackay et al. 1985).

Photolysis:  $t_{1/2} = 3.5 \text{ h}$  estimated from lab. simulated UV photolysis (light intensity about 6 times of natural sunlight at noon on a summer day in Freeport) for 10 ppm to react with 5 ppm NO at  $27 \pm 1^\circ\text{C}$  (Dilling et al. 1976); probably would not occur (Callahan et al., 1979)  
 photocatalyzed mineralization by the presence of  $\text{TiO}_2$  with the rate of  $830 \text{ ppm min}^{-1} \cdot \text{g}^{-1}$  of catalyst (Ollis 1985);  
 $k = (4.08\text{--}6.27) \times 10^{-3} \text{ h}^{-1}$  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,  $k_{OH}$  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:

- $k_{OH} = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow system-LMR, Howard 1976)  
 Photooxidation  $t_{1/2} \sim 120 \text{ min}$  for reaction with  $\text{NO}_2$  under UV irradiation (Gay, Jr. et al 1976)  
 $k_{OH}^* = (2.37 \pm 0.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 234–420 K (discharge flow-resonance fluorescence, Chang & Kaufman 1977)  
 $k_{OH} = (0.27 \pm 0.08) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$  at 1 atm and  $305 \pm 2 \text{ K}$  (relative rate method, Winer et al. 1978)  
 $k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson et al. 1979,1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)  
 $k_{OH} = 2.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 5.3 d, loss of 17.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)  
 $k_{OH} = 1.2 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  estimated, and  $k_{O_3} = 3.6 \times 10^3 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at 300 K (Lyman 1982)

$k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the gas-phase reaction with ozone at  $296 \pm 2 \text{ K}$  (Atkinson et al. 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k < 1000 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen,  $k = 6.0 \text{ M}^{-1} \text{ h}^{-1}$  for  $RO_2$  radical (Mabey et al. 1982)

$k = (17 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water at pH 2 and  $20\text{--}23^\circ\text{C}$  (Hoigné & Bader 1983)

$k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Tuazon et al. 1984)

$k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs.}) = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a loss rate of  $0.10 \text{ d}^{-1}$ ,  $k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a loss rate of  $0.002 \text{ d}^{-1}$  at room temp. (Atkinson et al. 1985)

$k_{OH} = (2.86 \pm 0.40) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with reference to *n*-butane at  $23.2 \pm 1.1^\circ\text{C}$  and a calculated atmospheric lifetime  $\tau = 4.0 \text{ d}$  (Edney et al. 1986)

$k_{NO_3} = (1.5 \pm 0.7) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2 \text{ K}$  (relative rate method, Atkinson et al. 1987)

$k_{NO_3} = 1.5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated atmospheric lifetime  $\tau = 64 \text{ d}$ ,  $k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with lifetime  $\tau = 9.6 \text{ d}$  and  $k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with lifetime  $\tau > 1.5 \text{ yr}$  at room temp. (Atkinson et al. 1987)

$k_{OH}(\text{calc}) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs.}) = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH}^* = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \text{ K}$  (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 6.92 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (as per Atkinson 1987 and 1988, Müller & Klein 1991)

$k_{NO_3} = (2.81 \pm 0.17) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  relative to ethene at  $298 \pm 2 \text{ K}$  (Atkinson 1991)

$k(\text{aq.}) = (15 \pm 2) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $21 \pm 1^\circ\text{C}$ , with a half-life of 37 min at pH 7 (Yao & Haag 1991).

Hydrolysis: not an important process (Mabey et al. 1982);

$k = 0.065 \text{ month}^{-1}$  at  $25^\circ\text{C}$  with  $t_{1/2} = 10.7 \text{ months}$  (Dilling et al. 1975; quoted, Howard et al. 1991);

$k = 9.0 \times 10^{-5} \text{ h}^{-1}$  (Mackay et al. 1985);

abiotic hydrolysis or dehydrohalogenation  $t_{1/2} = 10.7 \text{ months}$  (Olsen & Davis 1990)

$t_{1/2} = 320 \text{ d}$  at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: can be biodegraded by microorganisms in sea water;

$t_{1/2}(\text{aerobic}) = 6 \text{ months to } 1 \text{ yr}$  based on acclimated soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991)

$k = 1.1 \text{ yr}^{-1}$  with  $t_{1/2} = 230 \text{ d}$  (Roberts et al. 1982; quoted, Olsen & Davis 1990)

$t_{1/2}(\text{anaerobic}) = 98 \text{ d to } 4.5 \text{ yr}$ , based on sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991);

$k = 0.06 \text{ yr}^{-1}$  with biodegradation  $t_{1/2} = 33 \text{ d}$ , microcosm constructed with crushed rock and water containing low microbial biomass depleted all TCE in 21 months of incubation (Barrio-Lage et al. 1987, quoted, Olsen & Davis 1990)

$k \sim 0.02 \text{ min}^{-1}$  in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989);

$k = 0.08 \text{ yr}^{-1}$  with  $t_{1/2} = 43 \text{ d}$  (Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 180 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 98 \text{ d}$  in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of  $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

$k_1 = 10.5 \text{ h}^{-1}$  (flagfish, calculated-BCF  $\times k_2$ , McCarty et al. 1992)

$k_2 = 0.398 \text{ h}^{-1}$  (flagfish, estimated-one compartment first-order kinetics, McCarty et al. 1992)

#### Environmental Half-Lives:

Air: tropospheric  $t_{1/2} = 6.0 \text{ wk}$ , when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition  $t_{1/2} = 3.5 \text{ h}$  with NO and  $t_{1/2} = 2.9 \text{ h}$  with  $NO_2$  under simulated atmospheric conditions (Dilling et al. 1976);

photooxidation  $t_{1/2} \sim 120 \text{ min}$  for reaction with  $NO_2$  under UV irradiation (Gay, Jr. et al. 1976)

residence time of 5.3 d, loss of 17.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 27\text{--}272$  h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991);  
atmospheric lifetime  $\tau = 4.0$  d, based on the photooxidation rate constant in the gas phase at  $23.2 \pm 1.1^\circ\text{C}$  (Edney et al. 1986);

atmospheric lifetimes  $\tau = 64$  d for the reaction with  $\text{NO}_3$  for a 12-h nighttime average concn. of  $2.4 \times 10^9$  molecule/ $\text{cm}^3$ ,  $\tau = 9.6$  d for the reaction with OH radical for a 12-h average concn. of  $1.0 \times 10^6$  molecule  $\text{cm}^{-3}$ , and  $\tau > 1.5$  yr for the reaction with  $\text{O}_3$  for a 24-h average concn. of  $7 \times 10^{11}$  molecule/ $\text{cm}^3$  (Atkinson et al. 1987);

$t_{1/2} \sim 3.7$  d (Yeh & Kastenberg 1991).

Surface water: estimated  $t_{1/2} = 1.2\text{--}90$  d in surface waters at various locations in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

half-lives from marine mesocosm:  $t_{1/2} = 28$  d in the spring at  $8\text{--}16^\circ\text{C}$ ,  $t_{1/2} = 13$  d in the summer at  $20\text{--}22^\circ\text{C}$  and  $t_{1/2} = 15$  d in the winter at  $3\text{--}7^\circ\text{C}$  when volatilization dominates, and  $t_{1/2} = 10.7$  d and  $8.6$  d for experiments with and without  $\text{HgCl}_2$  as poison, respectively, in September 9–15 (Wakeham et al. 1983)

Biodegradation  $t_{1/2}$ (aerobic) = 100 d,  $t_{1/2}$ (anaerobic) = 400 d; hydrolysis  $t_{1/2} = 320$  d at pH 7 in natural waters (Capel & Larson 1995)

$t_{1/2} = 4320\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} \sim 90$  d (Yeh & Kastenberg 1991);

measured rate constant  $k = (15 \pm 2) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $21 \pm 1^\circ\text{C}$ , with  $t_{1/2} = 37$  min at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 7704\text{--}39672$  h, based on hydrolysis half-life (Dilling et al. 1975; quoted, Howard et al. 1991) and anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991)

$t_{1/2} \sim 2.0$  yr in the ground water in the Netherlands (estimated, Zoeteman et al. 1981);

$t_{1/2} \sim 86$  d (Yeh & Kastenberg 1991).

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

$t_{1/2} = 4320\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} \sim 43$  d in upper soil and  $t_{1/2} \sim 86$  d in lower soil (Yeh & Kastenberg 1991).

Sediment:  $t_{1/2} \sim 43$  d (estimated, Yeh & Kastenberg 1991).

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

$t_{1/2} < 10$  d, subject to plant uptake via volatilization (Ryan et al. 1988).

**TABLE 5.1.1.30.1**

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

$$S/(\text{wt}\%) = 0.10494 + 4.9038 \times 10^{-5} \cdot (t/^\circ\text{C}) + 6.4541 \times 10^{-6} \cdot (t/^\circ\text{C})^2 - 1.8808 \times 10^{-8} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 1.4049 - 8.2223 \times 10^{-3} \cdot (T/\text{K}) + 1.3218 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Vallaud et al. 1957		Horvath 1982		Tse et al. 1992		Wright et al. 1992	
in Horvath 1982		summary of literature data		activity coefficient		activity coefficient	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
10	1280	0	1049	20	1483	20	1340
20	1285	10	1061	30	1450	30	1409
25	1288	20	1083	40	1468	40	1308
30	1290	25	1099				
40	1305	30	1117				
50	1330	40	1160				
		50	1212				
		60	1271				
		70	1335				
		80	1405				
		eq. 1	$S/\text{wt}\%$				

(Continued)

TABLE 5.1.1.30.1 (Continued)

2.

Horvath & Getzen 1999a				Knauss et al. 2000	
summary of literature data				batch equilibrium-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>
at 1.0 MPa					
0	1450	40	1260	21	1417
5	1410	45	1270	50	1450
10	1370	50	1280	75	1878
15	1330	55	1300	99	2872
20	1310	60	1330	117	5268
25	1280				
30	1279	eq. 2	S/wt%		
35	1260	temp range 273–333 K			

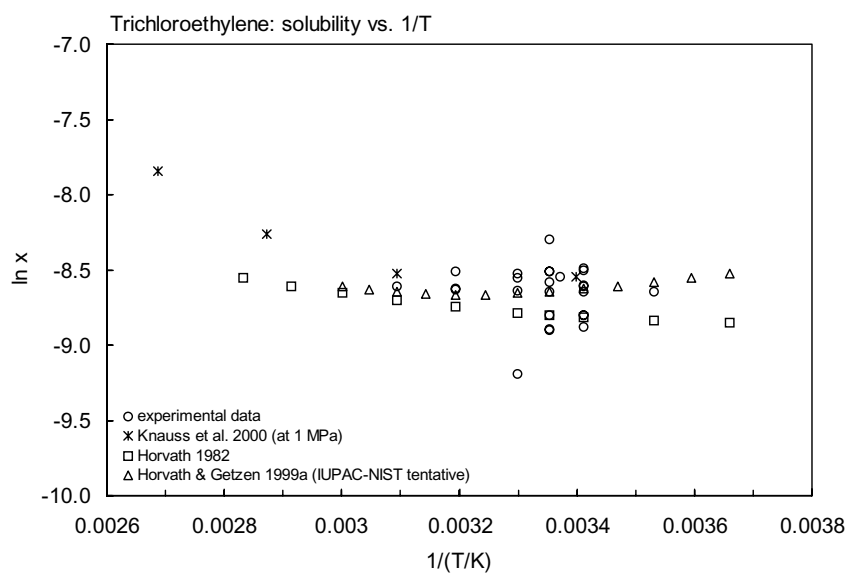
FIGURE 5.1.1.30.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.2

Reported vapor pressures of trichloroethylene at various temperatures and the coefficients for the vapor pressure equations

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

Hertz & Rathmann 1912		McDonald 1944		Stull 1947	
		ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.0	9733	17.8	4239	-43.8	133.3
30.0	12266	19.85	7226	-22.8	666.6
38.0	18532	20.99	7506	-12.4	1333
44.15	23598	24.4	8813	-1.0	2666
45.0	24398	25.5	9546	11.9	5333
51.0	31197	27.4	10319	20.0	7999
65.0	31329	30.2	11999	31.4	13332
77.0	74927	31.2	12426	48.0	26664
87.15	101325	34.39	14292	67.0	53329
		38.49	17305	86.7	101325
		39.29	18025		
		42.41	20545	mp/°C	-73
		44.51	22425		
		46.44	24318		
		51.05	29264		
		55.8	35210		
		60.5	41876		
		65.07	48889		
		71.44	61115		
		76.93	72988		
		80.38	81966		
		85.82	97018		
		86.47	98992		

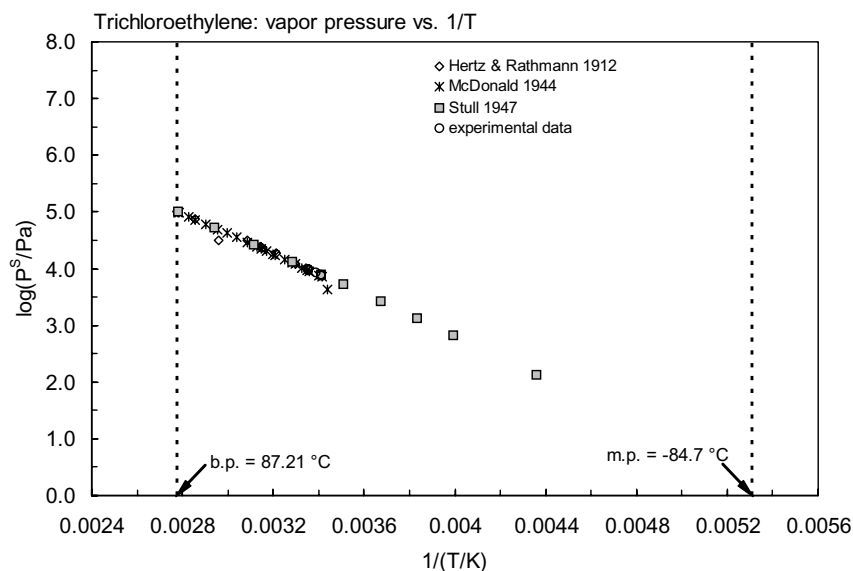


FIGURE 5.1.1.30.2 Logarithm of vapor pressure versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.3

Reported Henry's law constants of trichloroethylene 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)	$\log (k_H/\text{atm}) = A - B/(T/K)$	(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		Gossett 1987		Ashworth et al. 1988		Tancredi & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
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)
1.0	240	9.6	383	10	545.1	25	768
1.0	254.4	17.5	324.2	15	675.8	26.5	797.2
1.2	231.2	24.8	970.7	20	853.2	27.4	999.5
2.5	307.1	34.6	1510	25	1034	28.9	979.4
7.0	366.4			30	1297	28.9	828.7
10.0	424.4	eq. 4	H/(atm m <sup>3</sup> /mol)			29.7	881.2
12.0	464.7	A	11.37	eq. 4	H/(atm m <sup>3</sup> /mol)	29.9	1159
12.0	484.8	B	4780	A	7.845	33.3	1019
12.9	523.4			B	3702	35.6	1386
14.0	565.2					38.3	1554
18.0	683.9					40	1484
18.0	692.3					44.7	1638
18.0	683.9					45	2724
19.0	717.7					47.2	2504
19.2	761.1						



TABLE 5.1.1.30.3 (Continued)

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancréde & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
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)
19.5	723.2					eq. 1a	K <sub>AW</sub>
24.3	979.6					A	6.664
25.2	984.7					B	2141
25.3	995.3						
26.0	1005						
26.0	1028						
26.1	1018						
eq. 3	k <sub>H</sub> /atm						
A	22.68						
B	4735						

2.

Tse et al. 1992		Wright et al. 1992		Robbins et al. 1993		Dewulf et al. 1995	
activity coefficient		activity coefficient		headspace-GC		EPICS-GC	
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)
20	709	20	756	25	1043	2.0	231.05
30	1155	30	1152	30	1330	6.0	290.1
40	1753	40	1753	40	1672	10.0	327.2
				45	2270	18.2	615.3
				50	2665	25.0	870.1
						eq. 1	K <sub>AW</sub>
						A	11.121
						B	3648

3.

Peng & Wan 1997		Knauss et al. 2000		Bierwagen & Keller 2001		Görgényi et al. 2002	
static headspace-GC		calculated-P/C(measured)		SPME-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
15	575	21	703.4	15	585	2.0	246
20	709	50	2552	25	823	6.0	348.6
25	885	75	4934	30	1114	10	447
30	1167	99	6854	40	1523	18	718
35	1309	117	6127			25	995
40	1650			eq 1	K <sub>AW</sub>	30	1308
45	2005			A	9.9697	40	1871
				B	3287.5	50	2765
eq. 3	k <sub>H</sub> /atm					60	3601
A	8.62					eq. 1	K <sub>AW</sub>
B	1736					A	12.13
						B	3908.2

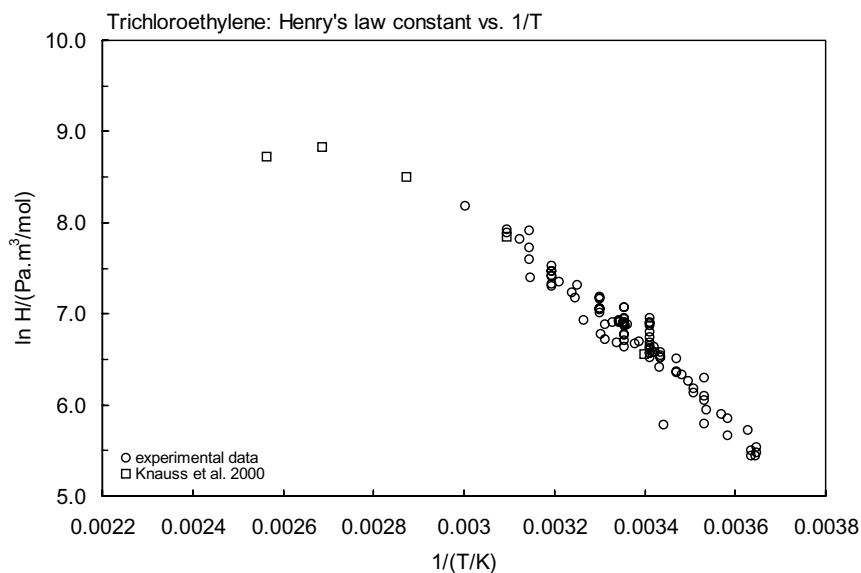


FIGURE 5.1.1.30.3 Logarithm of Henry's law constant versus reciprocal temperature for trichloroethylene.

**TABLE 5.1.1.30.4**  
Reported octanol-water partition coefficients of  
trichloroethylene at various temperatures

Dewulf et al. 1999

EPICS-GC

t/°C	log K <sub>OW</sub>
2.2	2.18
6.0	2.18
10.0	2.28
14.1	2.24
18.7	2.29
24.8	2.20

change in enthalpy:

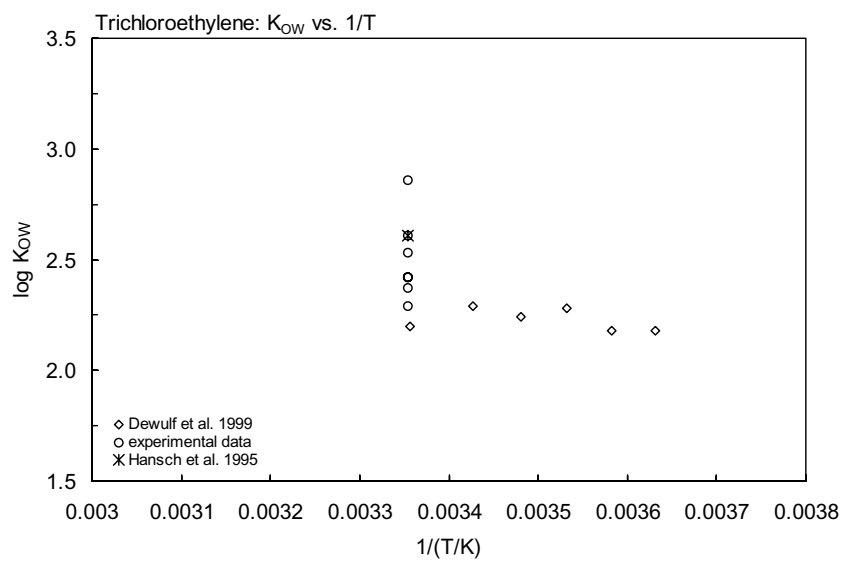
$$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 3.4$$

(-8.4 to 15.2)

enthalpy of transfer

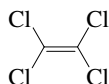
$$\Delta H_{oct}/(\text{kJ mol}^{-1}) = 2.7$$

(-9.0 to 14.5)



**FIGURE 5.1.1.30.4** Logarithm of  $K_{OW}$  versus reciprocal temperature for trichloroethylene.

## 5.1.1.31 Tetrachloroethylene



Common Name: Tetrachloroethylene

Synonym: ethylene tetrachloride, perchloroethene, perchloroethylene, tetrachloroethene, 1,1,2,2-tetrachloro-ethylene

Chemical Name: tetrachloroethylene

CAS Registry No: 127-18-4

Molecular Formula:  $C_2Cl_4$ ,  $CCl_2=CCl_2$

Molecular Weight: 165.833

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

-22.3 (Lide 2003)

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

121.3 (Lide 2003)

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

1.62272, 1.61446 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959)

1.6227 (Horvath 1982; Weast 1982–83)

1.62283, 1.61431 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

102.0 ( $20^{\circ}C$ , calculated-density)

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

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

39.61, 34.72 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

10.56 (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):

150 (selected from literature or measured in DuPont laboratories, data also presented in graph, temp range  $0-80^{\circ}C$ , McGovern 1943)

150 ( $20^{\circ}C$ , McConnell et al. 1975; Pearson & McConnell 1975)

130, 120, 140 (1.5, 20,  $25^{\circ}C$ , selected from literature, Dilling 1977)

200 ( $20^{\circ}C$ , shake flask-GC, Chiou et al. 1977)

400 (shake flask-GC, Freed et al. 1979)

136 ( $37^{\circ}C$ , shake flask-GC, Sato & Nakijima 1979)

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

200 (shake flask-titration/turbidity, Coca & Diaz 1980, Coca et al. 1980)

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

150\* (summary of literature data, temp range  $0-80^{\circ}C$ , Horvath 1982)

242 ( $23-24^{\circ}C$ , shake flask-GC, Broholm et al. 1992)

286\* ( $19.5^{\circ}C$ , shake flask-GC/TC, measured range  $0-91.8^{\circ}C$ , Stephenson 1992)

256 (activity coeff. by inert gas stripping-GC, Li et al. 1993)

258.8 ( $20^{\circ}C$ , limiting activity coeff. by inert air stripping-GC, Hovorka & Dohnal 1997)

206\* (tentative value, temp range  $0-70^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 0.26479 - 1.5487 \times 10^{-3} \cdot (T/K) + 2.4477 \times 10^{-6} \cdot (T/K)^2$ , temp range 273–343 K (equation derived from reported solubility data, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

192.3\* ( $22^{\circ}C$ , batch equilibrium-GC, sample prepared at 1.0 MPa, measure range  $22-161^{\circ}C$ , Knauss et al. 2000)

215 (deionized water, batch equilibrium, Ladaa et al. 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):

- 2666 (extrapolated, data presented in graph, McGovern 1943)  
 2397\* (Antoine eq. regression, temp range -20.6 to 120.8°C, Stull 1947)  
 2462 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)  
 $\log(P/\text{mmHg}) = 7.02003 - 1415.5/(221.0 + t/^\circ\text{C})$ ; temp range 34–187°C (Antoine eq. for liquid state, Dreisbach 1959)  
 2453\* (vapor-liquid equilibrium VLE data, measured range 27.887–108°C, Polák et al. 1970)  
 $\log(P/\text{mmHg}) = 7.05854 - 1438.947/(233.368 + t/^\circ\text{C})$ ; temp range 27.887–108°C (ebulliometry, Polák et al. 1970)  
 4524\* (37.088°C, temp range 37.088–119.650°C, Boublik & Aim 1972; quoted, Boublik et al. 1984)  
 2394 (calculated-Antoine eq., Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 9240.5/(T/\text{K})] + 8.026207$ ; temp range -20.6 to 120.8°C (Antoine eq., Weast 1972–73)  
 2388 (calculated-Antoine eq., Boublik et al. 1973)  
 $\log(P/\text{mmHg}) = 6.97183 - 1386.915/(217.526 + t/^\circ\text{C})$ ; temp range 37–119°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 1866 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)  
 640, 1893, 2480 (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)  
 2417, 2456 (calculated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.10343 - 1387.956/(217.64 + t/^\circ\text{C})$ , temp range: 37–120°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.19467 - 1445.722/(224.074 + t/^\circ\text{C})$ , temp range: 26.9–108°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 2465 (Daubert & Danner 1986; quoted, Howard 1990)  
 2462 (selected, Riddick et al. 1986)  
 $\log(P/\text{kPa}) = 6.10170 - 1386.90/(217.52 + t/^\circ\text{C})$ , temp range not specified (Antoine eq., Riddick et al. 1986)  
 2415 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.1017 - 1386.9/(-55.63 + T/\text{K})$ , temp range: 310–393 K, (Antoine eq., Stephenson & Malanowski 1987)  
 2479, 4319 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)  
 $\log(P/\text{mmHg}) = 30.4038 - 1.5265 \times 10^3/(T/\text{K}) - 8.783 \cdot \log(T/\text{K}) - 2.6364 \times 10^{-9} \cdot (T/\text{K}) + 9.4381 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 142–306 K (vapor pressure eq., Yaws 1994)

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):

- 2718 (exptl.-1/K<sub>AW</sub> = C<sub>w</sub>/C<sub>A</sub>, Hine & Mookerjee 1975)  
 248, 581 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)  
 1621 (20°C, batch stripping-GC, Mackay et al. 1979)  
 2006 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)  
 $\log(H/\text{atm}) = 10.38 - 2159.0/(T/\text{K})$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)  
 1635\* (equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)  
 $\ln(k_H/\text{atm}) = 16.05 - 3539/(T/\text{K})$ ; temp range 1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 1528 (20°C, gas stripping-GC, Munz & Roberts 1982)  
 1316 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)  
 1317; 1175 (20°C, EPICS-GC; gas stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)  
 $\ln[H/(\text{atm m}^3/\text{mol})] = 13.12 - 5119/(T/\text{K})$ ; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)  
 $\ln[H/(\text{atm m}^3/\text{mol})] = 11.32 - 4622/(T/\text{K})$ ; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)  
 2908 (adsorption isotherm, Urano & Murata 1985)  
 1445 (20°C, multiple equilibration, Munz & Roberts 1986)  
 1852\* (EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)  
 $\ln[H/(\text{atm m}^3/\text{mol})] = 12.45 - 4918/(T/\text{K})$ ; temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)  
 1445 (20°C, EPICS-GC, Munz & Roberts 1987)  
 $\log K_{AW} = 5.92 - 1802/(T/\text{K})$ ; temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

- 2908 (gas stripping-GC, Warner et al. 1987)  
 1304 (20°C, EPICS-GC, Yurteri et al. 1987)  
 1733\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 10.65 - 4368/(T/K)$ ; temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)  
 1363\* (tap water, EPICS-GC, temp range 25–47.2°C, Tancréde & Yanagisawa 1990)  
 $\log K_{AW} = 7.481 - 2279/(T/K)$ ; temp range 25–47.2°C (EPICS-GC, Tancréde & Yanagisawa 1990)  
 2721 (computed value, Yaws et al. 1991)  
 1759\* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)  
 $\ln (1/K_{AW}) = -5.13 + 1736/(T/K)$ ; temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)  
 1599 ( $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)  
 1723\* (static headspace-GC, temp range 25–45°C, Robbins et al. 1993)  
 1490\* (EPICS-GC/FID, temp range 2–25°C, Dewulf et al. 1995)  
 717, 1914 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)  
 $\ln K_{AW} = -4528/(T/K) + 0.01080\cdot Z + 14.655$ ; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)  
 1319 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 1200 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)  
 1710\* (equilibrium headspace-GC, temp range 15–45°C, Peng & Wan 1997)  
 $\log (k_H/\text{atm}) = 9.06 - 1822/(T/K)$ , temp range 15–45°C (headspace-GC measurements, Peng & Wan 1997)  
 1260 (20°C, headspace equilibrium-GC, Peng & Wan 1998)  
 2200\* (sea water 36‰ NaCl, headspace-GC, temp range 15–45°C, Peng & Wan 1998)  
 $\log (k_H/\text{atm}) = 9.09 - 1795/(T/K)$ ; sea water 36‰ NaCl, temp range 15–45°C (headspace-GC measurements, Peng & Wan 1998)  
 1159.2 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 2890 (modified EPICS method-GC, Ryu & Park 1999)  
 1781\* (calculated-P/C(exptl. measured), temp range 22–161°C, Knauss et al. 2000)  
 1690 (static headspace method, Ladaa et al. 2001)  
 1299 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{AW} = 6.394 - 1955/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

- 2.60 (shake flask-GC, Chiou et al. 1977)  
 2.60 (shake flask, Hansch & Leo 1979)  
 2.53 (shake flask-LSC, Banerjee et al. 1980)  
 2.53 (shake flask-LSC, Veith et al. 1980,1983; Veith & Kosian 1982)  
 2.67 (RP-HPLC-RT correlation, Veith et al. 1980)  
 3.78 (HPLC-RT correlation, McDuffie 1981)  
 3.30, 2.72–3.57 (shake flask method: mean, range of mean values, OECD 1981)  
 3.40 (shake flask, Hansch & Leo 1985, 1987)  
 3.40 (correction of Ball & Roberts 1991 selection, Ball & Roberts 1992)  
 3.40 (recommended, Sangster 1993)  
 3.40 (recommended, Hansch et al. 1995)  
 2.27\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C Dewulf et al. 1999)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

- 3.48 (head-space GC/FID, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 1.59 (trout, Neely et al. 1974)  
 1.598 (trout muscle, calculated-ratio of rate const.  $k_1/k_2$ , Neely et al. 1974)  
 1.45–1.88 (calculated- $K_{OW}$ , Veith et al. 1979; Veith et al. 1980)  
 –1.70 (male Albino rats, Geyer et al. 1980)  
 1.69 (bluegill sunfish, Barrows et al. 1980)

- 1.49 (calculated-S, Kenaga 1980)
- 1.69 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
- 2.35 (calculated- $K_{OW}$ , Lyman et al. 1982)
- 2.40 (microorganisms-water, Mabey et al. 1982)
- 2.06 (rainbow trout, Veith & Kosian 1982)
- 1.70 (calculated-MCI  $\chi$ , Koch 1983)
- 1.70, 2.30 (quoted, calculated, Sabljic 1987)
- 1.60 (calculated-solvatochromic parameters, Hawker 1990)
- 2.40 (calculated- $K_{OW}$ , McCarty et al. 1992)
- 1.79 (rainbow trout, Saito et al. 1992)

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

- 2.38 (calculated, Kenaga & Goring 1980, Kenaga 1980)
- 2.32 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
- 2.14; 2.54, 2.89; 2.35, 2.57 (calculated- $K_{OW}$ ; calculated-S and mp; calculated-S, Karickhoff 1981)
- 2.23 (average of 3 sediments and 5 soils, batch equilibrium, Schwarzenbach & Westall 1981)
- 2.04 (Schwarzenbach & Westall 1981)
- 3.23 (calculated- $K_{OW}$ , Lyman et al. 1982)
- 2.38 (peaty soil, calculated- $K_{OM}$ , Friesel et al. 1984)
- 2.56 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)
- 2.56 (soil, Chiou et al. 1988)
- 2.00 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.76, 2.53 (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)
- 1.75 (untreated Marlette soil B<sub>t</sub> horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)
- 2.87, 2.78 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.64 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
- 3.29 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 4.03 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 2.39, 2.57 (20°C, calculated- $K_{OW}$ , Grathwohl 1990)
- 2.14 (calculated-molecular conductivity index, Olsen & Davis 1990)
- 2.45 (2.57% organic carbon in surface soil, Pignatello 1990,1991)
- 1.81–2.95 (calculated- $K_{OW}$ , Ball & Roberts 1991)
- 3.60 (Borden organic phase with no mineral sorption, Ball & Roberts 1991)
- 2.90 (Borden organic phase with no mineral sorption but with Curtis et al. 1986 correlation, Ball & Roberts 1992)
- 2.62, 2.79, 2.74, 2.80, 2.85, 2.78, 2.83 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon  $f_{OC}$  = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)
- 0.393–1.943 (19 soils from U.S. and China with polar organic carbon POC ranging from 2.89–59.9% and organic carbon OC ranging from 1.08–50.8%, batch sorption equilibrium, Kile et al. 1999)
- 1.13–2.11 (9 freshwater sediments from U.S. and China with polar organic carbon POC ranging from 5.36–52.5% and organic carbon OC ranging from 0.58–5.62%, batch sorption equilibrium, Kile et al. 1999)
- 2.32, 2.45, 2.22 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, 0.1  $\leq$  OC < 0.5%, average, Delle Site 2001)

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

- 1.70 (untreated A horizon Marlette soil, Lee et al. 1989)
- 2.56, 2.30(A horizon Marlette soil treated with HDTMA, DDTMA, Lee et al. 1989)
- 1.64 (untreated B<sub>t</sub> horizon Marlette soil, Lee et al. 1989)
- 2.75, 2.64 (treated B<sub>t</sub> horizon Marlette soil with HDTMA, DDTMA, Lee et al. 1989)
- 2.32, 1.90 (quoted, calculated-molecular conductivity index, Olsen & Davis 1990)
- 3.20; 2.40 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

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

Volatilization: evaporation  $t_{1/2}(\text{exptl}) = (27 \pm 3)$  min for 1 mg/L in water when stirred at 200 rpm at approximately 25°C in an open container of 65 mm deep and  $t_{1/2}(\text{calc}) = 0.56$  min (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation  $t_{1/2}(\text{exptl}) = 20\text{--}27.1$  min,  $t_{1/2}(\text{calc}) = 0.20, 26.5$  min at 20–25°C, and  $t_{1/2}(\text{exptl}) = 37.5$  min,  $t_{1/2}(\text{calc}) = 27$  min at 15°C from water (Dilling 1977)

ratio of evaporation rate constant to that of oxygen reaeration: a measured value of 0.44 to that of 0.40 as predicted (Smith et al. 1980);

$t_{1/2} = 5\text{--}12$  d from pond,  $t_{1/2} = 3$  h–7 d from river,  $t_{1/2} = 3.6\text{--}14$  d from lake were estimated using representative reaeration rates (Lyman et al. 1982; quoted, Howard 1990);

estimated  $t_{1/2} \sim 4.2$  h from water (Thomas 1982);

rate constants:  $k = 0.028$  d<sup>-1</sup>,  $t_{1/2} = 25$  d in spring at 8–16°C,  $k = 0.051$  d<sup>-1</sup>,  $t_{1/2} = 14$  d in summer at 20–22°C,  $k = 0.056$  d<sup>-1</sup>,  $t_{1/2} = 12$  d in winter at 3–7°C for the periods when volatilization appears to dominate, and  $k = 0.057$  d<sup>-1</sup>,  $t_{1/2} = 12.1$  d with HgCl<sub>2</sub>, and  $k = 0.058$  d<sup>-1</sup>,  $t_{1/2} = 12.0$  d without HgCl<sub>2</sub> as poison in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: photocatalyzed mineralization by the presence of TiO<sub>2</sub> with the rate of 6.8 ppm/min per gram of catalyst (Ollis 1985); rate constant of  $3.09 \times 10^{-3}$  h<sup>-1</sup> with H<sub>2</sub>O<sub>2</sub> under photolysis at 25°C in F-113 solution and with HO<sup>-</sup> 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 NO<sub>3</sub> radical and  $k_{\text{O}_3}$  with O<sub>3</sub> or as indicated, \*data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{O}_3} < 2 \times 10^{-23}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 297 K (Mathias et al. 1974; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{OH}} = 1.3 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a lifetime about 10 d (Yung et al. 1975; quoted, Callahan et al. 1979)

$k_{\text{OH}} = 1.7 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296 K (discharge flow system-LMR, Howard 1976)

$k_{\text{OH}}^* = (1.69 \pm 0.07) \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 297 K, measured range 297–420 K with calculated lifetime of 0.4–0.6 yr in troposphere (discharge flow system-RF, Chang & Kaufman 1977)

$k_{\text{OH}} = (0.13 \pm 0.04) \times 10^{10}$  cm<sup>3</sup> M<sup>-1</sup> s<sup>-1</sup> at 1 atm and  $305 \pm 2$  K (relative rate method, Winer et al. 1978)

$k_{\text{OH}} = 1.70 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (Atkinson et al. 1979, 1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{OH}} = 1.7 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>, residence time of 68 d, loss of 1.5% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = 1.0 \times 10^{11}$  cm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup>, and  $k_{\text{O}_3} = 1.0 \times 10^3$  cm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup> at 300 K (estimated, Lyman 1982)

$k \ll 100$  M<sup>-1</sup> h<sup>-1</sup> for singlet oxygen 25°C (Mabey et al. 1982)

completely degraded in an hour (Dimitriades et al. 1983; quoted, Howard 1990)

$k < 0.1$  M<sup>-1</sup> s<sup>-1</sup> for reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{O}_3} < 2 \times 10^{-23}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{\text{OH}} = 1.7 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (Tuazon et al. 1984)

$k_{\text{OH}}^* = 1.67 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K (recommended, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 4.2 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{\text{OH}}(\text{obs.}) = 1.7 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{\text{NO}_3} < 4.0 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at  $298 \pm 2$  K (relative rate method, Atkinson et al. 1987)

$k_{\text{NO}_3} < 4.0 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a calculated atmospheric lifetime  $\tau > 240$  d,  $k_{\text{OH}} = 1.7 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with lifetime  $\tau = 140$  d, and  $k_{\text{O}_3} < 2 \times 10^{-23}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a lifetime  $\tau > 2 \times 10^3$  yr at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{\text{OH}}(\text{obs.}) = 1.66 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}} = 2.34 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K,  $k_{\text{NO}_3} = 9.7 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296 K (Atkinson 1990)

$k_{\text{NO}_3} < 5.20 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> relative to ethene at  $298 \pm 2$  K (Atkinson 1991)

Hydrolysis:  $k = 0.079$  month<sup>-1</sup> at 25°C with  $t_{1/2} = 8.8$  months (Dilling et al. 1975; quoted, Callahan et al. 1979); abiotic hydrolysis or dehydrohalogenation  $t_{1/2} = 8.8$  months (Olsen & Davis 1990)

Biodegradation: aqueous aerobic  $t_{1/2} = 4320\text{--}8640$  h, based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater grab sample test data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2352\text{--}39672$  h, based on anaerobic screening test data (Bouwer et al. 1981; quoted, Howard et al. 1991);

first-order  $k = 1.1$  yr<sup>-1</sup> with  $t_{1/2} = 230$  d (Roberts et al. 1982; quoted, Olsen & Davis 1990)



$t_{1/2} = 34$  d (Wood et al. 1985; quoted, Olsen & Davis 1990).

$t_{1/2}(\text{aerobic}) = 180$  d,  $t_{1/2}(\text{anaerobic}) = 98$  d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant for bacteria  $k = 1 \times 10^{-10}$  ml cell<sup>-1</sup> h<sup>-1</sup> (Mabey et al. 1982).

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

$k_1 = 3.323$  h<sup>-1</sup>;  $k_2 = 0.0823$  h<sup>-1</sup> (trout muscle, Neely et al. 1974)

$k_1 = 11.4$  h<sup>-1</sup> (flagfish, calculated-BCF  $\times k_1$ , McCarty et al. 1992)

$k_2 = 0.0454$  h<sup>-1</sup> (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)

$k_1 = 3.30$  h<sup>-1</sup>;  $k_2 = 0.0833$  h<sup>-1</sup> (trout, Hawker & Connell 1985)

#### Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} = 12$  wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance  $t_{1/2} > 10$  d for the reaction with OH radical (Darnall et al. 1976);

lifetime  $\sim 10$  d, based on reaction with OH radical (Yung et al. 1975; quoted, Callahan et al. 1979);

photodecomposition  $t_{1/2} = 14.2$  h with NO and  $t_{1/2} = 8.3$  h with NO<sub>2</sub> under simulated atmospheric conditions (Dilling et al. 1976);

estimated N. troposphere residence time of 150 d by one compartment nonsteady state model (Singh et al. 1978);

lifetime of 1.0 yr in troposphere (Altshuller 1980);

residence time of 68 d, loss of 1.5% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

estimated troposphere residence time of 200–390 d (Lyman 1982);

$t_{1/2} = 384$ – $3843$  h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetimes:  $\tau > 240$  d for the reaction with NO<sub>3</sub> for a 12-h nighttime average concentration of  $2.4 \times 10^9$  molecule/cm<sup>3</sup>,  $\tau = 140$  d for the reaction with OH radical for a 12-h average concentration of  $1.0 \times 10^6$  molecule/cm<sup>3</sup>, and  $\tau > 2000$  yr for the reaction with O<sub>3</sub> for a 24-h average concentration of  $7 \times 10^{11}$  molecule/cm<sup>3</sup> (Atkinson et al. 1987).

Surface water: estimated  $t_{1/2} = 9.9$ – $32$  d in surface waters at various locations in case of a first order reduction process;  $t_{1/2} = 3$ – $30$  d in rivers,  $t_{1/2} = 30$ – $300$  d in lakes and ground waters (Zoeteman et al. 1980)

$t_{1/2} = 25$  d in spring at 8–16°C, 14 d in summer at 20–22°C and 12 d in winter at 3–7°C when volatilization dominates, and  $t_{1/2} = 12.1$  d and 12.0 d for experiments with and without HgCl<sub>2</sub> as poison respectively in September 9–15 in marine mesocosm (Wakeham et al. 1983)

$t_{1/2} = 4320$ – $8640$  h, based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater sample grab data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991);

calculated  $t_{1/2} = 10$  d and 32 d concentration reduction between sampling points on the Rhine River and a lake in the Rhine basin, respectively (Zoeteman et al. 1980; quoted, Howard 1990)

$t_{1/2}(\text{aerobic}) = 180$  d,  $t_{1/2}(\text{anaerobic}) = 98$  d in natural waters (Capel & Larson 1995).

Ground water:  $t_{1/2} = 8640$ – $17280$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

#### Sediment:

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

$t_{1/2} = 4320$ – $8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

$t_{1/2} = 14$  h, clearance from fish in simulated ecosystem (Neely 1980);

$t_{1/2} < 10$  d, subject to plant uptake via volatilization (Ryan et al. 1988);

$t_{1/2} = 0.4$ – $0.5$  d to eliminate from small fish (McCarty et al. 1992).

TABLE 5.1.1.31.1

Reported aqueous solubilities of tetrachloroethylene at various temperatures

$$S/(\text{wt}\%) = 1.49696 \times 10^{-2} - 7.8009 \times 10^{-6} \cdot (t/^{\circ}\text{C}) - 5.1403 \times 10^{-7} \cdot (t/^{\circ}\text{C})^2 + 3.6938 \times 10^{-8} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 0.26479 - 1.5487 \times 10^{-3} \cdot (T/\text{K}) + 2.4477 \times 10^{-6} \cdot (T/\text{K})^2 \quad (2)$$

Horvath 1982		Stephenson 1992		Horvath & Getzen 1999a		Knauss et al. 2000	
summary of literature data		shake flask-GC		summary of literature data		batch equilibrium-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>
at 1.0 MPa							
0	149.7	0	273	0	244	23	192.3
10	148.8	9.5	270	5	234	51	247.4
20	149	19.5	286	10	224	75	313.8
25	150.3	31.1	221	15	218	101	519
30	152.7	40.0	213	20	211	124	1006
40	162	50.1	273	25	206	150	1895
50	179.1	61.3	304	30	202	161	2513
60	206.3	71	377	35	200		
70	245.7	80.2	380	40	198		
80	299.7	91.8	523	45	198		
				50	199		
eq. 1	S/wt%			55	202		
				60	205		
				65	210		
				70	216		
				eq. 2	S/wt%		
				temp range 273–343 K			

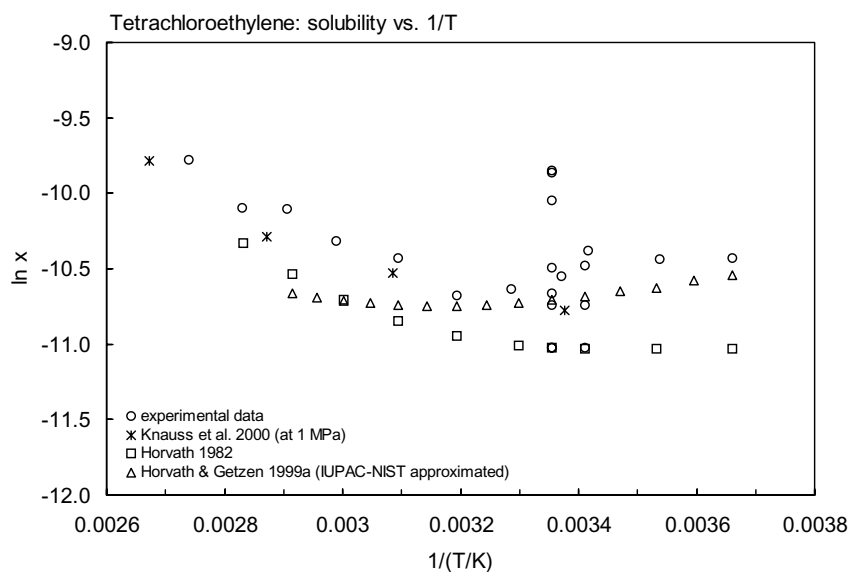


FIGURE 5.1.1.31.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.2

Reported vapor pressures of tetrachloroethylene 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)			
Stull 1947		Polak et al. 1970		Boublik & Aim 1972	
summary of literature data		vapor-liquid equilibrium		in Boublik et al. 1984	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-20.6	133.3	27.887	2869	37.088	4524
2.40	666.6	35.758	4274	46.239	6967
13.8	1333	41.702	5689	52.671	9306
26.3	2666	46.502	7101	58.697	12046
40.1	5333	57.065	11276	63.270	14549
49.2	7999	61.254	15412	68.545	17921
61.3	13332	68.065	17620	73.064	21314
79.8	26664	74.529	22541	78.165	25780
100.0	53329	81.957	29555	82.292	29923
120.8	101325	88.055	36557	87.183	35493
		94.568	45465	91.791	41470
mp/ $^{\circ}\text{C}$	-19.0	98.917	52316	97.291	49704
		104.269	61875	103.930	61295
		107.692	68694	111.548	77125
				119.650	97337
				eq. 2	P/kPa
				A	6.10343
				B	1387.956
				C	217.640
				bp	121.074

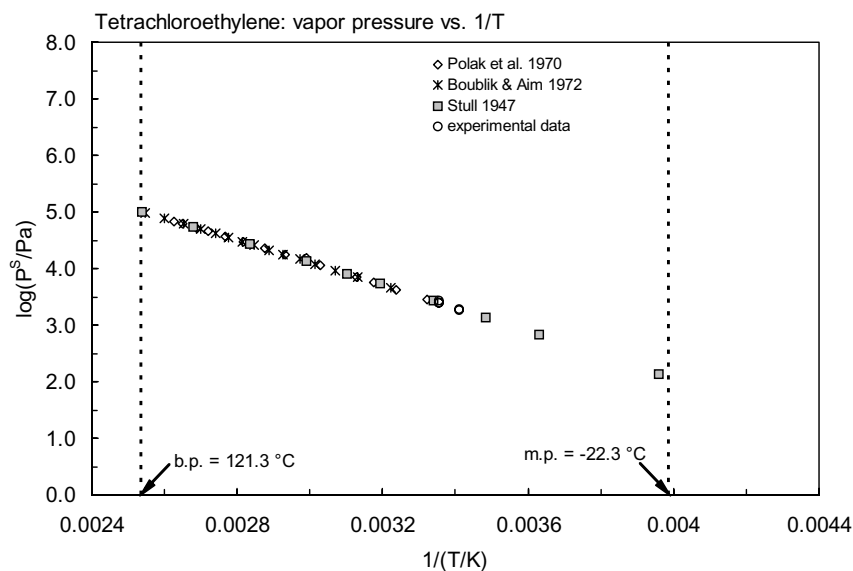


FIGURE 5.1.1.31.2 Logarithm of vapor pressure versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.3

Reported Henry's law constants of tetrachloroethylene 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)	$\log (k_H/\text{atm}) = A - B/(T/K)$	(3a)
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

1.

Leighton & Calo 1981		Gossett 1987		Tancredi & Yanagisawa 1990		Kolb et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		equilibrium headspace-GC	
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)
1.0	377.4	9.6	691	25	1363	40	1759
1.0	413.5	17.5	1186	26.5	1694	60	2080
1.2	430.6	24.8	1793	27.4	2224	70	3658
2.5	474.9	34.6	2857	28.9	2160	80	3375
7.0	572.9			28.9	2034		
10.0	675.2			29.7	2770	eq. 2	1/K <sub>AW</sub>
12.0	731.4	eq. 4	H/(atm m <sup>3</sup> /mol)	29.9	2998	A	-5.13
12.0	797.6	A	12.45	33.3	3057	B	-1736
12.9	826.0	B	4918	35.6	2413		
14.0	914.7			38.3	2745		
18.0	1122			40	4895		
18.0	1144	Ashworth et al. 1988		44.7	5549		
18.0	1145	EPICS-GC		45	6004		
19.0	1176	t/°C H/(Pa m <sup>3</sup> /mol)		47.2	5886		
19.2	1156						
19.5	1182	10	857.2	eq. 1a	K <sub>AW</sub>		

TABLE 5.1.1.31.3 (Continued)

Leighton & Calo 1981		Gossett 1987		Tancredi & Yanagisawa 1990		Kolb et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		equilibrium headspace-GC	
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)
24.3	1583	15	1125	A	7.481		
25.2	1623	20	1429	B	2279		
25.3	1651	25	1733				
26.0	1636	30	2482				
26.0	1712						
26.1	1679	eq. 4	H/(atm m <sup>3</sup> /mol)				
		A	10.65				
eq. 3	k <sub>H</sub> /atm	B	4368				
A	22.68						
B	4735						

2.

Robbins et al. 1993		Dewulf et al. 1995		Peng & Wan 1997		Knauss et al. 2000	
headspace-GC		EPICS-GC		equilibrium headspace-GC		calculated-P/C	
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)
25	1723	2.0	359.2	15	1016	22	1781
30	2340	6.0	2492	20	1272	51	5837
40	3070	10.0	602.7	25	1710	75	10328
45	2847	18.2	995.6	30	2160	101	18540
		25.0	1490	35	2713	124	19157
				40	3283	150	20200
		eq. 1	K <sub>AW</sub>	45	4108	161	19844
		A	14.655	eq. 3a	k <sub>H</sub> /atm		
		B	4528	A	9.06		
				B	1822		

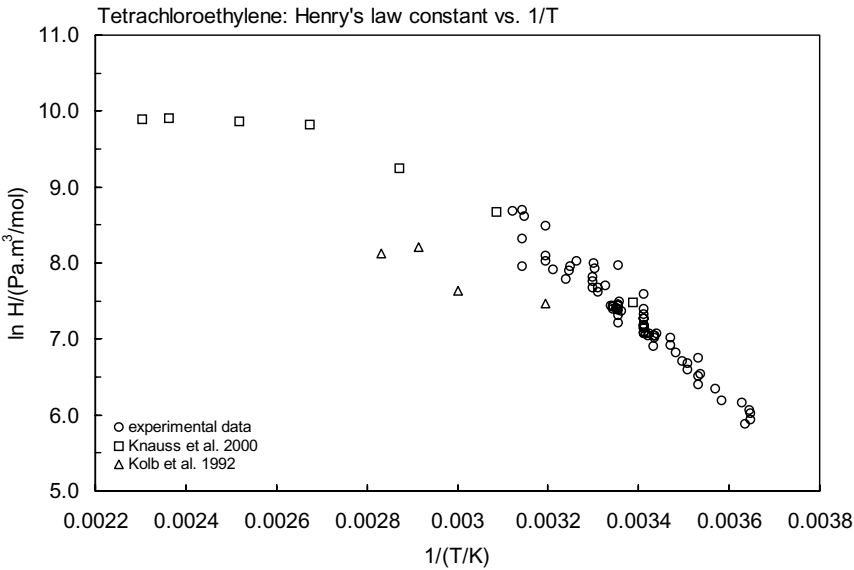


FIGURE 5.1.1.31.3 Logarithm of Henry's law constant versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.4

Reported octanol-water partition coefficients of tetrachloroethylene at various temperatures

Dewulf et al. 1999

EPICS-GC	
t/°C	log K <sub>OW</sub>
2.2	2.25
6.0	2.27
10.0	2.38
14.1	2.32
18.7	2.36
24.8	2.27

change in enthalpy:

$$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 2.6$$

(-11.1 to 16.3)

enthalpy of transfer

$$\Delta H_{\text{oct}}/(\text{kJ mol}^{-1}) = 4.7$$

(-9.0 to 18.4)

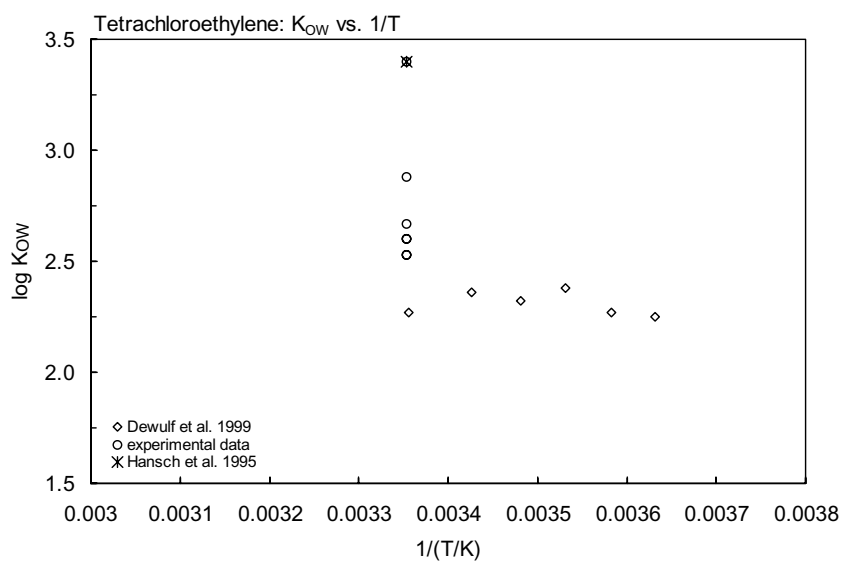
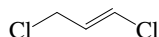


FIGURE 5.1.1.31.4 Logarithm of K<sub>OW</sub> versus reciprocal temperature for tetrachloroethylene.

## 5.1.1.32 1,3-Dichloropropene



Common Name: 1,3-Dichloropropene

Synonym: 1,3-dichloropropylene, 1,3-dichloro-1-propene, Telone II

Chemical Name: 1,3-dichloropropene

CAS Registry No: 542-75-6

Molecular Formula:  $C_3H_4Cl_2$ ,  $CH_2ClCH=CHCl$

Molecular Weight: 110.970

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

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

112.0 (*trans*-stereoisomer I, Horvath 1982; McNally & Grob 1984; Dean 1985; Lide 2003)

104.3 (*cis*-stereoisomer II, Horvath 1982; McNally & Grob 1984; Dean 1985; Lide 2003)

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

1.224 (*trans*-stereoisomer I, Horvath 1982; McNally & Grob 1984)

1.217 (*cis*-stereoisomer II, Horvath 1982; McNally & Grob 1984)

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

91.2 (*trans*-stereoisomer I,  $20^{\circ}C$ , calculated-density)

90.7 (*cis*-stereoisomer II,  $20^{\circ}C$ , calculated from density)

108.4 (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  $25^{\circ}C$ , F: 1.0

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

2800 (*trans*-stereoisomer I, Dilling 1977)

2700 (*cis*-stereoisomer II, Dilling 1977)

2723 (recommended, Horvath 1982)

1071 (*trans*-stereoisomer I, headspace-GC, McNally & Grob 1983)

1088 (*cis*-stereoisomer II, headspace-GC, McNally & Grob 1983)

1020 ( $30^{\circ}C$ , *trans*-stereoisomer I, headspace-GC, McNally & Grob 1984)

911 ( $30^{\circ}C$ , *cis*-stereoisomer II, headspace-GC, McNally & Grob 1984)

1000 ( $20^{\circ}C$ , Wauchope et al. 1992)

2250 (Wauchope et al. 1992)

4533, 4311, 4223 ( $20, 30, 40^{\circ}C$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated):

4533, 5733 (*trans*-, *cis*-stereoisomer, data from Dow Chemicals, Dilling 1977)

435, 569 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

3333 ( $20^{\circ}C$ , selected, Mills et al. 1982)

3334 ( $20^{\circ}C$ , quoted, Warner et al. 1987)

3866 ( $20^{\circ}C$ , Wauchope et al. 1992)

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

232 (calculated-P/C, Dilling 1977)

137 (calculated-P/C, Warner et al. 1987)

122, 198, 302 ( $20, 30, 40^{\circ}C$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

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

1.98 (selected, Mills et al. 1982)

1.41 (quoted, Verhaar et al. 1992)

1.84 (*cis/trans*, calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

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

1.505 (soil, selected, Wauchope et al. 1992)

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

Volatilization:  $t_{1/2} = 31$  min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975)

$t_{1/2}(\text{exptl}) = 29.6$  min,  $t_{1/2}(\text{calc}) = 2.4$  min, 23.8 min for *cis*-stereoisomer, and  $t_{1/2}(\text{calc}) = 3.2$  min, 24.6 min for *trans*-stereoisomer from water (Dilling 1977)

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:

$k_{OH} = (7.74 \pm 0.2) \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> *cis*-isomer,  $k_{OH} = (1.31 \pm 0.05) \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for *trans*-isomer at  $22 \pm 2^\circ\text{C}$ , calculated  $t_{1/2} = 12$  h and 7 h for the *cis*- and *trans*-isomer, respectively (relative rate method, Tuazon et al. 1984)

$k_{O_3} = 1.5 \times 10^{-19}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> *cis*-isomer,  $k_{O_3} = 6.7 \times 10^{-19}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for *trans*-isomer at room temp., calculated  $t_{1/2} = 52$  d and 12 d for *cis*- and *trans*-isomer, respectively (relative rate method, Tuazon et al. 1984)

$k_{OH}(\text{calc}) = 1.1 \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}(\text{obs.}) = 7.5 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for *cis*-isomer;  $k_{OH}(\text{calc}) = 1.3 \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}(\text{obs.}) = 1.26 \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for *trans*-isomer at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH}(\text{calc}) = 8.8 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}(\text{obs.}) = 8.45 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for *cis*-isomer;  $k_{OH}(\text{calc}) = 10.0 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}(\text{obs.}) = 14.4 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for *trans*-isomer at room temp. (SAR [structure-activity relationship], Atkinson 1987)

Hydrolysis:  $t_{1/2} = 133$ –271 h, based on measured rate constants for hydrolysis at pH 7 and  $25^\circ\text{C}$  (Mill et al. 1985; quoted, Howard et al. 1991) and pH 5 and  $20^\circ\text{C}$  (McCall 1987; quoted, Howard et al. 1991); rate of hydrolysis is, however, independent of pH over the range of pH 5 to pH 10 (McCall 1987).

Biodegradation: aqueous aerobic  $t_{1/2} = 168$ –672 h, based on unacclimated aqueous aerobic biodegradation screening studies (Tabak et al. 1981; Krijgheld & Van der Gen 1986; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 672$ –2688 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 or Half-Lives:

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 0.24$ –2.4 h from air for the reaction with OH radicals (Darnall et al. 1976);

$t_{1/2}(\text{calc}) = 12$  h and 7 h for the *cis*- and *trans*-isomer, respectively, for reactions with OH radical;  $t_{1/2}(\text{calc}) = 52$  d and 12 d for *cis*- and *trans*-isomer, respectively, for reactions with  $O_3$  at room temp. (Tuazon et al. 1984).

$t_{1/2} = 4.66$ –80.3 h, based on measured rate constants for reaction with OH radical and ozone (Howard et al. 1991)

Surface water:  $t_{1/2} = 133$ –271 h, based on measured rate of hydrolysis at pH 7 and  $25^\circ\text{C}$  (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and  $20^\circ\text{C}$  (McCall 1987; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 133$ –271 h, based on measured rate of hydrolysis at pH 7 and  $25^\circ\text{C}$  (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and  $20^\circ\text{C}$  (McCall 1987; quoted, Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 133$ –271 h, based on measured rate of hydrolysis at pH 7 and  $25^\circ\text{C}$  (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and  $20^\circ\text{C}$  (McCall 1987; quoted, Howard et al. 1991).

Biota:



## 5.1.1.33 Chloroprene



Common Name: Chloroprene

Synonym: 2-chloro-1,3-butadiene

Chemical Name: 2-chloro-1,3-butadiene

CAS Registry No: 126-99-8

Molecular Formula:  $C_4H_5Cl$ ,  $CH_2=CClCH=CH_2$

Molecular Weight: 88.536

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

-130 (Kirk-Othmer 1985; Verschueren 1983; Stephenson & Malanowski 1987; Lide 2003)

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

59.4 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

69.145 (Boublik et al. 1984)

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

0.9583 (Weast 1982–83; Dean 1985)

0.9580 (Verschueren 1983)

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

92.4 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

102.3 (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  $25^{\circ}C$ , F: 1.0

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

964000 ( $20^{\circ}C$ , saturation concentration, Verschueren 1983)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

26660, 36660 ( $20^{\circ}C$ ,  $30^{\circ}C$ , Verschueren 1983)

28740 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.30955 - 793.85/(181.137 + t/^{\circ}C)$ , temp range:  $20$ – $60^{\circ}C$  (Antoine eq. from reported exptl. data Boublik et al. 1984)

28780 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.16150 - 783.45/(197.7 + t/^{\circ}C)$ ; temp range  $20$ – $60^{\circ}C$  (Antoine eq., Dean 1985, 1992)

29450 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.652 - 1545.3/(T/K)$ ; temp range:  $279$ – $333\ K$  (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.6519 - 1545.0/(T/K)$ ; temp range  $243$ – $263\ K$  (Antoine eq.-II, Stephenson & Malanowski 1987)

23200 (quoted, Howard 1989)

$\log(P/mmHg) = 8.9353 - 1.9176 \times 10^3/(T/K) + 0.73836 \cdot \log(T/K) - 8.4743 \times 10^{-3} \cdot (T/K) + 6.0224 \times 10^{-6} \cdot (T/K)^2$ ; temp range  $143$ – $525\ K$  (vapor pressure eq., Yaws 1994)

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

3242 (estimated by bond contribution method, Howard 1989)

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

2.03 (Howard 1989)

Bioconcentration Factor,  $\log BCF$ :

1.342 (estimated- $K_{ow}$ , Lyman et al. 1982; quoted, Howard 1989)

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

2.498 (soil, estimated- $K_{ow}$ , Lyman et al. 1982)

1.699 (soil, molecular topology and QSAR, Sabljic 1984)

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

Volatilization:  $t_{1/2} \sim 3$  h from a model river 1 m deep with a current velocity of 1 m/s and a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 2.9$ –27.8 h, based on estimated rate constants for the reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 672$ –4320 h, based on aqueous aerobic screening test data for vinyl chloride (Helfgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2688$ –17280 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 or Half-Lives:

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 0.24$ –2.4 h from air for the reaction with OH radicals (Darnall et al. 1976);

$t_{1/2} = 1.8$  h for the reaction with photochemically produced hydroxyl radicals and  $t_{1/2} = 12$  h for the reaction with ozone in atmosphere (Cupitt 1980; quoted, Howard 1989);

$t_{1/2} = 2.9$ –27.8 h, based on estimated rate constants for reaction with hydroxyl radicals and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Surface water: estimated  $t_{1/2} = 6.7$ –53 d in surface waters at various locations in case of a first order reduction process; and  $t_{1/2} = 3$ –30 d in rivers,  $t_{1/2} = 30$ –300 d in lakes and ground waters (Zoeteman et al. 1980)

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

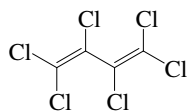
Ground water:  $t_{1/2} = 1344$ –8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

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

Biota:

## 5.1.1.34 Hexachlorobutadiene



Common Name: Hexachlorobutadiene

Synonym: HCBd, perchloro-1,3-butadiene

Chemical Name: 1,1,2,3,4,4-hexachloro-1,3-butadiene

CAS Registry No: 87-68-3

Molecular Formula:  $C_4Cl_6$ ,  $Cl_2C=CClClC=CCl_2$

Molecular Weight: 260.761

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

-21.0 (Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)

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

215 (Horvath 1982; Lide 2003)

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

1.682 (Horvath 1982)

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

155.2 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

206.8 (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  $25^{\circ}C$ , F: 1.0

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

0.20 (Melnikov 1971)

2.00 ( $20^{\circ}C$ , Pearson & McConnell 1975)

3.23 (shake flask-HPLC, Banerjee et al. 1980)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

20.0 ( $20^{\circ}C$ , Pearson & McConnell 1975)

$\log(P/kPa) = 6.06503 - 1520.873/(163.685 + t/^{\circ}C)$ ; temp range  $70$ – $200^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.4781 - 1783.8/(-84.48 + T/K)$ ; temp range  $343$ – $484\ K$  (Antoine eq., Stephenson & Malanowski 1987)

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

2604 (calculated-P/C, Warner et al. 1987)

1044 (batch stripping, Warner et al. 1987)

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

4.74 (HPLC-RT correlation, Konemann et al. 1979)

4.78 (shake flask-HPLC, Banerjee et al. 1980)

4.63 (calculated-fragment const., Könemann 1981)

4.90 (shake flask-GC, both phases, Chiou 1985)

4.78 (recommended, Sangster 1993)

4.78 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

4.70 (Thomann 1989)

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

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

Volatilization:

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 2965\text{--}28650$  h, based on an estimated rate constant for vapor phase reaction with OH radicals (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: no hydrolyzable groups, rate constant at pH 7 is zero (Kollig et al. 1987).

Biodegradation: aqueous aerobic  $t_{1/2} = 672\text{--}4320$  h, based on monitoring data and acclimated aqueous screen test data (Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2688\text{--}17280$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: tropospheric  $t_{1/2} \sim 1.0$  wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

$t_{1/2} = 2865\text{--}28650$  h, based on estimated photooxidation half-life in air (Howard et al. 1991).

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

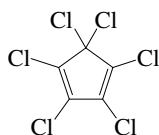
Ground water:  $t_{1/2} = 1344\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

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

Biota:

## 5.1.1.35 Hexachlorocyclopentadiene



Common Name: Hexachlorocyclopentadiene

Synonym: 1,2,3,4,5,5-hexachlorocyclopentadiene, perchlorocyclopentadiene, HCCPD

Chemical Name: 1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene

CAS Registry No: 77-47-4

Molecular Formula:  $C_5Cl_6$

Molecular Weight: 272.772

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

-9 (Lide 2003)

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

239 (Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ): 1.702

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

160.3 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

210.1 (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  $25^{\circ}C$ , F: 1.0

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

0.805 (Shake flask-LSC Lu et al. 1974)

1.80 (Zepp et al. 1979)

0.805 (Callahan et al. 1979; Dobbs et al. 1980; Geyer et al. 1981; Warner et al. 1987; Isnard & Lambert 1988)

1.80 ( $28^{\circ}C$ , vapor saturation or shake flask-GC, Wolfe et al. 1982)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

10.84 (Verschuereen 1977; Warner et al. 1987)

10.67 (Wolfe et al. 1982)

11.90 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.4813 - 2804.32/(T/K)$ ; temp range 335–512 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -9.7942 - 3.3161 \times 10^3/(T/K) + 10.171 \cdot \log(T/K) - 2.1115 \times 10^{-2} \cdot (T/K) + 9.2045 \times 10^{-6} \cdot (T/K)^2$ ; temp range 284–746 K (vapor pressure eq., Yaws 1994)

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

2736 (concentration ratio-GC, Wolfe et al. 1982)

1662 (batch stripping; Warner et al. 1987)

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

5.04 (HPLC-RT correlation, McDuffie 1981)

5.04 ( $28^{\circ}C$ , concentration ratio-GC, Wolfe et al. 1982)

5.26 (HPLC-RT correlation, Eadsforth 1986)

5.04 (recommended, Sangster 1993)

5.04 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

2.53, 2.97, 3.21, 2.65 (algae, snail, mosquito, fish, Lu et al. 1975)

1.47 (fathead minnow, Veith et al. 1979)

3.04, 3.21 (*Chlorella*, calculated-solubility, Geyer et al. 1981)

- 1.47, 4.19 (quoted, calculated- $K_{OW}$ , Mackay 1982)  
 3.18, 3.89 (estimated-S and  $K_{OW}$ , Isnard & Lambert 1988)

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

- 4.08 (sediment organic carbon, calculated- $K_{OW}$ , Wolfe et al. 1982)

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

Volatilization: appears to be important in flowing waters (Callahan et al. 1979).

Photolysis: near-surface photolysis is an important process with a rate constant  $k = 4.9 \text{ d}^{-1}$  with  $t_{1/2} = 11 \text{ min}$  (Callahan et al. 1979);

direct photolysis in natural waters in midday sunlight of Athens, Georgia at latitude  $34^\circ\text{N}$  and  $83^\circ\text{W}$  with  $t_{1/2} < 10 \text{ min}$ , and near-surface photolysis rate constant  $k(\text{calc}) = 3.9 \text{ h}^{-1}$  on cloudless days averaged over both light and dark periods for a year (Wolfe et al. 1982);

photolysis  $t_{1/2} = 1.0 \text{ min}$  to  $10.7 \text{ min}$ , based on photolysis studies in aqueous solutions (Butz et al. 1982; Wolfe et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation  $t_{1/2} = 1.0$  to  $8.9 \text{ h}$ , based on calculated rate constants for the vapor phase reactions with OH radicals and  $\text{O}_3$  in air (Cupitt 1980; quoted, Howard et al. 1991).

Hydrolysis: appears to be an important fate process with a rate constant  $k = 5.6 \times 10^{-7} \text{ s}^{-1}$  at  $25^\circ\text{C}$  with  $t_{1/2} = 14 \text{ d}$  (Callahan et al. 1979);

reaction rate constant was independent of pH range of about 3 to 10 under most environmental conditions and an extrapolated rate constant  $k = 4 \times 10^{-3} \text{ s}^{-1}$  was found at  $25^\circ\text{C}$  with  $t_{1/2} = 173 \text{ h}$  (Wolfe et al. 1982; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic  $t_{1/2} = 168$  to  $672 \text{ h}$ , based on aerobic aqueous screening test data (Tabak et al. 1981; Freitag et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 672$  to  $2688 \text{ h}$ , based on aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 1.0$  to  $8.9 \text{ h}$ , based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water:  $t_{1/2} = 1.0 \text{ min}$  to  $173 \text{ h}$ , based on photolysis and hydrolysis half-lives (Howard et al. 1991); measured rate constant  $k = (90 \pm 40) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $25 \pm 2^\circ\text{C}$ , with  $t_{1/2} = 6 \text{ min}$  at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 173$  to  $1344 \text{ h}$ , based on aerobic aqueous biodegradation and hydrolysis half-lives (Howard et al. 1991).

Sediment: hydrolysis rate constant in the sediment was assumed to be the same as that of water and decay rate constant  $k = 1.5$  to  $5.4 \times 10^{-5} \text{ s}^{-1}$  for natural pond sediment-water system (Wolfe et al. 1982).

Soil:  $t_{1/2} = 168$  to  $672 \text{ h}$ , based on aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota:

## 5.1.2 BROMOALKANES AND BROMOALKENES

## 5.1.2.1 Bromomethane



Common Name: Methyl bromide

Synonym: bromomethane, monobromomethane, Embafume, Terabol

Chemical Name: bromomethane, methyl bromide

CAS Registry No: 74-83-9

Molecular Formula:  $\text{CH}_3\text{Br}$

Molecular Weight: 94.939

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

−93.68 (Lide 2003)

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

3.5 (Lide 2003)

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

1.6755, 1.6617 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Dreisbach 1961)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

56.7 ( $20^{\circ}\text{C}$ , calculated-density)

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

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

23.26, 24.098 ( $25^{\circ}\text{C}$ , at bp, Riddick et al. 1986)

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  $25^{\circ}\text{C}$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

13410\* (vapor saturation-gravitational method, measured range  $10$ – $32^{\circ}\text{C}$ , Haight 1951)

20700, 24140 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , gravitational method, Glew & Moelwyn-Hughes 1953)

14400 (Irmann 1965; Hine & Mookerjee 1975)

13400 (Jolles 1966; Günther et al. 1968)

12930 (Korenman et al. 1971)

900 ( $20^{\circ}\text{C}$ , Verschueren 1977, 1983)

15223\* (summary of literature data, temp range  $5$ – $80^{\circ}\text{C}$ , Horvath 1982)

17500 ( $20^{\circ}\text{C}$ , Windholz et al. 1983)

Vapor Pressure (Pa at  $25^{\circ}\text{C}$  and reported temperature dependence equations):

256550 (interpolated-Antoine eq. regression, temp range  $-96.3$  to  $3.6^{\circ}\text{C}$ , Stull 1947)

217700 (calculated-Antoine eq., Dreisbach 1959, 1961)

$\log(P/\text{mmHg}) = 6.95965 - 986.59/(238.32 + t/^{\circ}\text{C})$ ; temp range  $-58$  to  $53^{\circ}\text{C}$  (Antoine eq. for liquid state, Dreisbach 1959, 1961)

$\log(P/\text{mmHg}) = 6.95965 - 986.590/(238.32 + t/^{\circ}\text{C})$ ; pressure range of  $10$  to  $1500$  mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

183900 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 5925.9/(T/\text{K})] + 7.482362$ ; temp range  $-96.3$  to  $190^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)

218930 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 7.08823 - 1044.42/(244.684 + t/^{\circ}\text{C})$  (Antoine eq., Kudchadker et al. 1979)

187000 ( $20^{\circ}\text{C}$ , Thomas 1982)

216900, 219000 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.20369 - 1041.723/(244.36 + t/^{\circ}\text{C})$ ; temp range  $-69.9$  to  $4.5^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.2243 - 1049.898/(245.319 + t/^{\circ}\text{C})$ ; temp range  $-70$  to  $3.6^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.21313 - 1044.42/(224.684 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
217680 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.08455 - 986.59/(-34.83 + T/\text{K})$ ; temp range 201–296 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 29.3988 - 2.0406 \times 10^3/(T/\text{K}) - 7.9966 \cdot \log (T/\text{K}) - 4.1899 \times 10^{-10} \cdot (T/\text{K}) + 5.0174 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
temp range 179–467 K (vapor pressure eq., Yaws 1994)

218630 (selected and summary of literature data, temp range 179.48–318.15 K, Xiang 2002)

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

631\*; 621 (exptl.-concn ratio, measured range  $5$ – $80^{\circ}\text{C}$ ; calculated-P/C, Glew & Moelwyn-Hughes 1953)

$\log \{H/(\text{mmHg} \cdot \text{L/mol})\} = 73.022 - 22.261 \cdot \log (T/\text{K}) - 4254.8/(T/\text{K})$ ; temp range 278.16–253.16 K (Glew & Moelwyn-Hughes 1953)

733\* ( $29.43^{\circ}\text{C}$ , concentration ratio, measured range  $29.44$ – $49.59^{\circ}\text{C}$ , Swain & Thornton 1962)

652 (calculated as  $1/K_{\text{AW}} C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)

533 ( $20^{\circ}\text{C}$ , calculated-P/C, Mackay & Shiu 1981)

19958 ( $20^{\circ}\text{C}$ , calculated-P/C, Mabey et al. 1982)

1317 (calculated-P/C, Thomas 1982)

20260 ( $20$ – $25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

10690 (calculated-P/C, Mackay & Shiu 1990)

687.4 (computed value, Yaws et al. 1991)

204, 515 ( $0$ ,  $22^{\circ}\text{C}$ , distilled water, headspace-GC, Elliott & Rowland 1993)

596\* (gas-liquid equilibrator-GC, measured range  $1.1$ – $30.5^{\circ}\text{C}$ , De Bruyn & Saltzman 1997)

490 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 3.468 - 1221/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

1.19 (shake flask-GC, Leo et al. 1975)

1.19 (Hansch & Leo 1979; Hansch & Leo 1985)

1.19 (recommended, Sangster 1989)

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

2.11 (calculated-infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

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

0.623 (microorganisms-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)

0.672 (calculated- $K_{\text{OW}}$ , Lyman et al. 1982)

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

2.236, 2.241, 2.215 (Naaldwijk loamy sand, Aalsmeer loam, Boskoop peaty clay, Howard 1989)

0.771 (sediment-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)

2.10 (calculated-S, Lyman et al. 1982)

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

Volatilization: estimated experimental  $t_{1/2} = 27$  min 1 mg/L when stirred at 200 rpm in water at approximately  $25^{\circ}\text{C}$  in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979);

$t_{1/2} \sim 30$  min (Mills et al. 1982);

$t_{1/2} = 3.0$  h in a model river (estimated, Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} \sim 0.2$  and  $0.5$  d for the volatilization from 1 and 10 cm of soil, respectively (Jury et al. 1984; quoted, Howard 1989).

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:

$k_{OH}^* = (4.14 \pm 0.43) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 245–375 K with lifetime of 1.32 yr in the troposphere (flash photolysis-RF, Davis et al. 1976)

$k_{OH} = 3.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow system, Howard & Evenson 1976)

$k_{OH} = 4.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , residence time of 289 d, loss of 0.4% in one day or 12 sunlit hour at 300 K (Singh et al. 1981)

$k_{OH} = 2.4 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at 300 K (estimated, Lyman 1982)

$k_{OH}^* = 3.93 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 0.1 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation  $t_{1/2} = 1633\text{--}16327 \text{ h}$  in air, based on measured rates for reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: first-order  $k = 4.0 \times 10^{-7} \text{ s}^{-1}$  with a maximum  $t_{1/2} = 20 \text{ d}$  at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979);

$k = 4.09 \times 10^{-7} \text{ s}^{-1}$  with  $t_{1/2} = 20 \text{ d}$  at pH 7 and 25°C (Mabey & Mill 1978)

$t_{1/2} = 470\text{--}912 \text{ h}$ , based on measured first-order hydrolysis rate constants (Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard 1989; Howard et al. 1991);

$k = 1.44 \times 10^{-3} \text{ h}^{-1}$  at pH 7 and 25°C (Callahan et al. 1979; quoted, Mabey et al. 1982)

$k = 3 \times 10^{-7} \text{ s}^{-1}$  at 25°C with  $t_{1/2} = 26.7 \text{ d}$  (Castro & Belser 1981; quoted, Howard 1989).

Biodegradation: aerobic  $t_{1/2}(\text{aq.}) = 168\text{--}672 \text{ h}$ , based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991);

anaerobic  $t_{1/2}(\text{aq.}) = 672\text{--}2688 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Tabak et al. 1981; quoted, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

lifetime of 3.8 yr in the troposphere (Altshuller 1980);

$t_{1/2} = 0.29 \text{ y}$  in the atmosphere for the reaction with  $2 \times 10^6 \text{ OH radicals/cm}^3$  at 25°C (Dilling 1982; quoted, Howard 1989);

$t_{1/2} = 289 \text{ d}$  estimated as toxic chemical residence time with rate constant of  $4 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction with OH radicals at 300 K (Singh et al. 1980,1981; quoted, Howard 1989);

$t_{1/2} = 1633\text{--}16327 \text{ h}$ , based on measured rates for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 20 \text{ d}$  at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2} = 168\text{--}672 \text{ h}$ , based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 336\text{--}912 \text{ h}$ , based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic waste water inoculum and hydrolysis half-life (Tabak et al. 1981; Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 168\text{--}672 \text{ h}$ , based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Biota:

**TABLE 5.1.2.1.1****Reported aqueous solubilities of bromomethane at various temperatures**

$$S/(\text{wt}\%) = 1.4019 - 6.3562 \times 10^{-2} \cdot (t/^{\circ}\text{C}) + 1.71977 \times 10^{-3} \cdot (t/^{\circ}\text{C})^2 - 2.8262 \times 10^{-5} \cdot (t/^{\circ}\text{C})^3 \\ + 2.5268 \times 10^{-7} \cdot (t/^{\circ}\text{C})^4 - 9.3470 \times 10^{-10} \cdot (t/^{\circ}\text{C})^5 \quad (1)$$

Haight 1951		Horvath 1982	
gravitational method		summary of literature data	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
10	26790	5	35000
17	18300	10	27997
25	13410	20	18401
32	11490	25	15223
		30	12804
		40	9517
		50	7430
		60	5919
		70	4757
		eq. 1	S/wt%

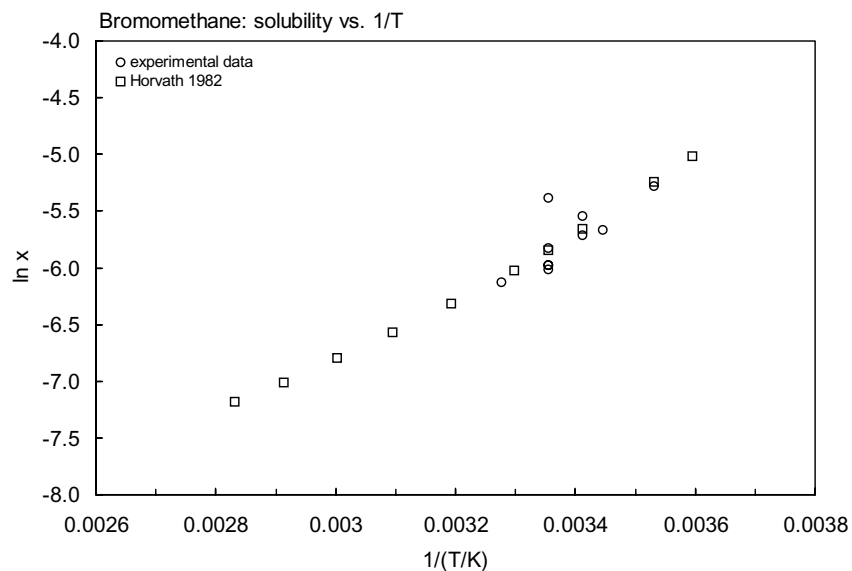
**FIGURE 5.1.2.1.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for bromomethane.

TABLE 5.1.2.1.2  
Reported Henry’s law constants of bromomethane 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)			
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
$\log H = A - B \cdot \log (T/K) - C/(T/K)$		(6)			
Glew & Moelwyn-Hughes 1953		Swain & Thornton 1962	De Bruyn & Saltzman 1997		
concentration ratio		concentration ratio	gas-liquid membrane equilibrators-GC		
t/°C	H/(Pa m³/mol)	t/°C H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	
				pure water	seawater 35‰ NaCl
5.0	276	29.43 729	1.1	205.5	253.9 255.2
10.0	340	29.43 733	5.0	261.8	321.7 320.6
14.98	427	29.44 744	10.0	334.4	424.0 417.0
20.0	532	40.35 980	13.4	380.9	471.3 460.6
24.97	631	40.35 992	18.0	440.5	536.1 -
30.0	744	40.35 1005	19.4	458.5	- 539.0
40.05	1005	49.59 1253	21.2	494.3	- 566.1
50.04	1301		25.0	596.0	708.6 666.1
60.03	1653		30.5	666.6	810.6 761.8
70.0	1987				
80.0	2400				
25.0	622				
eq 6	P/(mmHg·L/mol)				
A	73.022				
B	22.261				
C	4254.8				

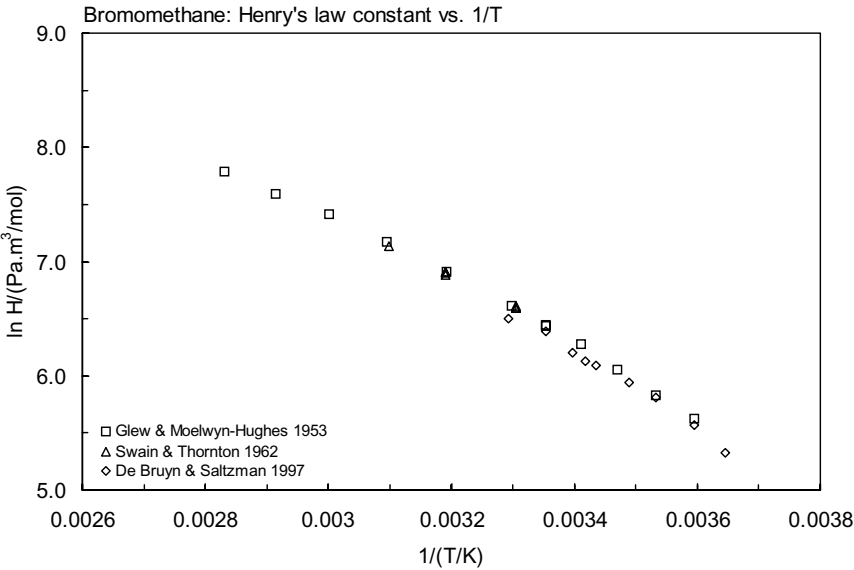
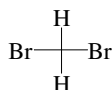


FIGURE 5.1.2.1.2 Logarithm of Henry’s law constant versus reciprocal temperature for bromomethane.

## 5.1.2.2 Dibromomethane



Common Name: Dibromomethane

Synonym: methylene bromide

Chemical Name: dibromomethane, methylene bromide

CAS Registry No: 74-95-3

Molecular Formula:  $\text{CH}_2\text{Br}_2$

Molecular Weight: 173.835

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

-52.5 (Weast 1982-83; Lide 2003)

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

97.0 (Horvath 1982; Weast 1982-83; Lide 2003)

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

2.4970, 2.4842 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Dreisbach 1961)

2.4970 (Horvath 1982; Weast 1982-83)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

70.1 (Stephenson & Malanowski 1987)

76.2 (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  $25^{\circ}\text{C}$ , F: 1.0

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

11480\* ( $20^{\circ}\text{C}$ , volumetric method, measured range  $0$ – $30^{\circ}\text{C}$ , Rex 1906)

11700, 11930 ( $15^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , shake flask-interferometer, Gross & Saylor 1931)

11486 (Seidell 1940; quoted, Deno & Berkheimer 1960)

17500 (shake flask-residue volume method, Booth & Everson 1948)

11000 (O'Connell 1963; Jolles 1966)

11442\* (summary of literature data, Horvath 1982)

11500 (Dean 1985)

12800\*, 11400 ( $19.3^{\circ}\text{C}$ ,  $29.5^{\circ}\text{C}$ , shake flask-GC/TC, measured range  $0$ – $90.1^{\circ}\text{C}$ , Stephenson 1992)

11420, 12030, 12270, 12580 ( $20$ ,  $30$ ,  $35$ ,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)

11114, 12060, 13052 ( $20$ ,  $30$ ,  $40^{\circ}\text{C}$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

12300 ( $20^{\circ}\text{C}$ , limiting activity coeff.  $\gamma^{\infty}$  by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

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

4626, 7518 ( $20^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , Rex 1906)

5775\* (Antoine eq. regression, temp range  $-35.1$  to  $98.6^{\circ}\text{C}$ , Stull 1947)

6034 (calculated by formula, Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.0625 - 1327.8/(220.58 + t/^{\circ}\text{C})$ ; temp range  $17$ – $236^{\circ}\text{C}$  (Antoine eq. for liquid state, Dreisbach 1961)

5767 (calculated-Antoine eq., Weast 1972-73)

$\log(P/\text{mmHg}) = [-0.2185 \times 8722.0/(T/\text{K})] + 8.028019$ ; temp range  $-35.1$  to  $98.6^{\circ}\text{C}$  (Antoine eq., Weast 1972-73)

5922 (Antoine eq. regression, Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 7.82594 - 1784.9/(263.73 + t/^{\circ}\text{C})$  (Antoine eq., Kudchadker et al. 1979)

6034 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.1874 - 1327.8/(-52.57 + T/\text{K})$ ; temp range  $290$ – $409$  K (Antoine eq., Stephenson & Malanowski 1987)

4650, 7730, 9840, 12383 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)  
 $\log(P/\text{mmHg}) = 35.3525 - 3.0445 \times 10^3/(T/K) - 9.5792 \cdot \log(T/K) + 5.8258 \times 10^{-10} \cdot (T/K) + 2.9443 \times 10^{-6} \cdot (T/K)^2$ ;  
 temp range 221–611 K (vapor pressure eq., Yaws 1994)  
 6084.6 (selected and summary of literature data, temp range 220.61–413.15 K, Xiang 2002)

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

90.0 (calculated- $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)  
 73.16 (calculated-bond method, Hine & Mookerjee 1975)  
 86.13 (batch stripping-GC, Nicholson et al. 1984)  
 86.03 (Munz & Roberts 1989)  
 70.9, 111.5, 142, 172 (20, 30, 35, 40°C, infinite dilution activity coeff.  $\gamma^\infty$ -GC, Tse et al. 1992)  
 72.7, 141, 252 (20, 30, 40°C, activity coeff.  $\gamma^\infty$ -differential pressure transducer, Wright et al. 1992)  
 281, 513 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 25.4, 48.3, 81.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)  
 $\ln K_{AW} = 11.70 - 4418/(T/K)$ ; seawater of salinity of 30.4‰, temp range 0–20°C (Moore et al. 1995)  
 66.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 68.94 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C or as indicated:

2.50 (Hansch et al. 1968)  
 1.70 (recommended, Sangster 1993)  
 1.70 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)  
 1.70, 1.65, 1.64 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)  
 1.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

3.07 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

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

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

Volatilization:

Photolysis: photocatalyzed mineralization by the presence of  $\text{TiO}_2$  with the rate of 4.1 ppm/min-g of catalyst (Ollis 1985).

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:

$k(\text{aq.}) = (6.1 \pm 0.61) \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$  was measured in 66.7% dioxane-water at 35.7°C (Hine et al. 1956; quoted, Roberts et al. 1992)

$k_{OH} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and estimated residence time of 46 d at 300 K (Singh et al. 1980)

$k_{OH} = 5 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , estimated at 300 K (Lyman 1982)

$k(\text{aq.}) = 4.0 \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with OH radical in aqueous solution with reference to  $\text{CH}_3\text{CCl}_3$  (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{O_3}(\text{aq.}) \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 21°C, with  $t_{1/2} \geq 80$  d at pH 7 (Yao & Haag 1991).

$k_{OH}(\text{aq.}) = (9.0 \pm 3.0) \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

Hydrolysis: rate constant  $k = 1.2 \times 10^{-10} \text{ s}^{-1}$  with  $t_{1/2} = 183$  yr at pH 7 and 25°C (Mabey & Mill 1978)

$t_{1/2} = 183$  yr at pH 7 and 25°C, based on overall hydrolysis rate constant (Mill et al. 1982; quoted, Howard et al. 1991).

Biodegradation:

$k = 2.1 \times 10^{-4} \text{ min}^{-1}$  with  $t_{1/2} = 24$  min in anoxic sediment-water suspension (Jafvert & Wolfe 1987)

$t_{1/2}$ (aq. aerobic) = 168–672 h, based on unacclimated aerobic screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 672–2688 h, based on unacclimated aqueous aerobic half-life (Howard et al. 1991).

Biotransformation:

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

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2}$  = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

estimated as toxic chemical residence time of 46 d with rate constant of  $2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction with OH radical at 300 K (Singh et al. 1980);

photooxidation  $t_{1/2}$  = 851–8510 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2}$  = 183 yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2}$  = 55 h in anoxic sediment-water suspension (Jafvert & Wolfe 1987);

$t_{1/2}$  = 168–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured  $k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and 21°C, with  $t_{1/2} \geq 80 \text{ d}$  at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2}$  = 336–1344 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:  $t_{1/2}$  = 55 h in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

Soil:  $t_{1/2}$  = 168–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

**TABLE 5.1.2.2.1**

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

$$S/(\text{wt}\%) = 1.1594 - 4.3267 \times 10^{-3} \cdot (t/^\circ\text{C}) + 1.8201 \times 10^{-4} \cdot (t/^\circ\text{C})^2 - 1.3335 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

1.

Rex 1906		Horvath 1982		Stephenson 1992		Tse et al. 1992	
volumetric method		summary of literature data		shake flask-GC		activity coefficient	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	11730	5	11594	0	11700	20	11420
10	11460	10	11330	9.7	11300	30	12030
20	11480	20	11350	19.3	12800	35	12270
30	11760	25	11442	29.5	11400	40	12580
		30	11574	39.5	12000		
				49.5	12700		
				59.9	13600		
				69.9	13600		
				79.8	16100		
				90.1	15100		
Gross & Saylor 1931						Wright et al. 1992	
shake flask-interferometer						activity coefficient	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$					$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
15	11700					20	11114
30	11930					30	12060
						40	13052

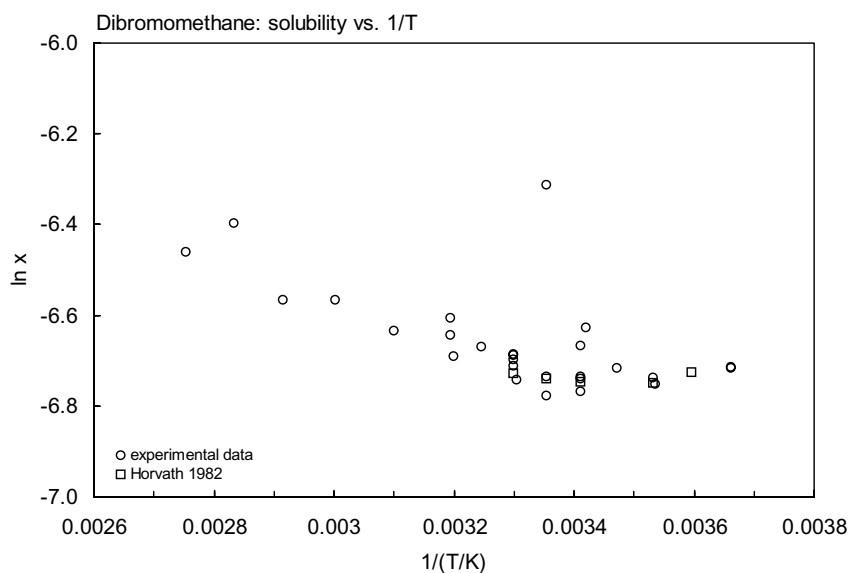


FIGURE 5.1.2.2.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for dibromomethane.

TABLE 5.1.2.2.2

Reported vapor pressures of dibromomethane at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
-35.1	133.3
-13.2	666.6
-2.40	1333
9.70	2666
23.3	5333
31.6	7999
42.3	13332
58.5	26664
79.0	53329
98.6	101325
mp/°C	-52.8

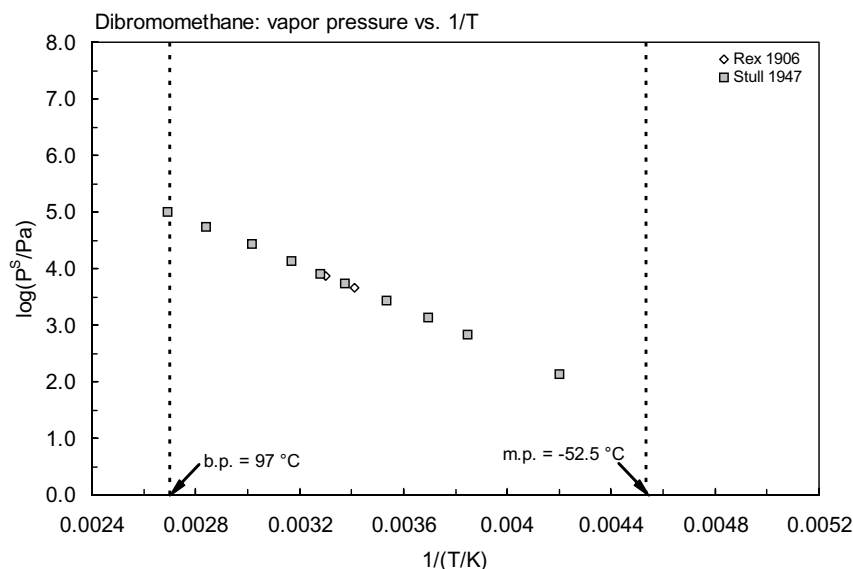


FIGURE 5.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for dibromomethane.

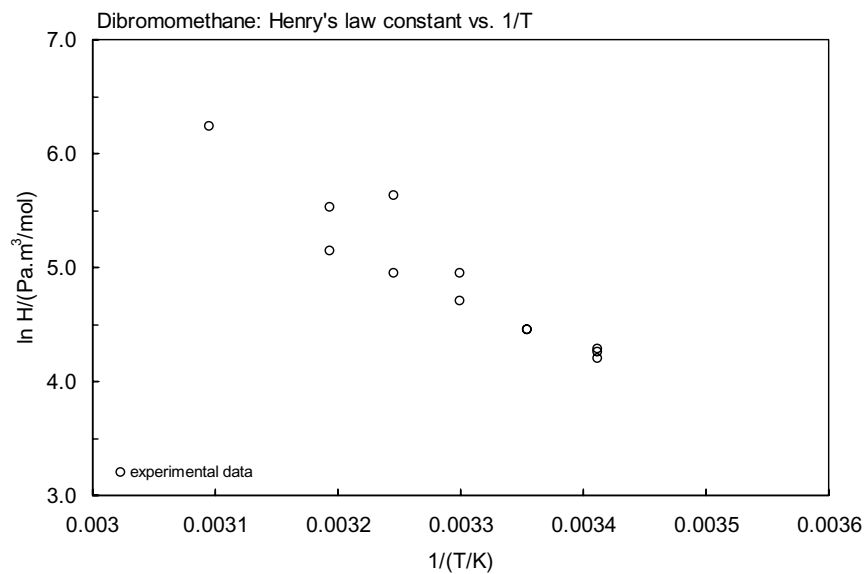
TABLE 5.1.2.2.3

Reported Henry's law constants of dibromomethane 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

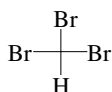
Tse et al. 1992		Wright et al. 1992		Bhatia & Sandler 1995		Moore et al. 1995	
activity coefficient		activity coefficient		activity coefficient		gas stripping-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
20	70.9	20	72.7	35	281	seawater, salinity 30.4‰	
30	111.5	30	141	50	513	0	25.4
35	142	40	252			10	48.3
40	172					20	81.9
						eq. 1	$K_{AW}$
						A	$11.70 \pm 0.03$
						B	$4418 \pm 154$





**FIGURE 5.1.2.2.3** Logarithm of Henry's law constant versus reciprocal temperature for dibromomethane.

## 5.1.2.3 Tribromomethane



Common Name: Tribromomethane

Synonym: bromoform, methenyl tribromide

Chemical Name: tribromomethane

CAS Registry No: 75-25-2

Molecular Formula:  $\text{CHBr}_3$

Molecular Weight: 252.731

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

8.69 (Lide 2003)

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

149.1 (Lide 2003)

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

2.8910 (Kahlbaum & Arndt 1898; Riddick et al. 1986)

2.8917, 2.8909 (Kudchadker et al. 1979)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

87.42 ( $20^{\circ}\text{C}$ , calculated-density)

99.5 (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  $25^{\circ}\text{C}$ , F: 1.0

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

3010, 3190 ( $15^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , shake flask-interferometer, Gross & Saylor 1931)

3110 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

3190 ( $30^{\circ}\text{C}$ , Seidell 1941)

3033 (Verschuereen 1977)

3100 (recommended, Horvath 1982)

3931 ( $30^{\circ}\text{C}$ , headspace-GC, McNally & Grob 1984)

3200 ( $30^{\circ}\text{C}$ , Dean 1985)

3180 ( $30^{\circ}\text{C}$ , selected, Riddick et al. 1986)

3235, 3452, 3695 (20, 30,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)

3978, 4555, 3467 (20, 35,  $50^{\circ}\text{C}$ , activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)

3163 ( $20^{\circ}\text{C}$ , equilibrium air stripping-GC, Hovorka & Dohnal 1997)

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

987\* ( $30^{\circ}\text{C}$ , temp range  $30$ – $110^{\circ}\text{C}$ , Kireev & Simnikow 1941; quoted, Boublik et al. 1984)

667\* ( $22^{\circ}\text{C}$ , summary of literature data, temp range  $22$ – $150.5^{\circ}\text{C}$ , Stull 1947)

2453\* ( $47.207^{\circ}\text{C}$ , temp range  $47.207$ – $139.055^{\circ}\text{C}$ , Boublik & Aim 1972; quoted, Boublik et al. 1984)

815 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 9673.3/(T/K)] + 7.875367$ ; temp range  $22$ – $150^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)

715 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.82182 - 1376.748/(200.966 + t/^{\circ}\text{C})$ ; temp range  $30$ – $100^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

720 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 7.03141 - 1511.50/(214.21 + t/^{\circ}\text{C})$  (Antoine eq., Kudchadker et al. 1979)

717 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 5.97839 - 1294.382/(202.729 + t/^{\circ}\text{C})$ ; temp range  $30$ – $100.8^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- $\log (P/\text{mmHg}) = 6.8218 - 1376.7/(201.0 + t/^{\circ}\text{C})$ ; temp range 30–101°C (Antoine eq., Dean 1985, 1992)  
 790 (quoted, Riddick et al. 1986)  
 727 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.20911 - 1544.81/(-54.77 + T/\text{K})$ ; temp range 320–412 K (Antoine eq., Stephenson & Malanowski 1987)  
 543, 981, 1704 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)  
 $\log (P/\text{mmHg}) = -10.2943 - 2.170 \times 10^3/(T/\text{K}) + 9.1193 \cdot \log (T/\text{K}) - 1.6495 \times 10^{-2} \cdot (T/\text{K}) + 7.4917 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
 temp range 281–696 K (vapor pressure eq., Yaws 1994)  
 685.5 (selected and summary of literature data, temp range 281.2–478.15 K, Xiang 2002)

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

- 68.3 (calculated- $1/K_{AW}$ ,  $C_W/C_A$ , Hine & Mookerjee 1975)  
 7.66 (calculated-bond method, Hine & Mookerjee 1975)  
 62.3, 62.0 (calculated-P/C, recommended, Mackay & Shiu 1981, 1990)  
 56.7 (20°C, calculated-P/C, Mabey et al. 1982)  
 43.6, 43.6; 58.8 (20°C, batch stripping-GC, calculated-P/C, distilled water, Nicholson et al. 1984)  
 46.6, 41.54, 43.6 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 116.0 - 5670/(T/\text{K})$ ; temp range 10–30°C (air stripping-GC, Nicholson et al. 1984)  
 54.2 (EPICS-LSC, Munz & Roberts 1987, 1989)  
 $\log K_{AW} = 4.729 - 1905/(T/\text{K})$ ; temp range 10–30°C (EPICS-LSC measurements, Munz & Roberts 1987)  
 53.9 (gas stripping-GC, Warner et al. 1987)  
 56.7 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 40.5, 70.9, 122 (20, 30, 40°C, infinite dilution activity coeff.  $\gamma^{\infty}$ -GC, Tse et al. 1992)  
 34.0, 71.6, 207 (20, 35, 50°C, activity coeff.  $\gamma^{\infty}$ -differential pressure transducer, Wright et al. 1992)  
 43.6 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 182, 536 (10, 20°C, gas stripping-GC, Moore et al. 1995)  
 14.3, 29.2, 52.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)  
 $\ln K_{AW} = 13.16 - 4973/(T/\text{K})$ ; seawater of salinity of 30.4‰, temp range: 0–20°C (Moore et al. 1995)  
 42.65 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 5.476 - 2120/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)  
 104.4 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

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

- 2.30 (calculated as per Tute 1971, Callahan et al. 1979)  
 2.38 (calculated-f const., Mabey et al. 1982; Valsaraj 1988)  
 2.67 (recommended, Hansch et al. 1995)

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

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

- 1.80 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)

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

- 2.07 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)

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

- Volatilization: calculated  $t_{1/2} = 63$  min to 24.2 d (using Langbein & Durum 1967 published  $O_2$  reaeration values) and  $t_{1/2} = 65.6$  d both from rivers and streams (Kaczmar et al. 1984).  
 Photolysis: photocatalyzed mineralization by the presence of  $\text{TiO}_2$  with the rate of 6.2 ppm/min per gram of catalyst (Ollis 1985).  
 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:  
 $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 0.5 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation  $t_{1/2} = 1299\text{--}12989$  h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k = 4.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$  for reaction with OH radical in water with reference to  $\text{CH}_3\text{CCl}_3$  (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{\text{OH}}(\text{aq.}) = (1.3 \pm 0.6) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

Hydrolysis: a maximum  $t_{1/2} = 686$  yr has been estimated at pH 7 and  $25^\circ\text{C}$  from experimental data at  $100\text{--}150^\circ\text{C}$  (Radding et al. 1977) which corresponds to a first-order rate constant  $k = 3.2 \times 10^{-11} \text{ s}^{-1}$  (Radding et al. 1977; Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard et al. 1991);

rate constant  $k = 3.2 \times 10^{-11} \text{ s}^{-1}$  with  $t_{1/2} = 686$  yr at pH 7 and  $25^\circ\text{C}$  (Mabey & Mill 1978)

rate constant  $k = 2.5 \times 10^{-9} \text{ h}^{-1}$  assigned by analogy to trichloromethane (Mabey et al. 1982).

Biodegradation:  $t_{1/2} = 672\text{--}4320$  h in soil, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991); anaerobic  $t_{1/2} = 2688\text{--}17280$  h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated rate constant  $k \sim 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 1299\text{--}12989$  h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 686$  yr at pH 7 and  $25^\circ\text{C}$  based on hydrolysis rate constant (Mabey & Mill 1978)

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

Sediment:

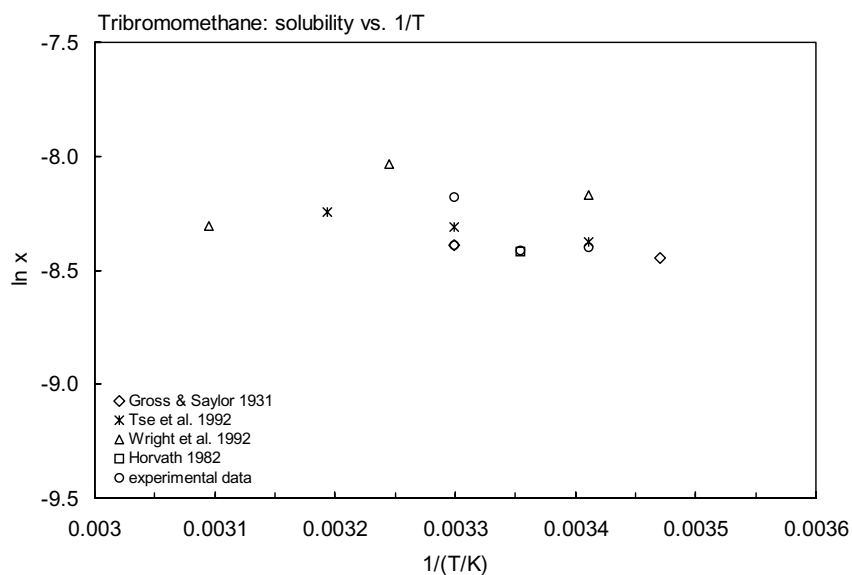
Soil:  $t_{1/2} = 672\text{--}4320$  h, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991).

Biota:

**TABLE 5.1.2.3.1**

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

Gross & Saylor 1931		Tse et al. 192		Wright et al. 1992	
shake flask-interferometer		activity coefficient		activity coefficient	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
15	3010	20	3235	20	3978
30	3190	30	3452	35	4555
		40	3695	50	3467



**FIGURE 5.1.2.3.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for tribromomethane.

**TABLE 5.1.2.3.2**

**Reported vapor pressures of tribromomethane 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)		

Kireev & Simnikow 1941		Stull 1947		Boublik & Aim 1972			
in Boublik et al. 1984		summary of literature data		in Boublik et al. 1984			
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
30.0	987	-	133.3	47.207	2453	123.929	49704
35.0	1267	22.0	666.6	59.767	4524	130.982	61295
40.0	1747	34.0	1333	69.518	6967	139.055	77125
50.0	2946	48.0	2666	76.389	9306	bp/ $^{\circ}\text{C}$	78.177
60.0	4693	63.6	5333	82.821	12046		at 10 mmHg
70.0	7399	73.4	7999	87.709	14549	Antoine eq.	
80.0	11306	85.9	13332	93.356	17921	eq. 2	P/kPa
90.0	16852	106.1	26664	98.173	21314	A	6.20467
110.0	24198	127.9	53329	103.595	25780	B	1541.946
		150.5	101325	108.003	29923	C	218.084
				113.216	35493		
		mp/ $^{\circ}\text{C}$	8.5	118.078	41470		

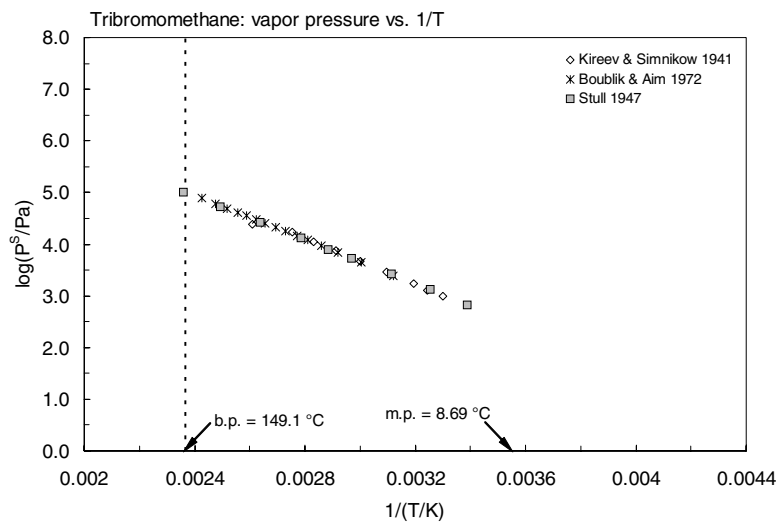


FIGURE 5.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for tribromomethane.

## 5.1.2.4 Bromoethane (Ethyl bromide)



Common Name: Ethyl bromide

Synonym: bromoethane, monobromoethane

Chemical Name: ethyl bromide, bromoethane

CAS Registry No: 74-96-4

Molecular Formula:  $C_2H_5Br$ ,  $CH_3CH_2Br$

Molecular Weight: 108.965

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

-118.60 (Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

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

38.5 (Lide 2003)

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

1.4594, 1.4492 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959)

1.4505 ( $25^{\circ}C$ , Riddick et al. 1986)

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

75.12 (calculated from density)

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

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

27.55, 26.48 ( $25^{\circ}C$ , at bp, Riddick et al. 1986)

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

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

9140\* ( $20^{\circ}C$  volumetric method, measured range  $0-30^{\circ}C$ , Rex 1906)

9600 ( $17.5^{\circ}C$ , volumetric method, Fühner 1924)

8880 ( $30^{\circ}C$ , van Arkel & Vles 1936)

9064 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

9000 (shake flask-interferometry, Donahue & Bartell 1952)

8939\* (summary of literature data, temp range  $0-30^{\circ}C$ , Horvath 1982)

9100 (Dean 1985; Riddick et al. 1986)

9000\* (tentative value, temp range  $0-^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 13.2481 - 8.0012 \times 10^{-2} \cdot (T/K) + 1.29448 \times 10^{-4} \cdot (T/K)^2$ , temp range  $273-303 K$  (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

51440, 75140 ( $20^{\circ}C$ ,  $30^{\circ}C$ , Rex 1906)

70095\* ( $28.145^{\circ}C$ , temp range  $28.145-75.365^{\circ}C$ , Zmaczynski 1930)

53329\* ( $21^{\circ}C$ , summary of literature data, temp range  $-74.3$  to  $38.4^{\circ}C$ , Stull 1947)

62460 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.91995 - 1090.81/(231.71 + t/^{\circ}C)$ ; temp range  $-32$  to  $110^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

$\log (P/mmHg) = 6.91995 - 1090.81/(231.71 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/mmHg) = [-0.2185 \times 6843.1/(T/K)] + 7.635277$ ; temp range  $74.3$  to  $229.5^{\circ}C$  (Antoine eq., Weast 1972-73)

62230 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.11352 - 1121.957/(234.741 + t/^{\circ}C)$ ; temp range  $28.145-75.4^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.9886 - 1121.9/(234.7 + t/^{\circ}\text{C})$ ; temp range 28–75°C (Antoine eq., Dean 1985, 1992)

62470 (lit; average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.04485 - 1090.81/(231.71 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

62470 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04485 - 1090.81/(-41.44 + T/\text{K})$ ; temp range 225–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.66835 - 1151.96/(12.999 + T/\text{K})$ ; temp range 334–504 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.77490 - 1602.405/(25.282 + T/\text{K})$ ; temp range 326–454 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.99873 - 1619.697/(T/\text{K})$ ; temp range 452–503 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 38.1816 - 2.517 \times 10^3/(T/\text{K}) - 10.329 \cdot \log (T/\text{K}) - 2.3368 \times 10^{-10} \cdot (T/\text{K}) + 5.4956 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 155–504 K (vapor pressure eq., Yaws 1994)

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

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

751 (computed value, Yaws et al. 1991)

767 ( $\gamma^{\infty}$  from gas stripping-GC, Li et al. 1993)

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

1.60 (calculated- $\pi$  const., Hansch et al. 1968)

1.61 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979, 1987)

1.61 (recommended, Sangster 1989)

1.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{AW}$  at 25°C:

1.53 (calculated-measured  $\gamma^{\infty}$  in pure octanol and vapor pressure P, Abraham et al. 2001)

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:

Hydrolysis:  $k = 2.64 \times 10^{-7} \text{ s}^{-1}$  with  $t_{1/2} \sim 30 \text{ d}$  at pH 7 and 25°C (Mabey & Mill 1978)

$k = 9.4 \times 10^{-4} \text{ h}^{-1}$  at pH 7 and 25°C with  $t_{1/2} \sim 30 \text{ d}$  (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water:  $t_{1/2} \sim 30 \text{ d}$  at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)



TABLE 5.1.2.4.1

Reported aqueous solubilities of bromoethane at various temperatures

$$S/(\text{wt}\%) = 1.0557 - 0.01309 \cdot (t/^\circ\text{C}) + 3.3850 \times 10^{-4} \cdot (t/^\circ\text{C})^2 - 2.950 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 13.2481 - 8.0012 \times 10^{-2} \cdot (T/\text{K}) + 1.29448 \times 10^{-4} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0	10670	0	10557	0	10510
10	9650	10	9557	5	10080
20	9140	20	9057	10	9710
30	8960	25	8939	15	9410
		30	8880	20	9170
		eq. 1	S/wt%	25	9000
				30	8890
				eq. 2	S/wt%
				temp range 273–303 K	

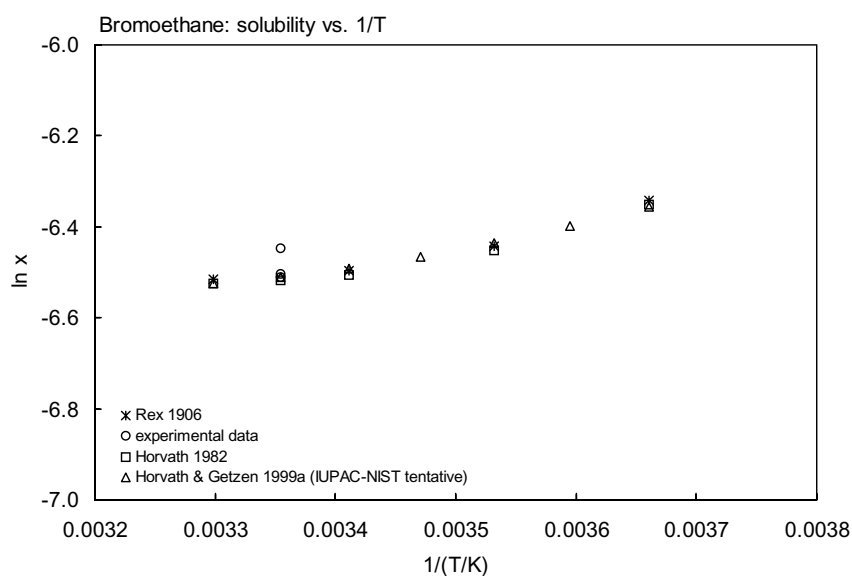
FIGURE 5.1.2.4.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for bromoethane.

TABLE 5.1.2.4.2

Reported vapor pressures of bromoethane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Zmaczynski 1930		Stull 1947	
		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
28.145	70095	-74.3	133.3
33.247	83515	-56.4	666.6
43.560	120803	-47.5	1333
48.771	143268	-37.8	2666
54.018	169066	-26.7	5333
59.300	198543	-19.5	7999
64.619	232113	-10.0	13332
69.94	270150	4.50	26664
75.365	312960	21.0	53329
		38.4	101325
		mp/°C	-117.8

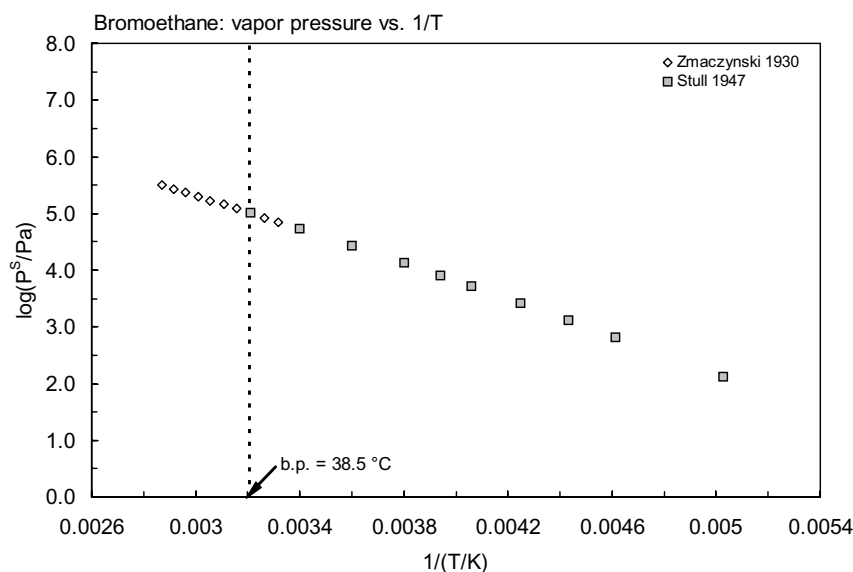
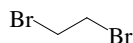


FIGURE 5.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for bromoethane.

## 5.1.2.5 1,2-Dibromoethane



Common Name: 1,2-Dibromoethane

Synonym: ethylene bromide, ethylene dibromide, *sym*-dibromoethane, EDB

Chemical Name: 1,2-dibromoethane

CAS Registry No: 106-93-4

Molecular Formula:  $C_2H_4Br_2$ ,  $CH_2BrCH_2Br$

Molecular Weight: 187.861

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

9.84 (Lide 2003)

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

131.6 (Lide 2003)

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

2.1792, 2.1688 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959; Horvath 1982)

2.1791, 2.1687 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

86.25 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

41.73, 36.35 ( $25^{\circ}C$ , at bp, Riddick et al. 1986)

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

10.03 (calculated, Dreisbach 1959)

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

3920, 4310 ( $15^{\circ}C$ ,  $30^{\circ}C$ , shake flask-interferometer, Gross & Saylor 1931)

4040\* (measured range  $0$ – $50^{\circ}C$ , van Arkel & Vles 1936)

4017 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

8600 (shake flask-volumetric method, Booth & Everson 1948)

4200 (measured by Dow Chemical, Dreisbach 1959)

3510\* ( $20^{\circ}C$ , shake flask-GC, measured range  $3$ – $34^{\circ}C$ , Chiou & Freed 1977)

2910 (shake flask-GC, Jones et al. 1977/78)

3520 (shake flask-GC, Chiou et al. 1979)

4320, 4321 ( $20^{\circ}C$ ,  $25^{\circ}C$ , shake flask-GC, Mackay et al. 1980)

4152\* (summary of literature data, Horvath 1982)

4310 ( $30^{\circ}C$ , Verschueren 1983)

4290 ( $30^{\circ}C$ , selected, Riddick et al. 1986)

3120 (shake flask-reverse phase polarography, Tokoro et al. 1988)

4120\*, 4310 ( $19.5^{\circ}C$ ,  $30.7^{\circ}C$ , shake flask-GC/TC, measured range  $10.0$ – $90.6^{\circ}C$ , Stephenson 1992)

4192 ( $20^{\circ}C$ , limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

3910\* (tentative value, temp range  $0$ – $75^{\circ}C$ . IUPAC-NIST Solubility Data Series, Hovath & Getzen 1999a)

$S/(wt\%) = 3.8651 - 2.7921 \times 10^{-2} \cdot (T/K) + 5.45647 \times 10^{-5} \cdot (T/K)^2$ , temp range  $273$ – $348$  K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

1333 ( $18.2^{\circ}C$ , summary of literature data, temp range  $-27$  to  $131.1^{\circ}C$ , Stull 1947)

1560 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 7.06245 - 1469.7/(220.0 + t/^{\circ}C)$ ; temp range  $43$ – $215^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

$\log (P/\text{mmHg}) = [-0.2185 \times 9229.4/(T/K)] + 7.93581$ ; temp range  $-27$  to  $304^\circ\text{C}$  (Antoine eq., Weast 1972–73)  
 1466, 2266 ( $20^\circ\text{C}$ ,  $30^\circ\text{C}$ , Verschuereen 1983)  
 1626 (interpolated-Antoine eq., Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 5.62666 - 1156.346/(2187.446 + t/^\circ\text{C})$ ; temp range  $52.56$ – $131.41^\circ\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{mmHg}) = 6.72148 - 1280.82/(201.75 + t/^\circ\text{C})$ ; temp range  $52$ – $131^\circ\text{C}$  (Antoine eq., Dean 1985, 1992)  
 1540 (lit. average, Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 4.32297 - 1560.3/(230.0 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 $\log (P_s/\text{kPa}) = 10.03 - 2863/(T/K)$ ; temp range  $228$ – $248$  K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_s/\text{kPa}) = 9.009 - 2606.5/(T/K)$ ; temp range  $251$ – $281$  K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.501 - 2181.1/(T/K)$ ; temp range  $283$ – $317$  K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.18375 - 1469.7/(-53.15 + T/K)$ ; temp range  $316$ – $488$  K (Antoine eq.-IV, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.16941 - 3200/(117.25 + T/K)$ ; temp range  $404$ – $578$  K (Antoine eq.-V, Stephenson & Malanowski 1987)  
 $\log (P/\text{mmHg}) = 16.8759 - 2.4267 \times 10^3/(T/K) - 3.0891 \cdot \log (T/K) - 6.0088 \times 10^{-10} \cdot (T/K) + 3.5901 \times 10^{-7} \cdot (T/K)^2$ ; temp range  $283$ – $650$  K (vapor pressure eq., Yaws 1994)

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

71.49 (calculated as  $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)  
 15.64, 110.7 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)  
 65.86\* (EPICS-GC, measured range  $10$ – $30^\circ\text{C}$ , Ashworth et al. 1988)  
 $\ln [H/(\text{atm m}^3 \text{ mol}^{-1})] = 5.703 - 3876/(T/K)$ ; temp range  $10$ – $30^\circ\text{C}$  (EPICS-GC, Ashworth et al. 1988)  
 71.49, 133.12 (quoted, calculated-QSAR, Nirmalakhandan & Speece 1988)  
 83.07 ( $20$ – $25^\circ\text{C}$  and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)  
 70.77 (computed value, Yaws et al. 1991)  
 52.6 ( $20^\circ\text{C}$ , equilibrium air stripping-GC, Hovorka & Dohnal 1997)  
 52.02 ( $20^\circ\text{C}$ , exponential saturator EXPSTAT technique, Dohnal & Hovorka 1999)  
 54.84 ( $20^\circ\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{AW} = 3.661 - 1556/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

1.96 (shake flask, Log P Database, Hansch & Leo 1987)  
 1.96 (recommended, Sangster 19943)  
 1.96 (recommended, Hansch et al. 1995)

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

0.778 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)  
 0.301 (calculated- $K_{OC}$  as per Kenaga & Goring 1978, Kenaga 1980)

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

1.556 (soil, equilibrium sorption isotherm, Chiou et al. 1979)  
 1.643 (soil, quoted, Kenaga 1980; Kenaga & Goring 1980)  
 1.699 (soil, calculated as per Kenaga & Goring 1978, Kenaga 1980)  
 1.643 (soil, selected, Jury et al. 1990)  
 1.64 (soil, organic carbon  $\text{OC} \geq 0.5\%$ , average, Delle Site 2001)

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

Volatilization: estimated volatilization  $t_{1/2} \sim 6.1$  h from water (Thomas 1982)

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:  
 $k_{OH} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296$  K (discharge flow system, Howard & Evenson 1976)

$k_{\text{OH}}(\text{calc}) = 2.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{\text{OH}} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a loss rate of  $0.01 \text{ d}^{-1}$ ,  $k_{\text{O}_3} < 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a loss rate of  $< 6 \times 10^{-7} \text{ d}^{-1}$  at room temp. (Atkinson 1985)

$k_{\text{O}_3}(\text{aq.}) \leq 0.014 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $22^\circ\text{C}$ , with a half-life of 28 d at pH 7 (Yao & Haag 1991).

Hydrolysis: EDB hydrolyzes to ethylene glycol and bromoethanol in water at pH 7 and  $25^\circ\text{C}$  with  $t_{1/2} = 5\text{--}10 \text{ d}$  (Leinster et al. 1978; quoted, Verschueren 1983);

$k = 9.9 \times 10^{-6} \text{ h}^{-1}$  at pH 7 and  $25^\circ\text{C}$  with a calculated  $t_{1/2} = 8.0 \text{ yr}$  (Jungclaus & Cohen 1986; quoted, Ellington 1989);

rate constant  $k = (8.9 \pm 0.1) \times 10^{-9} \text{ s}^{-1}$  in water at  $25^\circ\text{C}$  and pH 7.5 with an estimated half-life of 2.5 yr (Vogel & Reinhard 1986);

$t_{1/2} = 2.2 \text{ yr}$ , based on measured neutral hydrolysis rate constant at pH 7 and  $25^\circ\text{C}$  (Weintraub et al. 1986; quoted, Howard et al. 1991).

Biodegradation: aerobic  $t_{1/2}(\text{aq.}) = 672\text{--}4320 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation screening test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991);

anaerobic  $t_{1/2}(\text{aq.}) = 48\text{--}360 \text{ h}$ , based on anaerobic stream and pond water sediment die-away test data (Jafvert & Wolfe 1987; quoted, Howard et al. 1991).

Biotransformation:

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

#### Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); photooxidation  $t_{1/2} = 257\text{--}2567 \text{ h}$ , based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 672\text{--}4320 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation (Howard et al. 1991);  $k(\text{exptl}) \leq 0.014 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $22^\circ\text{C}$ , with  $t_{1/2} \geq 28 \text{ d}$  at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 470\text{--}2880 \text{ h}$ , based on data from anaerobic ground water ecosystem study (Wilson et al. 1986; quoted, Howard et al. 1991) and data from an aerobic ground water ecosystem study (Swindoll et al. 1987; quoted, Howard et al. 1991).

Sediment: calculated  $t_{1/2} = 1500 \text{ d}$  at  $25^\circ\text{C}$  and pH 7, based on studies in pure water and in barely saturated subsurface sediment at  $25\text{--}60^\circ\text{C}$  (Haag & Mill 1988).

Soil: estimated  $t_{1/2} \sim 3650 \text{ d}$  of volatilization loss from soil (Jury et al. 1990);

disappearance  $t_{1/2} < 2.0 \text{ d}$ , estimated from the volatilization loss of mixtures (Anderson et al. 1991);

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

Biota:

**TABLE 5.1.2.5.1**

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

$$S(\text{wt}\%) = 0.36583 + 1.4836 \times 10^{-3} \cdot (t/^\circ\text{C}) + 3.48175 \times 10^{-6} \cdot (t/^\circ\text{C})^2 + 6.47685 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S(\text{wt}\%) = 3.8651 - 2.7921 \times 10^{-2} \cdot (T/\text{K}) + 5.45647 \times 10^{-5} \cdot (T/\text{K})^2, \quad (2)$$

1.

Gross & Saylor 1931		van Arkel & Vles 1936		Chiou & Freed 1977		Horvath 1982	
shake flask-interferometer				shake flask-GC		summary of literature data	
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>
15	3920	0	3340	3	2960	5	3658
30	4310	20	4020	20	3510	10	3817
		35	4490	34	4150	20	4012
		50	5290			25	4152

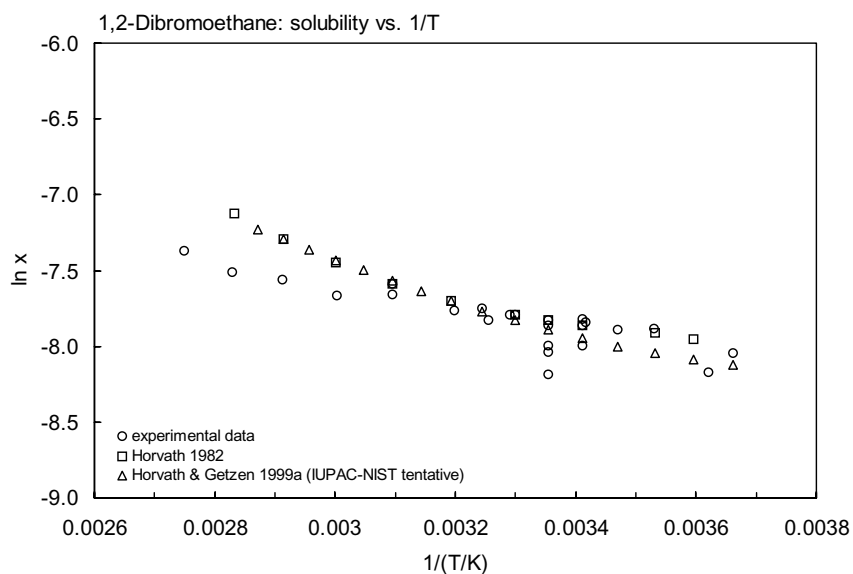
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TABLE 5.1.2.5.1 (Continued)

Gross & Saylor 1931		van Arkel & Vles 1936		Chiou & Freed 1977		Horvath 1982	
shake flask-interferometer				shake flask-GC		summary of literature data	
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>
						30	4310
						40	4722
						50	5297
						60	6073
						70	7089
						80	8384
						eq.1	S/wt%

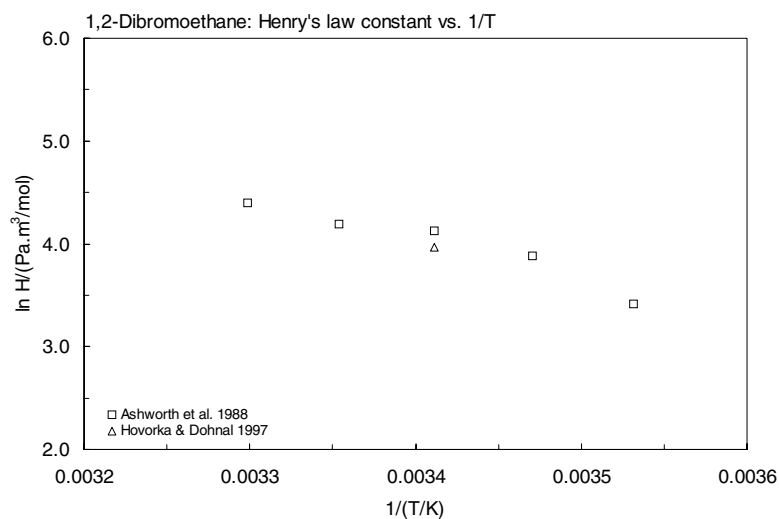
2.

Stephenson 1992		Horvath & Getzen 1999a			
shake flask-GC		tentative, IUPAC-NIST			
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
10.1	3950	0	3090	55	5780
19.5	4120	5	3200	60	6190
30.7	4310	10	3340	65	6630
39.6	4440	15	3500	70	7090
50	4930	20	3690	75	7580
59.9	4890	25	3910		
70.2	5420	30	4150	eq. 2	S/wt%
80.3	5720	35	4420		
90.6	6580	40	4720		
		45	5050		
		50	5400		

FIGURE 5.1.2.5.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,2-dibromomethane.

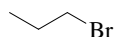
**TABLE 5.1.2.5.2**  
**Reported Henry's law constants of 1,2-dibromoethane**  
**at various temperatures**

Ashworth et al. 1988	
EPICS-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)
10	30.4
15	48.6
20	61.8
25	65.9
30	81.1
$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/\text{K})$	
A	5.703
B	3876



**FIGURE 5.1.2.5.2** Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dibromomethane.

## 5.1.2.6 1-Bromopropane



Common Name: 1-Bromopropane

Synonym: bromopropane, monobromopropane, *n*-propyl bromide, propyl bromide

Chemical Name: *n*-propyl bromide, 1-bromopropane

CAS Registry No: 106-94-5

Molecular Formula: C<sub>3</sub>H<sub>7</sub>Br, CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>Br

Molecular Weight: 122.992

Melting Point (°C):

−110.3 (Lide 2003)

Boiling Point (°C):

71.1 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.3536, 1.3452 (20°C, 25°C, Dreisbach 1961)

1.3537 (Horvath 1982)

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

90.86 (20°C, calculated-density)

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

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

31.88, 68.8 (25°C, 68.8°C, Riddick et al. 1986)

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

9.037 (quoted, Riddick et al. 1986)

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 or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

2450\* (20°C, volumetric method, measured range 0–30°C, Rex 1906)

2275 (19.5°C, shake flask, Fühner 1924)

2310 (30°C, shake flask-interferometer, Gross & Saylor 1931)

2312 (30°C, shake flask, Van Arkel & Vles 1936)

2454 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

2460 (calculated-K<sub>ow</sub>, Hansch et al. 1968)

2450 (20°C, exptl., Korenman et al. 1971)

2427\* (summary of literature data, Horvath 1982)

2300 (30°C, Dean 1985; Riddick et al. 1986)

2340\* (tentative value, IUPAC-NIST Solubility Data Series, temp range 0–30°C Horvath & Getzen 1999)

S/(wt%) = 9.0608 − 0.05911·(T/K) + 9.8925 × 10<sup>−5</sup>·(T/K)<sup>2</sup>, temp range 273–303 K (Horvath & Getzen 1999)

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):

14770, 22740 (20°C, 30°C, volumetric method Rex 1906)

13332\* (18°C, summary of literature data, temp range −53.0 to 71°C, Stull 1947)

18440 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 6.91065 − 1194.889/(225.51 + t/°C); temp range −6 to 107°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.91065 − 1194.889/(225.51 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

18300 (interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.09224 − 1232.529/(230.19 + t/°C); temp range 0–30°C (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)

18440 (selected, Riddick et al. 1986)

log (P/kPa) = 6.03960 − 1194.33/(225.223 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)



$\log (P_L/\text{kPa}) = 6.03555 - 1194.889/(-47.64 + T/K)$ ; temp range 250–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.03823 - 1193.612/(-48.005 + T/K)$ ; temp range 301–344 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -9.0284 - 1.8916 \times 10^3/(T/K) + 9.691 \cdot \log (T/K) - 2.7013 \times 10^{-2} \cdot (T/K) + 1.7877 \times 10^{-5} \cdot (T/K)^2$ ; temp range 163–544 K (vapor pressure eq., Yaws 1994)

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

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

1133, 1564 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

766.0 (calculated-QSAR, Nirmalakhandan & Speece 1988)

732 (computed value, Yaws et al. 1991)

950 ( $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)

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

2.10 (shake flask-GC, Fujita et al. 1964; Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)

2.10 (recommended, Sangster 1989, 1993)

2.10 (recommended, Hansch et al. 1995)

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:

Hydrolysis:  $k = 3.04 \times 10^{-7} \text{ s}^{-1}$  with estimated  $t_{1/2} = 26 \text{ d}$  at pH 7 and 25°C (Mabey & Mill 1978)

$k = 1.1 \times 10^{-3} \text{ h}^{-1}$  at pH 7 and 25°C with estimated  $t_{1/2} = 26 \text{ d}$ . (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: estimated  $t_{1/2} = 26 \text{ d}$  at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

Ground water:

Sediment:

Soil:

Biota:

TABLE 5.1.2.6.1

Reported aqueous solubilities of 1-bromopropane at various temperatures

$$S/(\text{wt}\%) = 0.2971 - 0.04225 \cdot (t/^\circ\text{C}) + 6.94998 \times 10^{-5} \cdot (t/^\circ\text{C})^2 + 5.00002 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 9.0608 - 0.05911 \cdot (T/\text{K}) + 9.8925 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0	2980	0	2971	0	2980
10	2630	10	2623	5	2760
20	2450	20	2444	10	2580
30	2470	25	2427	15	2450
		30	2464	20	2370
		eq. 1	S/wt%	25	2340
				30	2360
				eq. 2	S/wt%
				temp range 273–303 K	

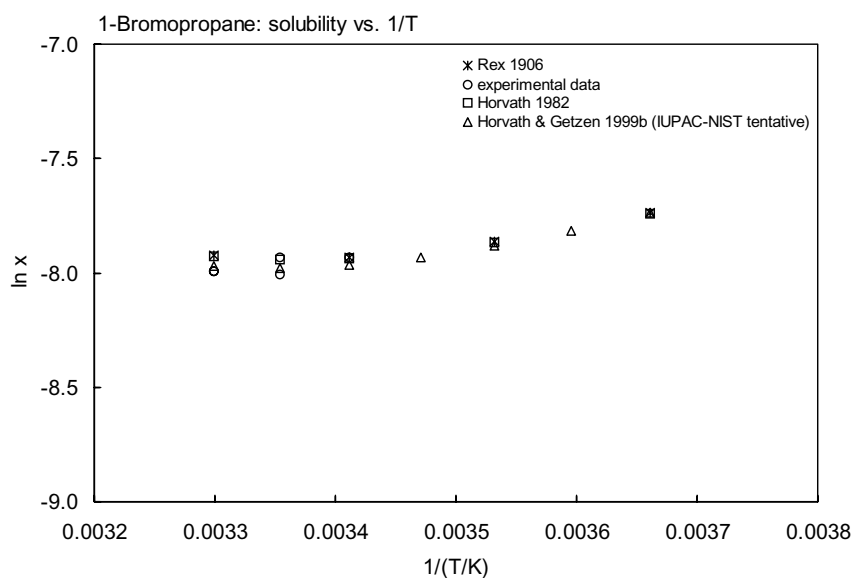


FIGURE 5.1.2.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-bromopropane.

TABLE 5.1.2.6.2

Reported vapor pressures of 1-bromopropane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Rex 1906		Stull 1947	
		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
0	5546	-52.0	133.3
10	9091	-33.4	666.6
20	14772	-23.3	1333
30	22745	-12.4	2666
		-0.30	5333
		7.50	7999
		18.0	13332
		34.0	26664
		52.0	53329
		71.0	101325
		mp/°C	-109.0

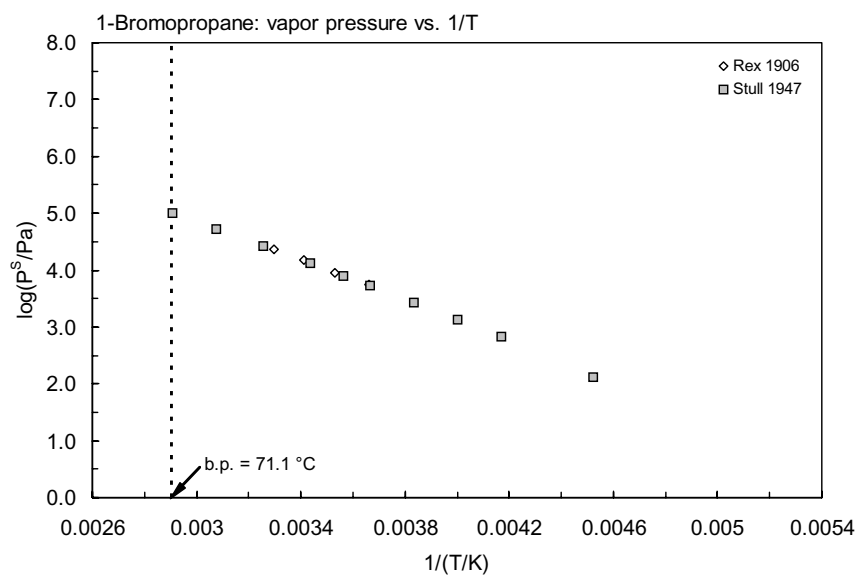


FIGURE 5.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1-bromopropane.

## 5.1.2.7 2-Bromopropane



Common Name: 2-Bromopropane

Synonym: isopropyl bromide

Chemical Name: 2-bromopropane, isopropyl bromide

CAS Registry No: 75-26-3

Molecular Formula:  $C_3H_7Br$ ,  $CH_3CHBrCH_3$

Molecular Weight: 122.992

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

−89.0 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

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

59.50 (Dean 1985; Lide 2003)

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

1.3140, 1.3060 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961; Riddick et al. 1986)

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

93.6 ( $20^{\circ}C$ , Stephenson & Malanowski 1987)

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

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

30.16, 28.4 ( $25^{\circ}C$ ,  $58.6^{\circ}C$ , Riddick et al. 1986)

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):

4180, 3650, 3180, 3180 (0, 10, 20,  $30^{\circ}C$ , volumetric method, Rex 1906)

2877 (shake flask-volumetric method, Fühner 1924)

3198 ( $30^{\circ}C$ , shake flask, Van Arkel & Vles 1936)

3162 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

2880, 2690 ( $20^{\circ}C$ , Korenman et al. 1971)

3000 (selected exptl., Horvath 1982)

2900 ( $18^{\circ}C$ , Dean 1985)

2860 ( $18^{\circ}C$ , selected, Riddick et al. 1986)

4160, 3640, 3170, 3170 (0, 10, 20,  $30^{\circ}C$ , tentative values of IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

23380, 35220 ( $20^{\circ}C$ ,  $30^{\circ}C$ , volumetric method Rex 1906)

26664 ( $23.8^{\circ}C$ , summary of literature data, temp range  $-61.8$  to  $60^{\circ}C$ , Stull 1947)

31500 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 6.61405 - 1072.9/(228.0 + t/^{\circ}C)$ ; temp range  $-19$  to  $95^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 7591.7/(T/K)] + 7.887729$ ; temp range  $-61.8$  to  $60^{\circ}C$  (Antoine eq., Weast 1972–73)

28780 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.09819 - 1200.652/(233.815 + t/^{\circ}C)$ ; temp range  $0$ – $30^{\circ}C$  (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)

31500 (selected, Riddick et al. 1986)

$\log(P/kPa) = 5.92741 - 1106.82/(222.851 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

31940 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.28473 - 858.03/(-71.18 + T/K)$ ; temp range  $236$ – $328\ K$  (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.91155 - 1098.573/(-51.268 + T/K)$ ; temp range  $299$ – $332\ K$  (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 31.3032 - 2.4924 \times 10^3/(T/K) - 8.4645 \cdot \log (T/K) + 1.6459 \times 10^{-10} \cdot (T/K) + 3.7859 \times 10^{-6} \cdot (T/K)^2;$$

temp range 184–532 K (vapor pressure eq., Yaws 1994)

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

1107	(calculated- $1/K_{\text{AW}}$ , $C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)
2479, 1564	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1082	(calculated-QSAR, Nirmalakhandan & Speece 1988)
978	(computed value, Yaws et al. 1991)
1192	( $\gamma^\infty$ from gas stripping-GC, Li et al. 1993)

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

1.90	(calculated- $\pi$ const., Hansch et al. 1968)
2.14	(recommended, Hansch et al. 1995)
1.80	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

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:

Hydrolysis:  $k = 3.86 \times 10^{-6} \text{ s}^{-1}$  with estimated  $t_{1/2} \sim 2.0 \text{ d}$  at pH 7 and  $25^\circ\text{C}$  (Mabey & Mill 1978)

$k = 1.4 \times 10^{-2} \text{ h}^{-1}$  at pH 7 and  $25^\circ\text{C}$  with estimated  $t_{1/2} \sim 2.0 \text{ d}$  (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986);

rate constants at  $25^\circ\text{C}$ :  $k = (379 \pm 41) \times 10^{-8} \text{ s}^{-1}$  in distilled water at pH 3–11 for equal or more than 72% conversion (Mill et al. 1980; quoted, Haag & Mill 1988),

$k = (383 \pm 33) \times 10^{-8} \text{ s}^{-1}$  in distilled water for 89% conversion,  $k = (372 \pm 64) \times 10^{-8} \text{ s}^{-1}$  in sediment-extracted water for 87% conversion, and  $k = (420 \pm 80) \times 10^{-8} \text{ s}^{-1}$  in sediment pores at pH 7.3 for 88% conversion (Haag & Mill 1988).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: estimated  $t_{1/2} \sim 2.0 \text{ d}$  at pH 7 and  $25^\circ\text{C}$  based on hydrolysis rate constant (Mabey & Mill 1978)

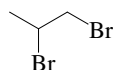
Ground water:

Sediment:  $t_{1/2} = 2.1 \text{ d}$ , based on neutral and base-catalyzed hydrolysis studies at  $25^\circ\text{C}$  in pure water and in barely saturated subsurface sediment at  $25\text{--}60^\circ\text{C}$  (Haag & Mill 1988).

Soil:

Biota:

## 5.1.2.8 1,2-Dibromopropane



Common Name: 1,2-Dibromopropane

Synonym: propylene bromide, propylene dibromide

Chemical Name: 1,2-dibromopropane

CAS Registry No: 78-75-1

Molecular Formula:  $C_3H_6Br_2$ ,  $CH_3CHBrCH_2Br$

Molecular Weight: 201.888

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

−55.49 (Lide 2003)

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

141.0 (Lide 2003)

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

1.93268, 1.92344 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959)

1.9324, 1.9241 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

1.9324 (Horvath 1982; Weast 1982–83)

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

104.5 ( $20^{\circ}C$ , calculated-density)

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

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

42.43, 35.52 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

8.937 (calculated, Dreisbach 1959; 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  $25^{\circ}C$ ):

1430 (measured by Dow Chemical, Dreisbach 1955–1961)

1463 (Hine & Mookerjee 1975)

1428 (recommended, Horvath 1982)

2000 (Dean 1985)

2986 (calculated-fragment const., Wakita et al. 1986)

1919 (predicted-MCI  $\chi$  and polarizability, Nirmalakhandan & Speece 1988)

1420 (calculated-AI, Okouchi et al. 1992)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

2000 ( $37.3^{\circ}C$ , Kahlbaum & Arndt 1898)

1036 (Antoine eq. regression, temp range  $-7.0$  to  $141.6^{\circ}C$ , Stull 1947)

1071 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.89105 - 1419.6/(212.0 + t/^{\circ}C)$ ; temp range  $50$ – $210^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

688 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.34875 - 1572.7/(212.0 + t/^{\circ}C)$ ; temp range  $56$ – $183^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 9801.9/(T/K)] + 8.073203$ ; temp range  $-7.0$  to  $141.6^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = 7.30398 - 1644.4/(232.0 + t/^{\circ}C)$ ; temp range  $0$ – $50^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.89105 - 1419.6/(212.0 + t/^{\circ}C)$ ; temp range  $50$ – $250^{\circ}C$  (Antoine eq., Dean 1985, 1992)

1072 (quoted from Dreisbach 1959, 1961, Riddick et al. 1986)

$\log(P/kPa) = 6.01595 - 1419.6/(212.0 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.47365 - 1572.7/(-61.15 + T/K)$ ; temp range  $329$ – $456$  K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.00898 - 1409.6/(-62.856 + T/K)$ ; temp range 312–403 K (Antoine eq., Stephenson & Malanowski 1987)

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

94.2	(calculated- $1/K_{AW}$ , $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)
21.1, 164	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
226.1	(calculated-QSAR, Nirmalakhandan & Speece 1988)
150	(computed value, Yaws et al. 1991)

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

2.54	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)
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Bioconcentration Factor,  $\log \text{BCF}$ :

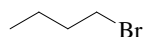
Sorption Partition Coefficient,  $\log K_{OC}$ :

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

Hydrolysis: rate constant  $k = (2.5 \pm 0.5) \times 10^{-8} \text{ s}^{-1}$  in water at 25°C and pH 7 with  $t_{1/2} \sim 320 \text{ d}$  (Vogel & Reinhard 1986).

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.9 1-Bromobutane (*n*-Butyl bromide)

Common Name: 1-Bromobutane

Synonym: *n*-butyl bromide, monobromobutane

Chemical Name: 1-bromobutane, *n*-butyl bromide, monobromobutane

CAS Registry No: 109-65-9

Molecular Formula:  $C_4H_9Br$ ,  $CH_3CH_2CH_2CH_2Br$

Molecular Weight: 137.02

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

-112.6 (Lide 2003)

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

101.6 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

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

1.2758, 1.2687 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961; Horvath 1982; Riddick et al. 1986)

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

107.9 ( $20^{\circ}C$ , calculated-density)

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

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

38.83, 31.85 ( $25^{\circ}C$ , normal bp, Dreisbach 1961)

36.60, 31.85 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

6.694 (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):

580 ( $16^{\circ}C$ , volumetric method, Fühner 1924)

608 ( $30^{\circ}C$ , shake flask-interferometer, Gross & Saylor 1931)

598 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

254 (shake flask-volumetric method, Booth & Everson 1948)

509 (exptl., Korenman et al. 1971)

600 (selected exptl., Horvath 1982)

869 (generator column-GC, Tewari et al. 1982)

601 (calculated-UNIFAC activity coeff., Arbuckle 1986)

608 ( $30^{\circ}C$ , quoted, Riddick et al. 1986)

680, 868, 871, 608 ( $16$ ,  $25$ ,  $25$ ,  $30^{\circ}C$ , reported values, IUPAC-NIST Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

10972 ( $20^{\circ}C$ , manometry, measured range  $20$ – $70^{\circ}C$ , Smyth & Engel 1929)

5333 ( $24.8^{\circ}C$ , summary of literature data, measured range  $-33.0$  to  $101.6^{\circ}C$ , Stull 1947)

5502 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 6.92254 - 1298.608/(219.70 + t/^{\circ}C)$ ; temp range  $19$ – $141^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 6.92254 - 1298.608/(219.70 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P/mmHg) = [-0.2185 \times 8789.1/(T/K)] + 8.028836$ ; temp range  $-33.0$  to  $101.6^{\circ}C$  (Antoine eq., Weast 1972–73)

5502 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.04744 - 1298.608/(219.70 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

5502 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.04744 - 1298.608/(-53.45 + T/K)$ ; temp range  $273$ – $400 K$  (Antoine eq.-I, Stephenson & Malanowski 1987)



$\log (P_L/\text{kPa}) = 6.1388 - 1349.142/(-48.003 + T/K)$ ; temp range 338–373 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 74.7061 - 4.0663 \times 10^3/(T/K) - 25.61 \cdot \log (T/K) + 1.3166 \times 10^{-2} \cdot (T/K) + 1.421 \times 10^{-13} \cdot (T/K)^2$ ; temp range 161–577 K (vapor pressure eq., Yaws 1994)

5506 (static method-manometer, measured range 278.15–323.15 K, Garriga et al. 2002)

$\ln (P/\text{kPa}) = 14.12331 - 3088.751/[(T/K) - 49.418]$ ; temp range 278.15–323.15 K (static method, Garriga et al. 2002)

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

1242 (calculated- $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

1600, 2313 (calculated-group contribution method, calculated-bond contribution Hine & Mookerjee 1975)

964.4 (calculated-QSAR, Nirmalakhandan & Speece 1988)

1223 (computed value, Yaws et al. 1991)

1215 ( $\gamma^\infty$  from gas stripping-GC, Li et al. 1993)

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

2.75 (generator column-GC, DeVoe et al. 1981; Wasik et al. 1981; Tewari et al. 1982)

2.75 (generator column-HPLC, DeVoe et al. 1981)

2.79 (estimated-activity coefficients, Wasik et al. 1981)

2.64 (estimated-activity coefficients, Schantz & Martire 1987)

2.75 (recommended, Sangster 1989)

2.75 (recommended, Hansch et al. 1995)

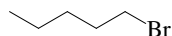
Bioconcentration Factor,  $\log \text{BCF}$ :

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

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.10 1-Bromopentane (*n*-Amyl bromide)

Common Name: 1-Bromopentane

Synonym: *n*-amyl bromide, monobromopentane, pentyl bromide

Chemical Name: *n*-amyl bromide, 1-bromopentane, monobromopentane, pentyl bromide

CAS Registry No: 110-53-2

Molecular Formula:  $C_5H_{11}Br$ ,  $CH_3CH_2CH_2CH_2CH_2Br$

Molecular Weight: 151.045

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

−88.0 (Lide 2003)

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

129.8 (Lide 2003)

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

1.2182, 1.2119 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961; Riddick et al. 1986)

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

124.0 ( $20^{\circ}C$ , calculated- density; Stephenson & Malanowski 1987)

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

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

41.78, 34.49 ( $25^{\circ}C$ , at normal bp, Dreisbach 1961)

41.43, 34.49 ( $25^{\circ}$ , bp, Riddick et al. 1986)

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

11.46 (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  $25^{\circ}C$ ):

127 (generator column-GC, Tewari et al. 1982)

141 (calculated-UNIFAC activity coeff., Arbuckle 1986)

127 (selected, Riddick et al. 1986)

127 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

1754 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 6.95580 - 1401.634/(214.38 + t/^{\circ}C)$ ; temp range  $41-171^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.95580 - 1401.634/(214.38 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

1680 (quoted, Riddick et al. 1986)

$\log (P/kPa) = 6.08070 - 11401.634/(214.38 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

1680 (interpolated-Antoine eq., Malanowski 1987)

$\log (P_L/kPa) = 6.0807 - 1401.634/(-58.77 + T/K)$ ; temp range 293–443 K (Antoine eq., Stephenson & Malanowski 1987)

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

2005 (computed value, Yaws et al. 1991)

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

3.37 (generator column-GC, DeVoe et al. 1981; Tewari et al. 1982)

3.37 (generator column-HPLC, DeVoe et al. 1981)

3.49 (generator column-GC, Wasik et al. 1981)

3.32 (estimated-measured activity coefficients, Schantz & Martire 1987)

3.37 (recommended, Sangster 1989)

3.37 (calculated-UNIFAC activity coeff., Dallos et al. 1993)

3.37 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

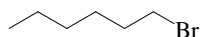
Sorption Partition Coefficient, log  $K_{OC}$ :

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h for the reaction with OH radicals in air (USEPA 1974; quoted, Darnall et al. 1976).

## 5.1.2.11 1-Bromohexane



Common Name: 1-Bromohexane

Synonym: *n*-hexyl bromide

Chemical Name: 1-bromohexane

CAS Registry No: 111-25-1

Molecular Formula:  $C_6H_{13}Br$ ;  $CH_3(CH_2)_4CH_2Br$

Molecular Weight: 165.071

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

−83.7 (Lide 2003)

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

155.3 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$ ):

1.1744, 1.1667 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

1.1744 ( $20^{\circ}C$ , Weast 1982–83)

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

140.6 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

46.77, 37.07 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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  $25^{\circ}C$ ):

25.75 (generator column-GC/FID, Tewari et al. 1982)

25.8 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

520 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.0023 - 1503.52/(209.5 + t/^{\circ}C)$ ; temp range  $63$ – $202^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.0023 - 1503.52/(209.5 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P_L/kPa) = 6.1272 - 1503.52/(T/K - 63.65)$ ; temp range 333–456 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

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

3.80 (generator column-GC, Tewari et al. 1982)

4.58 (HPLC-RT correlation, Burkhard et al. 1985)

3.80; 3.804 (generator column-GC; calculated-activity coeff.  $\gamma$ , Schantz & Martire 1987)

3.80 (recommended, Sangster 1989, 1993; Hansch et al. 1995)

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

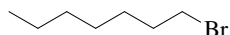
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

## 5.1.2.12 1-Bromoheptane



Common Name: 1-Bromoheptane

Synonym: heptyl bromide

Chemical Name: 1-bromoheptane

CAS Registry No: 629-04-9

Molecular Formula:  $C_7H_{15}Br$

Molecular Weight: 179.098

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

−56.1 (Dreisbach 1961; Weast 1982–83; Lide 2003)

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

178.9 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Density ( $g/cm^3$ ):

1.140, 1.1347 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

1.140 ( $20^{\circ}C$ , Weast 1982–83)

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

157.1 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

51.83, 39.59 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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  $25^{\circ}C$ ):

6.68 (generator column-GC/GID, Tewari et al. 1982; Miller et al. 1985)

6.68 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

163 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.0582 - 1603.71/(205.0 + t/^{\circ}C)$ ; temp range  $82$ – $228^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.0582 - 1603.71/(205.0 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P_L/kPa) = 6.1831 - 1603.71/(T/K - 68.15)$ ; temp range 333–483 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 43.3327 - 4.0389 \times 10^3/(T/K) - 12.105 \cdot \log(T/K) - 1.5959 \times 10^{-10} \cdot (T/K) + 3.0522 \times 10^{-6} \cdot (T/K)^2$ ; temp range 217–651 K (vapor pressure eq., Yaws 1994)

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

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

4.36 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

4.36; 4.44 (generator column-GC; calculated-activity coeff., Schantz & Mairtire 1987)

4.36 (recommended, Sangster 1989; 1994; Hansch et al. 1995)

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

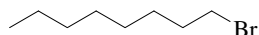
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

## 5.1.2.13 1-Bromooctane



Common Name: 1-Bromooctane

Synonym: octyl bromide

Chemical Name: 1-bromooctane

CAS Registry No: 111-83-1

Molecular Formula:  $C_8H_{17}Br$ ,  $CH_3(CH_2)_6CH_2Br$

Molecular Weight: 193.125

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

-55 (Dreisbach 1961; Weast 1982-83; Stephenson & Malanowski 1987; Lide 2003)

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

200.8 (Dreisbach 1961; Weast 1982-83; Lide 2003)

Density ( $g/cm^3$ ):

1.1122, 1.1072 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

1.1122 ( $20^{\circ}C$ , Weast 1982-83)

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

174.3 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

56.92, 42.04 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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)

1.67 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)

1.67 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)

1.72\* ( $24.9^{\circ}C$ , generator column-GC, measured range  $1.1-40.1^{\circ}C$ , Sarraute et al. 2004)

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):

50.66 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.1179 - 1701.61/(200.8 + t/^{\circ}C)$ ; temp range  $101-253^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.1179 - 1701.61/(200.8 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P_L/kPa) = 6.2428 - 1701.61/(T/K - 72.35)$ ; temp range  $373-475 K$  (Antoine eq., liquid, Stephenson & Malanowski 1987)

50.53\* ( $24.9^{\circ}C$ , calculated-Antoine eq. of Li & Rossini 1961, temp range  $1.1-40.1^{\circ}C$ , Sarraute et al. 2004)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ . Additional data at other temperatures designated \* are compiled at the end of this section):

5699\* (calculated-P/C, temp range  $1.1-40.1^{\circ}C$ , Sarraute et al. 2004)

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

4.89 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

4.89; 5.09 (generator column-GC; correlated-activity coeff., Schantz & Martire 1987)

4.89 (recommended, Sangster 1989, 1994; 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,  $t_{1/2}$ :

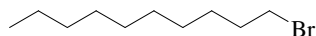
Half-Lives in the Environment:

**TABLE 5.1.2.13.1**

**Reported aqueous solubilities, vapor pressures and Henry's law constants of 1-bromooctane 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)			
Aqueous solubility		Vapor pressure		Henry's law constant	
Sarraute et al. 2004		Sarraute et al. 2004		Sarraute et al. 2004	
generator column-GC		extrapolated -Antoine eq.#		calculated-P/C	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
1.10	2.66	1.10	6.567	1.10	478.8
5.0	2.22	5.0	9.431	5.0	809.4
5.2	2.414	5.2	9.606	5.2	777.4
9.9	1.76	9.9	14.69	9.9	1600
9.9	1.77	9.9	14.68	9.9	1600
14.9	1.82	14.9	22.60	14.9	2395
24.9	1.715	24.9	50.53	24.9	5699
29.9	2.18	29.9	73.61	29.9	6500
34.0	2.78	34.0	105.5	34.0	7350
40.0	3.65	40.0	150.1	40.0	7941
40.1	3.48	40.1	150.6	40.1	8360
Antoine eq.					
#see <a href="#">ref.</a> Li & Rossini 1961					
eq. 2		P/mmHg			
A		7.1231			
B		1369.20			
C		204.4			
pressure range 10–1500 torr mmHg					

## 5.1.2.14 1-Bromodecane



Common Name: 1-Bromodecane

Synonym: decyl bromide

Chemical Name: 1-bromodecane

CAS Registry No: 112-29-8

Molecular Formula:  $C_{10}H_{21}Br$ ,  $CH_3(CH_2)_8CH_2Br$

Molecular Weight: 221.178

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

-29.2 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

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

240.6 (Dreisbach 1961; Weast 1982–83; Riddick et al. 1986; Lide 2003)

Density ( $g/cm^3$ ):

1.0702, 1.0656 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961; Riddick et al. 1986)

1.0702 ( $20^{\circ}C$ , Weast 1982–83)

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

206.7 ( $10^{\circ}C$ , Stephenson & Malanowski 1987)

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

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

67.12, 46.66 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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):

5.33 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.2336 - 1888.67/(193.3 + t/^{\circ}C)$ ; temp range  $135-297^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.2336 - 1888.67/(193.3 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

5.0 (quoted value from Dreisbach 1961, Riddick et al. 1986)

$\log(P/kPa) = 6.3585 - 1888.67/(193.3 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.3585 - 1888.67/(T/K - 79.85)$ ; temp range  $383-570 K$  (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

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

6.43 (HPLC-RT correlation, McDuffie 1981)

6.35, 5.84 (HPLC-RT correlation; calculated-CLOGP, Burkhard et al. 1985)

6.43 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

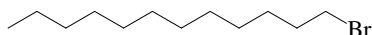
Sorption Partition Coefficient,  $\log K_{OC}$ :

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

Half-Lives in the Environment:



## 5.1.2.15 1-Bromododecane



Common Name: 1-Bromododecane

Synonym: lauryl bromide

Chemical Name: 1-bromododecane

CAS Registry No: 143-15-7

Molecular Formula:  $C_{12}H_{25}Br$ ,  $CH_3(CH_2)_{10}CH_2Br$

Molecular Weight: 249.231

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

-9.5 (Dreisbach 1961; Weast 1982-83; Lide 2003)

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

276 (Dreisbach 1961; Weast 1982-83; Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$ ):

1.0399, 1.0355 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

1.0399 ( $20^{\circ}C$ , Weast 1982-83)

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

240.1 ( $20^{\circ}C$ , Stephenson & Malanowski 1987)

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

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

77.38, 50.91 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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):

$\log(P/mmHg) = 7.3390 - 2061.93/(186.6 + t/^{\circ}C)$ ; temp range 165-237 $^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.3390 - 2061.93/(186.6 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini. 1961)

$\log(P/kPa) = 6.4639 - 2061.93/(T/K - 86.55)$ ; temp range 411-610 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

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

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

6.98; 6.90 (HPLC-RT correlation; calculated-CLOPG, Burkhard et al. 1985)

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

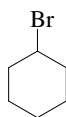
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

## 5.1.2.16 Bromocyclohexane



Common Name: Bromocyclohexane

Synonym: cyclohexyl bromide

Chemical Name: bromocyclohexane

CAS Registry No: 108-85-0

Molecular Formula:  $C_6H_{11}Br$

Molecular Weight: 163.055

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

-56.5 (Weast 1982-83; Lide 2003)

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

166.2 (Weast 1982-83; Lide 2003)

Density ( $g/cm^3$ ):

1.33585, 1.32976 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.3359 ( $20^{\circ}C$ , Weast 1982-83)

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

122.06, 122.6 ( $20^{\circ}C$ ,  $25^{\circ}C$ , calculated-density)

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

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

37.59, 44.80 (normal bp,  $25^{\circ}C$ , Dreisbach 1955)

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

8.70 (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  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

421 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 6.97980 - 1572.19/(217.38 + t/^{\circ}C)$ ; temp range  $68-260^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log P/mmHg = 6.97980 - 1572.19/(t/^{\circ}C + 217.38)$ ; temp range  $68-200^{\circ}C$  (Antoine eq., Dean 1992)

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

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

3.20 (shake flask-GC, Canton & Wagman 1983)

3.20 (recommended, Sangster 1993)

3.20 (selected, 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:

## 5.1.2.17 Vinyl bromide



Common Name: Vinyl bromide

Synonym: bromoethene, bromoethylene, ethylene bromide

Chemical Name: bromoethene

CAS Registry No: 593-60-2

Molecular Formula:  $C_2H_3Br$ ,  $CH_2 = CHBr$

Molecular Weight: 106.949

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

-139.54 (Dreisbach 1959; Riddick et al. 1986; Lide 2003)

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

15.80 (Dreisbach 1959; Dean 1985; Riddick et al. 1986; Lide 2003)

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

1.4933, 1.4738( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1959; Riddick et al. 1986)

1.4930 (Dean 1985)

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

71.6 ( $20^{\circ}C$ , calculated-density)

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

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

22.60, 23.45 ( $25^{\circ}C$ , bp, Dreisbach 1959; Riddick et al. 1986)

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

5.121 (Dreisbach 1959; 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):

4310 ( $30^{\circ}C$ , shake flask-interferometry, Saylor & Gross 1931)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

101325 ( $15.8^{\circ}C$ , summary of literature data, temp range  $-95.4$ – $15.8^{\circ}C$ , Stull 1947)

137700 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.66715 - 953.4/(236.0 + t/^{\circ}C)$ ; temp range  $-60$  to  $60^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1959)

145350 (extrapolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 6076.9/(T/K)] + 7.490979$ ; temp range  $-95.4$  to  $15.8^{\circ}C$  (Antoine eq., Weast 1972–73)

144330, 139840 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.03256 - 1494.17/(281.722 + t/^{\circ}C)$ ; temp range  $-66$ – $11.9^{\circ}C$  (Antoine eq. derived from exptl data of Mehl 1934, Boublik et al. 1984)

$\log(P/kPa) = 6.08611 - 1083.017/(249.845 + t/^{\circ}C)$ ; temp range  $-87.5$ – $16.0^{\circ}C$  (Antoine eq. derived from exptl data of Guyer et al. 1937, Boublik et al. 1984)

137700 (selected lit. value, Riddick et al. 1986)

$\log(P/kPa) = 5.79205 - 953.4/(236.0 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

140480 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.03266 - 1014.0/(-37.15 + T/K)$ ; temp range 224–319 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -10.9281 - 1.1619 \times 10^3/(T/K) + 9.3115 \cdot \log(T/K) - 2.2655 \times 10^{-2} \cdot (T/K) - 4.531 \times 10^{-5} \cdot (T/K)^2$ ; temp range 135–473 K (vapor pressure eq., Yaws 1994)

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

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

- 1.57 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)
- 1.57 (recommended, Sangster 1993)

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 see reference:

$k_{\text{OH}} = 6.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $25.4^\circ\text{C}$  (Perry et al. 1977)

$k_{\text{OH}}(\text{calc}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 6.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1985)

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 672\text{--}4320 \text{ h}$ , based on aqueous screening test data for vinyl chloride (Heffgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2880\text{--}17280 \text{ h}$ , based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 9.4\text{--}94 \text{ h}$ , based on measured rate constant for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

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

Ground water:  $t_{1/2} = 1344\text{--}69000 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation of vinyl chloride from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

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

Biota:

## 5.1.3 IODOALKANES

## 5.1.3.1 Iodomethane (Methyl iodide)



Common Name: Methyl iodide

Synonym: iodomethane, moniodomethane

Chemical Name: methyl iodide

CAS Registry No: 74-88-4

Molecular Formula: CH<sub>3</sub>I

Molecular Weight: 141.949

Melting Point (°C):

-66.4 (Lide 2003)

Boiling Point (°C):

42.43 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

2.2790, 2.265 (20°C, 25°C, Dreisbach 1961)

2.2792, 2.265 (20°C, 25°C, Riddick et al. 1986)

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

62.28 (20°C, calculated-density)

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

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

27.97, 27.338 (25°C, bp, Riddick et al. 1986)

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 or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

14190\* (20°C, volumetric method, measured range 0–30°C, Rex 1906)

13630 (20°C, Merckel 1937)

14200 (Seidell 1940; Seidell 1941)

log [C/(mol/L)] = -110.278 + 37.621·log (T/K) + 4823/(T/K); temp range 278.16–322.91 K (Glew &amp; Moelwyn-Hughes 1953)

13900\* (recommended, temp range 0–40°C, Horvath 1982)

14000 (20°C, Verschueren 1983; Riddick et al. 1986)

14000 (Dean 1985)

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):

44180, 64440(20°C, 30°C, Rex 1906)

75860\* (34.4°C, temp range 0.10–34.4°C, Thompson &amp; Linnett 1936)

53329\* (25.3°C, summary of literature data, temp range -55.0 to 25.3°C, Stull 1947)

log (P/mmHg) = 22.974 - 5.346·log (T/K) - 2132/(T/K); temp range 278.16–322.91 K (Glew &amp; Moelwyn-Hughes 1953)

54120 (calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.87991 - 1093.235/(230.94 + t/°C); temp range -29 to 76°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.87991 - 1093.235/(230.94 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li &amp; Rossini 1961)

49704\* (22.879°C, temp range -13.819 to 41.427°C, Boublik &amp; Aim 1972; quoted, Boublik et al. 1984)

47750 (interpolated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 6616.5/(T/K)] + 7.403018$ ; temp range  $-55.0$  to  $254.8^\circ\text{C}$  (Antoine eq., Weast 1972-73)

53980 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log (P/\text{mmHg}) = 6.97241 - 1138.29/(t/^\circ\text{C} + 235.774)$ ; temp range  $-14$  to  $42^\circ\text{C}$  (Antoine eq., Kudchadker et al. 1979)

54120 (lit. average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.09731 - 1138.29/(235.774 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

53960 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.10541 - 1142.67/(-36.87 + T/K)$ ; temp range  $228$ – $337$  K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = A6.17197 - 1240.17/(-17.887 + T/K)$ ; temp range  $315$ – $502$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -20.3718 - 1.2536 \times 10^3/(T/K) + 13.645 \cdot \log (T/K) - 2.6955 \times 10^{-2} \cdot (T/K) + 1.6389 \times 10^{-5} \cdot (T/K)^2$ ; temp range  $207$ – $528$  K (vapor pressure eq., Yaws 1994)

54009 (selected summary of literature data, temp range  $206.71$ – $363.15$  K, Xiang 2002)

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

541\*, 536 (exptl.-concn ratio, measured range  $0$ – $49^\circ\text{C}$ , calculated-P/C, Glew & Moelwyn-Hughes 1953)

$\log \{H/(\text{mmHg} \cdot \text{L/mol})\} = 133.252 - 42.967 \cdot \log (T/K) - 6955.2/(T/K)$ ; temp range  $273.16$ – $322.91$  K (Glew & Moelwyn-Hughes 1953)

653\* ( $29.43^\circ\text{C}$ , concn ratio, measured range  $29.43$ – $40.34^\circ\text{C}$ , Swain & Thornton 1962)

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

$\ln K_{AW} = 10.34 - 3541/(T/K)$ ; measured range  $5$ – $33^\circ\text{C}$  (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

287 (computed value, Yaws et al. 1991)

159, 442 ( $0$ ,  $20^\circ\text{C}$ , distilled water, headspace-GC, Elliott & Rowland 1993)

429 ( $20^\circ\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 1996)

414 ( $20^\circ\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{AW} = 4.059 - 1416/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

1.69 ( $19^\circ\text{C}$ , shake flask, Collander 1951)

1.51 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

1.51 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^\circ\text{C}$ :

2.16 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

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: photooxidation  $t_{1/2} = 535$ – $5348$  h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).

Hydrolysis:  $k = 7.28 \times 10^{-8} \text{ s}^{-1}$  at pH 7 (extrapolated to  $25^\circ\text{C}$ ) with  $t_{1/2} = 110$  d (Mabey & Mill 1978).

Biodegradation: aqueous aerobic  $t_{1/2} = 1168$ – $672$  h, based on estimated aerobic half-life (Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 672$ – $2688$  h, based on estimated aerobic half-life (Howard et al. 1991).

Biotransformation:

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

## Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);  $t_{1/2} = 535\text{--}5348$  h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 168\text{--}672$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water:  $t_{1/2} = 336\text{--}1344$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 168\text{--}672$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

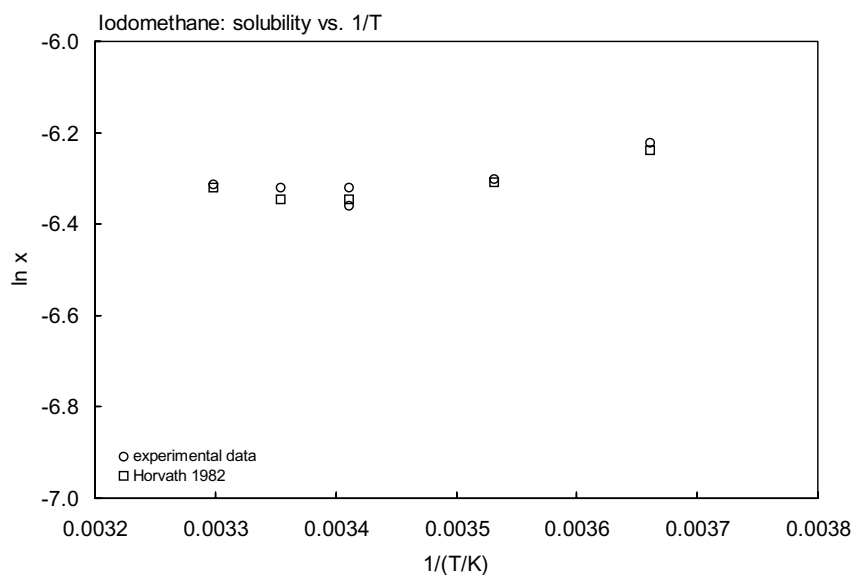
Biota:

**TABLE 5.1.3.1.1**

**Reported aqueous solubilities of iodomethane (methyl iodide) at various temperatures**

$$S/(\text{wt}\%) = 1.53863 - 0.012169 \cdot (t/^\circ\text{C}) + 1.2714 \times 10^{-4} \cdot (t/^\circ\text{C})^2 + 4.834 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

Rex 1906		Horvath 1982	
volumetric method		summary of literature data	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	15650	0	15386
10	14460	10	14345
20	14190	20	13848
30	14290	25	13848
		30	14185
		40	15646
		eq. 1	$S/\text{wt}\%$



**FIGURE 5.1.3.1.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for iodomethane.

TABLE 5.1.3.1.2

Reported vapor pressures of iodomethane (methyl iodide) at various temperatures and the coefficients for the vapor pressure equations

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

Thompson & Linnett 1936		Stull 1947		Boublik & Aim 1972	
		summary of literature data		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0.10	18932			-13.819	9306
4.30	22798	-55.5	666.6	-8.883	12046
11.70	31331	-45.8	1333	-5.101	14549
34.4	75860	-35.0	2666	-0.780	17921
		-24.2	5333	2.954	21314
		-16.9	7999	7.146	25780
		-7.0	13332	10.542	29923
		8.0	26664	14.567	35493
		25.3	53329	18.341	41470
		42.4	101325	22.879	49704
				28.342	61295
		mp/°C	-64.4	34.600	77125
				41.427	97913
				eq. 2	P/kPa
				A	6.11297
				B	1146.368
				C	236.677
				bp	42.431

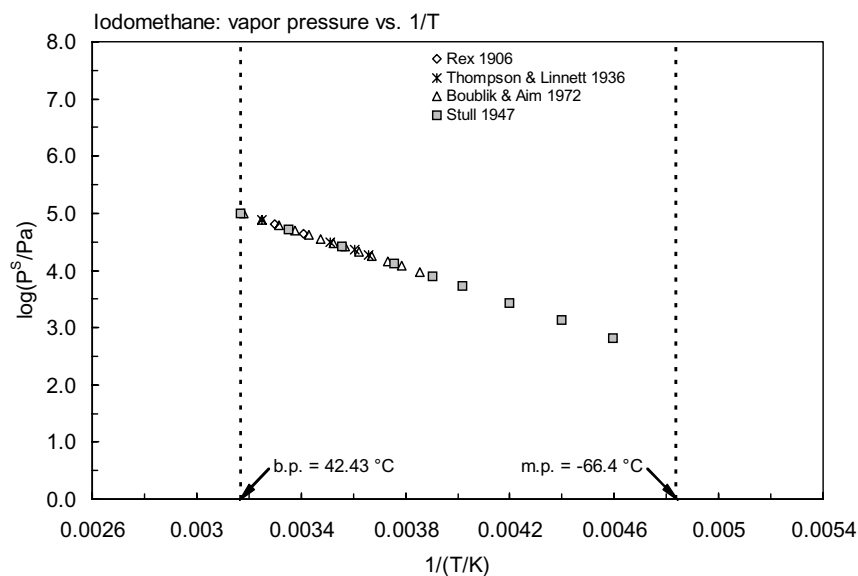
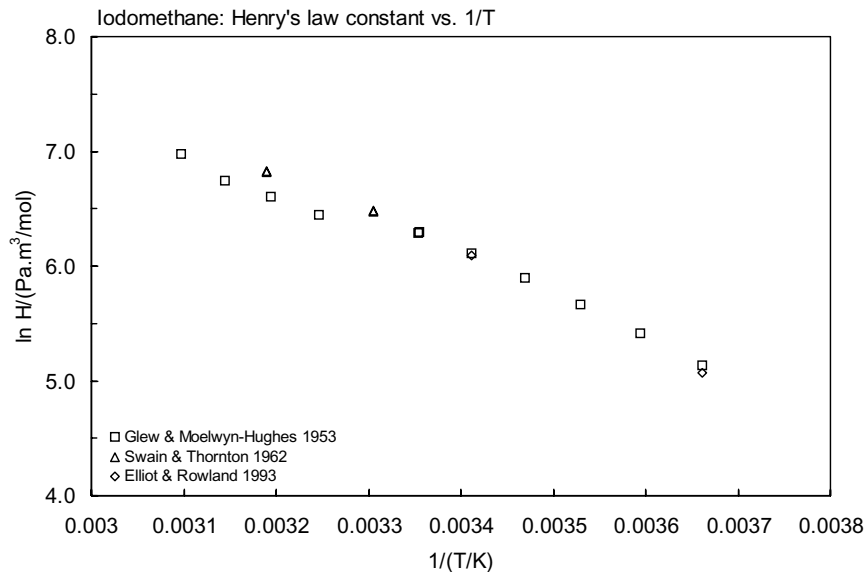


FIGURE 5.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodomethane.



**TABLE 5.1.3.1.3**  
**Reported Henry’s law constants of iodomethane (methyl iodide) 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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)			
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
$\log H = A - B \cdot \log (T/K) - C/(T/K)$		(6)			
<b>Glew &amp; Moelwyn-Hughes 1953</b>		<b>Swain &amp; Thornton 1962</b>		<b>Elliot &amp; Rowland 1993</b>	
<b>concentration ratio</b>		<b>concentration ratio</b>		<b>headspace-GC</b>	
<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>	<b>t/°C</b>	<b>H/(Pa m³/mol)</b>
0	169.9	29.45	653	0	159
5.03	224.8	29.44	651	20	442
10.2	288.0	40.35	923		
15.12	364.0	40.34	913		
19.94	450.6				
24.92	541.2				
34.92	630.6				
39.86	738.6				
44.87	850.6				
49.75	1072				
25.0	536				
eq 6	P/(mmHg·L/mol)				
A	71.005				
B	21.656				
C	4043.9				



**FIGURE 5.1.3.1.3** Logarithm of Henry’s law constant versus reciprocal temperature for iodomethane.

## 5.1.3.2 Iodoethane (Ethyl iodide)



Common Name: Ethyl iodide

Synonym: iodoethane

Chemical Name: ethyl iodide, iodoethane,

CAS Registry No: 75-03-6

Molecular Formula:  $C_2H_5I$ ,  $CH_3CH_2I$

Molecular Weight: 155.965

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

-111.1 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)

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

72.30 (Rex 1906; Dreisbach 1961; Horvath 1982; Riddick et al. 1986; Lide 2003)

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

1.9358, 1.9245 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

1.9357, 1.9244 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

80.6 ( $20^{\circ}C$ , calculated from density)

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

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

31.93, 29.77 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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):

4030\* ( $20^{\circ}C$ , volumetric method, measured range  $0-30^{\circ}C$ , Rex 1906;)

3910 ( $22.5^{\circ}C$ , volumetric method, Fühner 1924)

4040 ( $30^{\circ}C$ , shake flask-interferometry, Gross & Saylor 1931)

4040 ( $30^{\circ}C$ , shake flask, Van Arkel & Vles 1936)

3915 ( $20^{\circ}C$ , Merckel 1937)

3918 (Seidell 1940, 1941; quoted, Deno & Berkheimer 1960; Hansch et al. 1968; Hine & Mookerjee 1975)

3915 ( $22.5^{\circ}C$ , Saracco & Spaccamela Marchetti 1958)

3920 ( $20^{\circ}C$ , exptl., Korenman et al. 1971)

4041\* (summary of literature data temp range  $0-30^{\circ}C$ , Horvath 1982)

3880 ( $30^{\circ}C$ , selected, Riddick et al. 1986)

4000\* (tentative value, temp range  $0-30^{\circ}C$ , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 8.5757 - 5.5568 \times 10^{-2} \cdot (T/K) + 9.43918 \times 10^{-5} \cdot (T/K)^2$ , temp range 273–303 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

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):

14280, 22150 ( $20^{\circ}C$ ,  $30^{\circ}C$ , Rex 1906)

21678\* ( $30^{\circ}C$ , manometry, measured range  $30-60^{\circ}C$ , Smyth & Engel 1929)

14612\* ( $20^{\circ}C$ , temp range  $-19.36$  to  $20.4^{\circ}C$ , Milazzo 1944)

13332\* ( $18^{\circ}C$ , summary of literature data, temp range  $-54.4$  to  $72.4^{\circ}C$ , Stull 1947)

18160 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/mmHg) = 6.83198 - 1175.709/(225.26 + t/^{\circ}C)$ ; temp range  $-6$  to  $109^{\circ}C$ , (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.83198 - 1175.709/(225.26 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/mmHg) = [-0.2185 \times 6843.1/(T/K)] + 7.635277$ ; temp range  $-74.3$  to  $229.5^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log (P/\text{kPa}) = 7.12695 - 1823.148/(285.30 + t/^{\circ}\text{C})$ ; temp range  $-19.36$  to  $20.4^{\circ}\text{C}$  (Antoine eq. derived from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.06765 - 1222.410/(228.368 + t/^{\circ}\text{C})$ , temp range  $30$ – $60^{\circ}\text{C}$  (Antoine eq. derived from reported experimental data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.959 - 1232.0/(229.0 + t/^{\circ}\text{C})$ ; temp range  $30$ – $60^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)

$\log (P/\text{kPa}) = 5.95688 - 1175.709/(225.26 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986) 18430 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.95686 - 1175.709/(-47.89 + T/\text{K})$ ; temp range  $249$ – $369$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 31.4422 - 2.5719 \times 10^3/(T/\text{K}) - 8.4867 \cdot \log (T/\text{K}) - 9.0736 \times 10^{-11} \cdot (T/\text{K}) + 3.571 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range  $162$ – $561$  K (vapor pressure eq., Yaws 1994)

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

732 (calculated- $1/K_{\text{AW}}$ ,  $C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)

840 (calculated-QSAR, Nirmalakhandan & Speece 1988)

545 (computed value, Yaws et al. 1991)

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

2.00 (shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)

2.00 (recommended, Sangster 1989, 1993)

2.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{\text{OA}}$  at  $25^{\circ}\text{C}$ :

2.59 (calculated-measured infinite dilution activity coeff. and vapor pressure  $P$ , Abraham et al. 2001)

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

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

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

Hydrolysis: rate constant  $k = 1.62 \times 10^{-7} \text{ s}^{-1}$  with  $t_{1/2} = 49$  d at  $25^{\circ}\text{C}$  and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4$ – $24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water:  $t_{1/2} = 49$  d at  $25^{\circ}\text{C}$  and pH 7 (Mabey & Mill 1978)

Ground water:

Sediment:

Soil:

Biota:

**TABLE 5.1.3.2.1****Reported aqueous solubilities of 1-iodoethane at various temperatures**

$$S/(\text{wt}\%) = 0.4391 - 3.24498 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 4.49991 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 1.15001 \times 10^{-6} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 8.5757 - 5.5568 \times 10^{-2} \cdot (T/\text{K}) + 9.43918 \times 10^{-4} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999a	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0	4410	0	4391	0	4400
10	4140	10	4123	5	4220
20	4030	20	4014	10	4090
30	4150	25	4041	15	4010
		30	4133	20	3980
		eq. 1	S/wt%	25	4000
				30	4050
				eq. 2	S/wt%
				temp range 273–303 K	

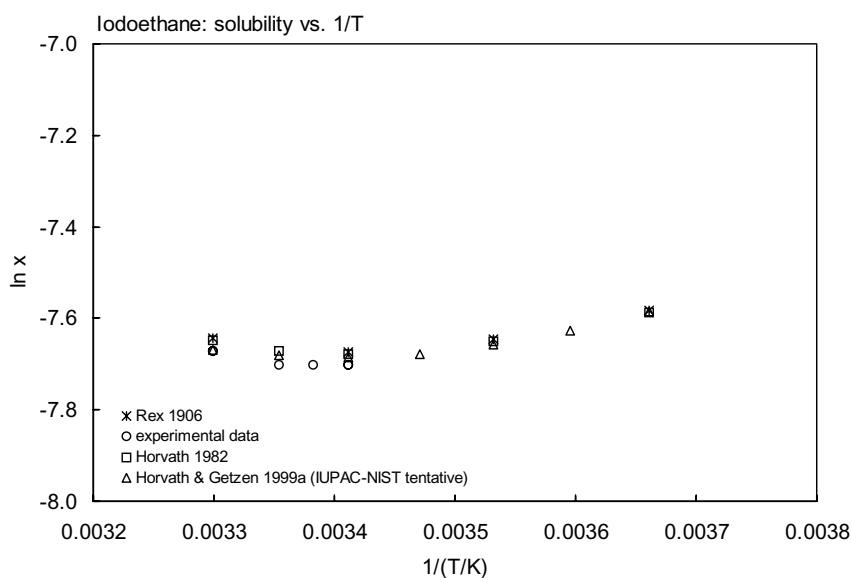
**FIGURE 5.1.3.2.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for iodoethane.

TABLE 5.1.3.2.2

Reported vapor pressures of iodoethane at various temperatures and the coefficients for the vapor pressure equations

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

Smyth & Engel 1929		Milazzo 1944		Stull 1947	
Manometry				summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.0	21678	-19.36	1867	-54.4	133.3
40.0	32637	0.040	5533	-34.3	666.6
50.0	47329	9.34	8666	-24.3	1333
60.0	67448	10.4	9066	-13.1	2666
		20.4	14612	-0.90	5333
				7.2	7999
				18.0	13332
				34.1	26664
				52.3	53329
				72.4	101325
				mp/°C	-105

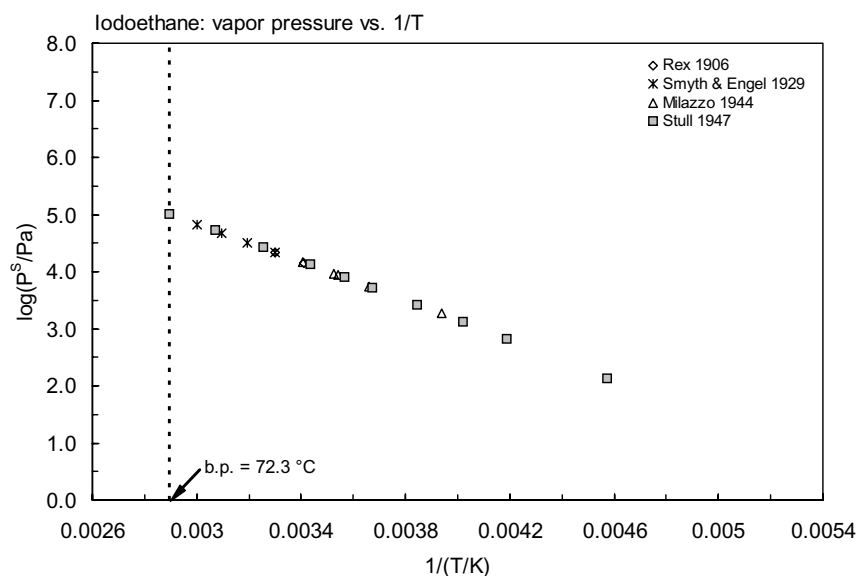
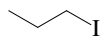


FIGURE 5.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for iodoethane.

## 5.1.3.3 1-Iodopropane



Common Name: 1-Iodopropane

Synonym: monoiodopropane, *n*-propyl iodide, propyl iodide

Chemical Name: 1-iodopropane, monoiodopropane, *n*-propyl iodide, propyl iodide

CAS Registry No: 107-08-4

Molecular Formula: C<sub>3</sub>H<sub>7</sub>I, CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>I

Molecular Weight: 169.992

Melting Point (°C):

−101.3 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):

102.5 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.7489, 1.7394 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)

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

97.2 (20°C, calculated-density)

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

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

45.98, 31.70 (25°C, bp, Dreisbach 1961)

36.25 (25°C, Riddick et al. 1986)

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

1070\* (20°C, volumetric method, measured range 0–30°C, Rex 1906)

867 (20°C, volumetric method, Fühner 1924)

1040 (30°C, shake flask-interferometer, Gross & Saylor 1931)

1037 (30°C, shake flask, Van Arkel & Vles 1936)

1073 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

872 (Seidell 1941)

1110 (calculated-K<sub>OW</sub>, Hansch et al. 1968)

1070, 1060 (23.5°C, elution chromatography, Schwarz 1980)

1051\* (summary of literature data, temp range 0–30°C, Horvath 1982)

1000 (Dean 1985)

1040 (30°C, quoted, Riddick et al. 1986)

1010\* (tentative value, temp range 0–30°C, IUPAC-NIST Series, Horvath & Getzen 1999b)

S/(wt%) = 3.4659 − 0.023046·(T/K) + 3.94424 × 10<sup>−5</sup>·(T/K)<sup>2</sup>, temp range 273–303 K (equation derived from literature data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

4679, 7305 (20°C, 30°C, volumetric method Rex, 1906)

5333 (23.6°C, summary of literature, data temp range −36.0 to 102.5°C, Stull 1947)

5745 (calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.81603 − 1267.062/(219.53 + t/°C); temp range 18–143°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.81603 − 1267.062/(219.53 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

log (P/mmHg) = [−0.2185 × 8467.1/(T/K)] + 7.824521; temp range −36.0 to 102.5°C (Antoine eq., Weast 1972–73)

5745 (quoted lit. average, Riddick et al. 1986)

log (P/kPa) = 5.94053 − 1267.062/(219.53 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

5745 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.6036 - 1160.5/(-59.55 + T/\text{K})$ ; temp range 171–271 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.94093 - 1267.062/(-52.62 + T/\text{K})$ ; temp range 271–402 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 1.2733 - 2.0214 \times 10^3/(T/\text{K}) + 4.1138 \cdot \log (T/\text{K}) - 1.2477 \times 10^{-2} \cdot (T/\text{K}) + 7.678 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 172–593 K (vapor pressure eq., Yaws 1994)

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

921 (calculated as  $1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}$ , reported as exptl., Hine & Mookerjee 1975)

1033, 1082 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1057 (calculated-QSAR, Nirmalakhandan & Speece 1988)

844 (computed value, Yaws et al. 1991)

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

2.50 (calculated- $\pi$  const., Hansch et al. 1968)

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

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

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

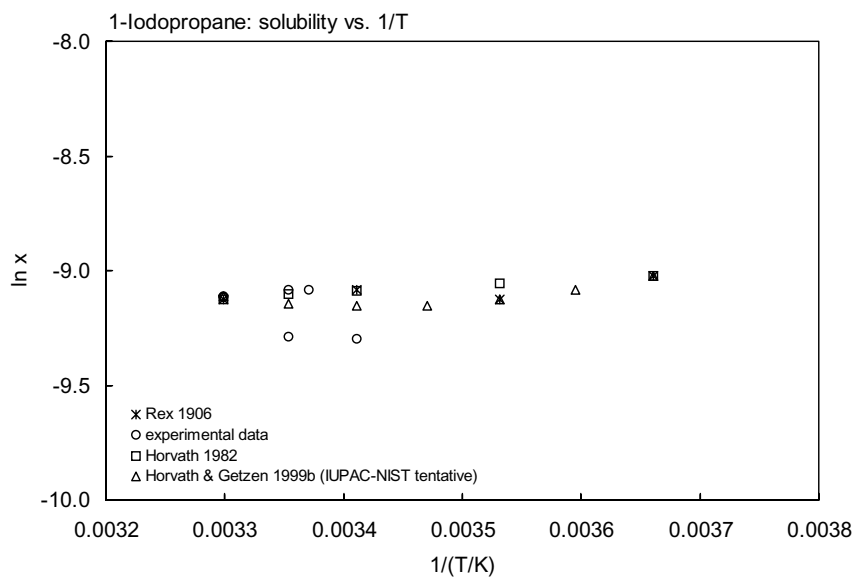
**TABLE 5.1.3.3.1**

**Reported aqueous solubilities of 1-iodopropane at various temperatures**

$$S/(\text{wt}\%) = 0.1139 - 4.86669 \times 10^{-4} \cdot (t/^\circ\text{C}) + 1.25003 \times 10^{-5} \cdot (t/^\circ\text{C})^2 - 2.8334 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 3.4659 - 0.023046 \cdot (T/\text{K}) + 3.94424 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999b	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	1140	0	1139	0	1140
10	1030	10	1100	5	1070
20	1070	20	1069	10	1030
30	1030	25	1051	15	1000
		30	1029	20	1000
				25	1010
		eq. 1	$S/\text{wt}\%$	30	1040
				eq. 2	$S/\text{wt}\%$
				temp range 273–303 K	



**FIGURE 5.1.3.3.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-iodopropane.



## 5.1.3.4 2-Iodopropane



Common Name: 2-Iodopropane

Synonym: isopropyl iodide

Chemical Name: 2-iodopropane, isopropyl iodide

CAS Registry No: 75-30-9

Molecular Formula:  $C_3H_7I$ ,  $CH_3CHICH_3$

Molecular Weight: 169.992

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

−90.0 (Riddick et al. 1986; Lide 2003)

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

89.50 (Riddick et al. 1986; Lide 2003)

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

1.7042, 1.6946 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

99.8, 100.3 ( $20^{\circ}C$ ,  $25^{\circ}C$ , calculated-density)

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

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

34.06 ( $25^{\circ}C$ , Riddick et al. 1986)

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):

1670, 1430, 1400, 1340 (0, 10, 20,  $30^{\circ}C$ , volumetric method, Rex 1906)

1343 ( $30^{\circ}C$ , shake flask, Van Arkel & Vles 1936)

1667, 1428, 1398, 1387, 1338 (0, 10, 20, 25,  $30^{\circ}C$ , summary of literature data, Horvath 1982)

$S/(wt\%) = 0.1667 - 4.23167 \times 10^{-3} \cdot t/^{\circ}C + 0.000224 \cdot (t/^{\circ}C)^2 - 3.98334 \times 10^{-6} \cdot (t/^{\circ}C)^3$  (Horvath 1982)

1400 ( $20^{\circ}C$ , selected, Riddick et al. 1986)

1670, 1430, 1400, 1340 (0, 10, 20,  $30^{\circ}C$ , reported exptl data of Rex 1906, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

7518, 11780 ( $20^{\circ}C$ ,  $30^{\circ}C$ , Rex 1906)

7999 ( $21.6^{\circ}C$ , summary of literature data, temp range  $-43.3$  to  $89.5^{\circ}C$ , Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 8243.4/(T/K)] + 7.873828$ ; temp range  $-43.3$  to  $89.5^{\circ}C$  (Antoine eq., Weast 1972–73)

5700 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.87492 - 1765.15/(T/K)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

9360 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2763 - 1414.85/(-31.45 + T/K)$ ; temp range 261–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.2724 - 989.55/(-69.18 + T/K)$ ; temp range 173–262 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 33.2023 - 2.7569 \times 10^3/(T/K) - 9.0585 \cdot \log(T/K) - 1.2099 \times 10^{-10} \cdot (T/K) + 3.5044 \times 10^{-6} \cdot (T/K)^2$ ; temp range 183–578 K (vapor pressure eq., Yaws 1994)

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

1133 (calculated- $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

2479, 1982 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1840 (calculated-QSAR, Nirmalakhandan & Speece 1988)

903 (computed value, Yaws et al. 1991)

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

Bioconcentration Factor,  $\log BCF$ :

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

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

Hydrolysis: rate constant  $k = 2.77 \times 10^{-6} \text{ s}^{-1}$  with  $t_{1/2} = 2.9 \text{ d}$  at  $25^\circ\text{C}$  and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water:  $t_{1/2} = 2.9 \text{ d}$  at  $25^\circ\text{C}$  and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)

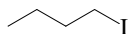
Ground water:

Sediment:

Soil:

Biota:

## 5.1.3.5 1-Iodobutane



Common Name: 1-Iodobutane

Synonym: *n*-butyl iodide, moniodobutane

Chemical Name: *n*-butyl iodide, 1-iodobutane, moniodobutane

CAS Registry No: 542-69-8

Molecular Formula:  $C_4H_9I$ ,  $CH_3CH_2CH_2CH_2I$

Molecular Weight: 184.018

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

−103.0 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)

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

130.53 (Dreisbach 1961; Riddick et al. 1986)

130.5 (Lide 2003)

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

1.6154, 1.6072 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961; Riddick et al. 1986)

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

113.9, 114.5 ( $20^{\circ}C$ ,  $25^{\circ}C$ , calculated- density, Riddick et al. 1986)

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

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

40.63, 33.40 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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  $25^{\circ}C$ ):

210 ( $17.5^{\circ}C$ , volumetric method, Fühner 1924)

202 ( $20^{\circ}C$ , Merckel 1937)

211 (Seidell 1940; quoted, Deno & Berkheimer 1960)

202 (Seidell 1941)

313 (Kakovsky 1957)

182 (selected exptl., Horvath 1982)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

1848 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/mmHg) = 6.82262 - 1358.860/(214.2 + t/^{\circ}C)$ ; temp range  $40-174^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.82262 - 1358.860/(214.20 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq., from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/kPa) = 5.94752 - 1358.860/(214.20 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

1848 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.94752 - 1358.86/(-58.95 + T/K)$ ; temp range 292–431 K (Antoine eq., Stephenson & Malanowski 1987)

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

1600 (calculated- $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

1426, 600 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1331 (calculated-QSAR, Nirmalakhandan & Speece 1988)

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

3.00 (calculated- $\pi$  const., Hansch et al. 1968)

2.51 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

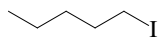
Sorption Partition Coefficient, log  $K_{OC}$ :

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).

## 5.1.3.6 1-Iodopentane



Common Name: 1-Iodopentane

Synonym: pentyl iodide

Chemical Name: 1-iodopentane

CAS Registry No: 628-17-1

Molecular Formula:  $C_5H_{11}I$ ,  $CH_3(CH_2)_3CH_2I$

Molecular Weight: 198.045

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

−85.6 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

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

157 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$ ):

1.5061, 1.5088 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1961)

1.5161 ( $20^{\circ}C$ , Weast 1982–83)

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

130.6 ( $20^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

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

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

43.33, 35.81 ( $25^{\circ}C$ , bp, Dreisbach 1961)

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):

585 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/mmHg) = 6.85172 - 1454.028/(209.17 + t/^{\circ}C)$ ; temp range  $61$ – $204^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.85172 - 1454.028/(209.17 + t/^{\circ}C)$ ; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log P_L/kPa = 5.97662 - 1454.028/(-63.98 + T/K)$ ; temp range 312–413 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  $\log K_B$ :

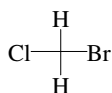
Sorption Partition Coefficient,  $\log K_{OC}$ :

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

Half-Lives in the Environment:

## 5.1.4 MIXED HALOGENATED HYDROCARBONS

## 5.1.4.1 Bromochloromethane



Common Name: Bromochloromethane

Synonym: chlorobromomethane, methylene bromochloride

Chemical Name: bromochloromethane, chlorobromomethane

CAS Registry No: 74-97-5

Molecular Formula:  $\text{CH}_2\text{BrCl}$

Molecular Weight: 129.384

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

-87.9 (Lide 2003)

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

68.0 (Lide 2003)

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

1.9344 (Dreisbach 1959; Weast 1982–83; Riddick et al. 1986)

1.9229 ( $25^{\circ}\text{C}$ , Dreisbach 1959)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

66.89 ( $20^{\circ}\text{C}$ , calculated-density)

73.8 (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  $25^{\circ}\text{C}$ , F: 1.0

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

15000 (O'Connell 1963)

9000 (Kirk-Othmer 1964, Irmann 1965, Dean 1985)

15000 (Jolls 1966)

14778 (at saturated pressure, recommended, Horvath 1982)

16690 (generator column-GC, Tewari et al. 1982)

38900 (calculated-UNIFAC activity coeff., Arbuckle 1986)

17000 (selected, Riddick et al. 1986)

Vapor Pressure (Pa at  $25^{\circ}\text{C}$  and reported temperature dependence equations):

18808 ( $24.06^{\circ}\text{C}$ , ebulliometric method, measured range  $15.72$ – $68^{\circ}\text{C}$ , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 6.38587 - 895.556/(186.703 + t/^{\circ}\text{C})$ ; temp range  $15.72$ – $68.0^{\circ}\text{C}$  (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)

19620 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/\text{mmHg}) = 6.86624 - 1132.3/(215.0 + t/^{\circ}\text{C})$ ; temp range  $-6$  to  $297^{\circ}\text{C}$  (Antoine eq. for liquid state, Dreisbach 1959)

19520 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.49606 - 942.267/(192.587 + t/^{\circ}\text{C})$ ; temp range  $15.7$ – $68^{\circ}\text{C}$  (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1973)

19520 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 6.41307 - 903.382/(187.594 + t/^{\circ}\text{C})$ ; temp range  $16$ – $68^{\circ}\text{C}$  (Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{kPa}) = 6.60056 - 932.609/(191.376 + t/^{\circ}\text{C})$ ; temp range  $15.7$ – $68^{\circ}\text{C}$  (Antoine eq. from reported exptl. data of McDonald & Shrader 1959, Boublik et al. 1984)

19530 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.51146 - 891.345/(-86.965 + T/\text{K})$ ; temp range  $226$ – $341$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 2.7704 - 2.0139 \times 10^3/(T/K) + 3.7817 \cdot \log (T/K) - 1.3241 \times 10^{-2} \cdot (T/K) + 8.1979 \times 10^{-6} \cdot (T/K)^2$ ;  
temp range 185–557 K (vapor pressure eq., Yaws 1994)  
19257 (selected summary of literature data, temp range 185.21–368.15 K, Xiang 2002)

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

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

1.41 (generator column-GC, Tewari et al. 1982)  
1.41 (recommended, Sangster 1993)  
1.41 (recommended, Hansch et al. 1995)

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:

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:

rate constant for the reaction with OH:  $k = (2.5 \pm 0.3) \times 10^{-6} \text{ M}^{-1} \text{ s}^{-1}$  was measured in 66.7% dioxane-water at 35.7°C (Hine et al. 1956; quoted, Roberts et al. 1992)

$k_{OH} = 1.11 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with atmospheric lifetime  $\tau = 0.43 \text{ yr}$  at 298 K, measured range 277–377 K (flash photolysis resonance fluorescence and discharge flow electron paramagnetic resonance, Orkin et al. 1997)

Hydrolysis: rate constant  $k = 1.2 \times 10^{-10} \text{ s}^{-1}$  with  $t_{1/2} = 44 \text{ yr}$  at pH 7 and 25°C (Mabey & Mill 1978)

Biodegradation:

Biotransformation:

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

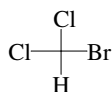
Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)

Atmospheric lifetime  $\tau = 0.21 \text{ yr}$  reduced from 0.43 yr due to reaction with OH with ocean removal (Orkin et al. 1997)

Surface water: hydrolysis rate constant  $k = 1.2 \times 10^{-10} \text{ s}^{-1}$  with  $t_{1/2} = 44 \text{ yr}$  at pH 7 and 25°C (Mabey & Mill 1978)

## 5.1.4.2 Bromodichloromethane



Common Name: Bromodichloromethane

Synonym: dichlorobromomethane

Chemical Name: bromodichloromethane, dichlorobromomethane

CAS Registry No: 75-27-4

Molecular Formula:  $\text{CHBrCl}_2$

Molecular Weight: 163.829

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

-57 (Lide 2003)

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

90.0 (Weast 1977; Lide 2003)

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

1.9710 ( $25^{\circ}\text{C}$ , Verschueren 1983)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

83.1 ( $20^{\circ}\text{C}$ , calculated-density)

94.7 (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  $25^{\circ}\text{C}$ , F: 1.0

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

4700 ( $22^{\circ}\text{C}$ , Mabey et al. 1981)

2968 ( $30^{\circ}\text{C}$ , headspace-GC, McNally & Grob 1984)

8880, 8668, 8506 ( $20, 30, 40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)

Vapor Pressure (Pa at  $25^{\circ}\text{C}$  or as indicated and reported temperature dependence equations):

6665 ( $20^{\circ}\text{C}$ , Dreisbach 1952;)

8555, 13440, 20444 ( $20, 30, 40^{\circ}\text{C}$ , DIPPR compilation, Tse et al. 1992)

Henry's Law Constant (Pa  $\text{m}^3/\text{mol}$  at  $25^{\circ}\text{C}$  and reported temperature dependence equations):

244.2 ( $20^{\circ}\text{C}$ , calculated-P/C, Mabey et al. 1982)

162 ( $20^{\circ}\text{C}$ , batch air stripping-GC, Nicholson et al. 1984)

162, 152, 152 ( $20^{\circ}\text{C}$ , batch stripping-GC, natural potable water samples, Nicholson et al. 1984)

$\ln [H/(\text{atm m}^3/\text{mol})] = 11.30 - 5210/(T/K)$ ; temp range  $10$ – $30^{\circ}\text{C}$  (air stripping-GC measurements, Nicholson et al. 1984)

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

243.1 ( $20$ – $25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

243 (calculated-P/C, Mackay & Shiu 1990)

162, 263, 405 ( $20, 30, 40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)

55.2, 106, 192 ( $0, 10, 20^{\circ}\text{C}$ , seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

$\ln K_{\text{AW}} = 13.43 - 4678/(T/K)$ ; seawater of salinity of 30.4‰, temp range:  $0$ – $10^{\circ}\text{C}$  (Moore et al. 1995)

185 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.143 - 2130/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

347 ( $37^{\circ}\text{C}$ , equilibrium headspace-GC, Batterman et al. 2002)

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

1.88 (calculated as per Tute 1971, Callahan et al. 1979; Mills et al. 1982)

2.10 (Hansch & Leo 1979)

2.10 (calculated, Mabey et al. 1982)

2.00 (recommended, Sangster 1993)



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

2.98; 2.97 (equilibrium headspace-GC; calculated- $K_{OW}/K_{AW}$ , Batterman et al. 2002)

Bioconcentration Factor,  $\log BCF$ :

1.544 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)

0.72–1.37 (estimated as per Lyman et al. 1982, Howard 1990)

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

1.785 (sediment-water, calculated- $K_{OW}$ , Mabey et al. 1982)

1.724–2.40 (estimated from  $S$  &  $K_{OW}$ , Swann et al. 1983; quoted, Howard 1990)

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

Volatilization: typical  $t_{1/2}$  ~35 h for a range of 33 min to 12 d was estimated from experimentally determined gas transfer rates (Kaczmar et al. 1984; quoted, Howard 1990).

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:

calculated rate constants at 25°C:  $k < 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 0.2 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982).

Hydrolysis: first-order rate constant  $k = 1.6 \times 10^{-10} \text{ s}^{-1}$  at pH 7 and 25°C with a maximum  $t_{1/2} = 137 \text{ yr}$  (Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard 1990).

Biodegradation:

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

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

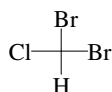
Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24 \text{ h}$  from air for the reaction with OH radical (Darnall et al. 1976);

$t_{1/2} = 3.92 \text{ months}$ , based on an estimated rate constant  $k = 8.522 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the vapor phase reaction with hydroxyl radical (GEMS 1987; quoted, Howard 1990).

Surface water: hydrolysis rate constant  $k = 1.6 \times 10^{-10} \text{ s}^{-1}$  with  $t_{1/2} = 137 \text{ yr}$  at pH 7 and 25°C (Mabey & Mill 1978)

## 5.1.4.3 Dibromochloromethane



Common Name: Dibromochloromethane

Synonym: chlorodibromomethane

Chemical Name: dibromochloromethane, chlorodibromomethane

CAS Registry No: 124-48-1

Molecular Formula:  $\text{CHBr}_2\text{Cl}$

Molecular Weight: 208.280

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

-22.0 (Dean 1985)

-20 (Lide 2003)

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

119–120 (Weast 1977; Weast 1982–83)

120 (Lide 2003)

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

2.451 (Weast 1982–83; Dean 1985)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

84.98 ( $20^{\circ}\text{C}$ , calculated-density)

97.1 (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  $25^{\circ}\text{C}$ , F: 1.0

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

4000 (calculated- $K_{\text{OW}}$ , Mabey et al. 1982)

5814, 6000, 6102 (20, 30,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)

Vapor Pressure (Pa at  $25^{\circ}\text{C}$  and reported temperature dependence equations):

10131 ( $20^{\circ}\text{C}$ , extrapolated-Antoine eq., Mabey et al. 1982)

2000 ( $20^{\circ}\text{C}$ , selected, Mills et al. 1982)

6667 ( $20^{\circ}\text{C}$ , Warner et al. 1987)

2324, 3877, 6232 (20, 30,  $40^{\circ}\text{C}$ , DIPPR compilation, Tse et al. 1992)

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

100 ( $20^{\circ}\text{C}$ , calculated-P/C, Mabey et al. 1982)

88.2; 88.1, 85.1 ( $20^{\circ}\text{C}$ , batch air stripping-GC; quoted lit. values, Nicholson et al. 1984)

86.1, 81.06, 78.02 ( $20^{\circ}\text{C}$ , batch stripping-GC, natural potable water samples, Nicholson et al. 1984)

$\ln [H/(\text{atm m}^3/\text{mol})] = 10.70 - 5210/(T/K)$ ; temp range  $10$ – $30^{\circ}\text{C}$  (air stripping-GC measurements, Nicholson et al. 1984)

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

120\* (EPICS-GC/FID, measured range  $10$ – $30^{\circ}\text{C}$ , Ashworth et al. 1988)

$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 14.62 - 6373/(T/K)$ ; temp range  $10$ – $30^{\circ}\text{C}$ , (EPICS measurements, Ashworth et al. 1988)

100 ( $20$ – $25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

81.06, 142, 223 (20, 30,  $40^{\circ}\text{C}$ , infinite dilution activity coeff.  $\gamma$ -GC, Tse et al. 1992)

28.2, 56.3, 103 (0, 10,  $20^{\circ}\text{C}$ , seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

$\ln K_{\text{AW}} = 13.62 - 4914/(T/K)$ ; seawater of salinity of 30.4‰, temp range:  $0$ – $10^{\circ}\text{C}$  (Moore et al. 1995)

85.3 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.296 - 2273/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

218 ( $37^{\circ}\text{C}$ , equilibrium headspace-GC, Batterman et al. 2002)

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

- 2.09 (calculated as per Tute 1971, Callahan et al. 1979)
- 2.24 (Hansch & Leo 1979)
- 2.24 (calculated, Mabey et al. 1982)
- 2.16 (recommended, Sangster 1993)
- 2.04 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C:

- 3.59 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)
- 3.33; 3.31 (equilibrium headspace-GC; calculated- $K_{OW}/K_{AW}$ , Batterman et al. 2002)

Bioconcentration Factor,  $\log BCF$ :Sorption Partition Coefficient,  $\log K_{OC}$ :Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Volatilization: calculated  $t_{1/2} = 43$  min to 16.6 d (using Langbein & Durum 1967 published  $O_2$  re-aeration values) and  $t_{1/2} = 45.9$  h both from rivers and streams (Kaczmar et al. 1984).

## Photolysis:

Oxidation: calculated rate constants at 25°C:  $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 0.5 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radicals (Mabey et al. 1982);

photooxidation  $t_{1/2} = 1025\text{--}10252$  h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: rate constant  $k = 8.0 \times 10^{-11} \text{ s}^{-1}$  with hydrolytic  $t_{1/2} = 274$  yr at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard et al. 1991);

$k = 2.88 \times 10^{-8} \text{ h}^{-1}$  at pH 7 and 25°C (analogy to chloroform as per Mabey & Mill 1978, Mabey et al. 1982).

Biodegradation: aqueous aerobic  $t_{1/2} = 672\text{--}4320$  h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 672\text{--}4320$  h, based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; Bouwer et al. 1981; quoted, Howard et al. 1991).

Biotransformation: estimated rate constant  $k = 1.0 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

## Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);  $t_{1/2} = 1025\text{--}10252$  h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 274$  yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2} = 672\text{--}4320$  h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 336\text{--}4320$  h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

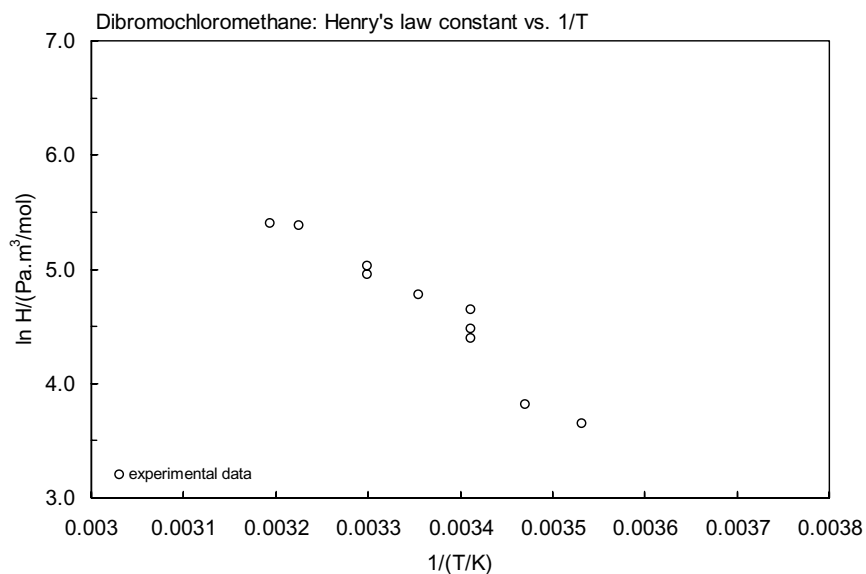
## Sediment:

Soil:  $t_{1/2} = 672\text{--}4320$  h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

## Biota:

**TABLE 5.1.4.3.1**  
**Reported Henry's law constants of dibromochloromethane**  
**at various temperatures**

Ashworth et al. 1988	
EPICS-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)
10	38.50
15	45.60
20	104.4
25	119.6
30	154.0
ln [H/(atm·m <sup>3</sup> /mol)] = A – B/(T/K)	
A	14.62
B	6373



**FIGURE 5.1.4.3.1** Logarithm of Henry's law constant versus reciprocal temperature for dibromochloromethane.

## 5.1.4.4 Chlorodifluoromethane (HCFC-22)



Common Name: Chlorodifluoromethane

Synonym: difluorochloromethane, Freon 22, CFC-22, CF-22

Chemical Name: chlorodifluoromethane

CAS Registry No: 75-45-6

Molecular Formula:  $\text{CHClF}_2$

Molecular Weight: 86.469

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

−157.42 (Lide 2003)

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

−40.7 (Lide 2003)

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

1.2090 ( $21^{\circ}\text{C}$ , Dean 1985)

1.1940 ( $25^{\circ}\text{C}$ , Kirk-Othmer 1985)

1.2136, 1.1942 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Riddick et al. 1986)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

71.2 ( $20^{\circ}\text{C}$ , calculated-density)

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

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

20.238 (bp, Riddick et al. 1986)

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

4.123 (Riddick et al. 1986)

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

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

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

2800, 2900 (quoted values, Irmann 1965)

3000 (DuPont 1966, 1969; quoted, Horvath 1982; Riddick et al. 1986)

2930 (selected, Hine & Mookerjee 1975)

3000 (Weast 1976; quoted, Horvath 1982)

2899\* (summary of literature data, temp range  $0$ – $60^{\circ}\text{C}$ , Horvath 1982)

3000 (Dean 1985)

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

101325\* ( $-40.8^{\circ}\text{C}$ , summary of literature data, temp range  $-122.8$  to  $-40.8^{\circ}\text{C}$ , Stull 1947)

1083100 (calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 5212.9/(T/\text{K})] + 7.730042$ ; temp range  $-122.8$  to  $85.3^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = 6.93892 - 808.919/(t/^{\circ}\text{C} + 240.161)$ ; temp range  $-79$  to  $-37^{\circ}\text{C}$  (Antoine eq., Kudchadker et al. 1979)

1027400 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.0741 - 815.920/(241.369 + t/^{\circ}\text{C})$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

35120, 570500 ( $-61.26^{\circ}\text{C}$ ,  $4.5^{\circ}\text{C}$ , Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.06382 - 808.919/(240.161 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

1043900 (Interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.33292 - 919.834/(-19.718 + T/\text{K})$ ; temp range  $170$ – $233$  K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.19138 - 863.436/(-26.04 + T/\text{K})$ ; temp range 230–275 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.35713 - 950.38/(-13.474 + T/\text{K})$ ; temp range 275–327 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.13064 - 1490.048/(64.627 + T/\text{K})$ ; temp range 324–366 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 40.3847 - 2.0731 \times 10^3/(T/\text{K}) - 12.317 \cdot \log (T/\text{K}) - 2.5116 \times 10^{-10} \cdot (T/\text{K}) + 1.0498 \times 10^{-5} \cdot (T/\text{K})^2$ ; temp range 116–369 K (vapor pressure eq., Yaws 1994)

132020 (238.15 K, selected summary of literature data, temp range 15.74–238.15 K, Xiang 2002)

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

$\log (H/\text{atm}) = 8.18 - 1469.55/(T/\text{K})$  (least-square regression of data from lit., Kavanaugh & Trussell 1980)

2980 (calculated as  $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

2478.8 (calculated-QSAR, Nirmalakhandan & Speece 1988)

3058 (computed value, Yaws et al. 1991)

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

1.08 (shake flask, Log P Database, Hansch & Leo 1987)

1.08 (recommended, Sangster 1993)

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  $NO_3$  radical and  $k_{O_3}$  with  $O_3$  or as indicated, \*data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^* = (4.75 \pm 0.48) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 297–434 K, with estimated lifetime of ~1.5 yr (flash photolysis-resonance fluorescence, Atkinson et al. 1975)

$k_{OH} = (3.4 \pm 0.7) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH}^* = (4.25 \pm 0.28) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 253–427 K, with calculated lifetime of 16–25 yr in troposphere (discharge flow-resonance fluorescence, Chang & Kaufman 1977)

$k_{OH} = 4.8 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K with lifetime of 43 yr in troposphere, measured range 250–350 K (FP-RF, Watson et al. 1977; quoted, Altshuller 1980)

$k_{OH} = (2.76 \pm 0.35) \times 10^9 \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 297 K (relative rate, Paraskevopoulos et al. 1981)

$k_{OH}(\text{calc}) = 6.8 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{OH}(\text{obs.}) = 4.68 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH}^* = 4.68 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

$k_{OH} = 4.7 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with an estimated tropospheric lifetime of 4.3 yr, Bunce et al. 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} = 2.4\text{--}24$  h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); lifetime of 44 yr in troposphere (Altshuller 1980);

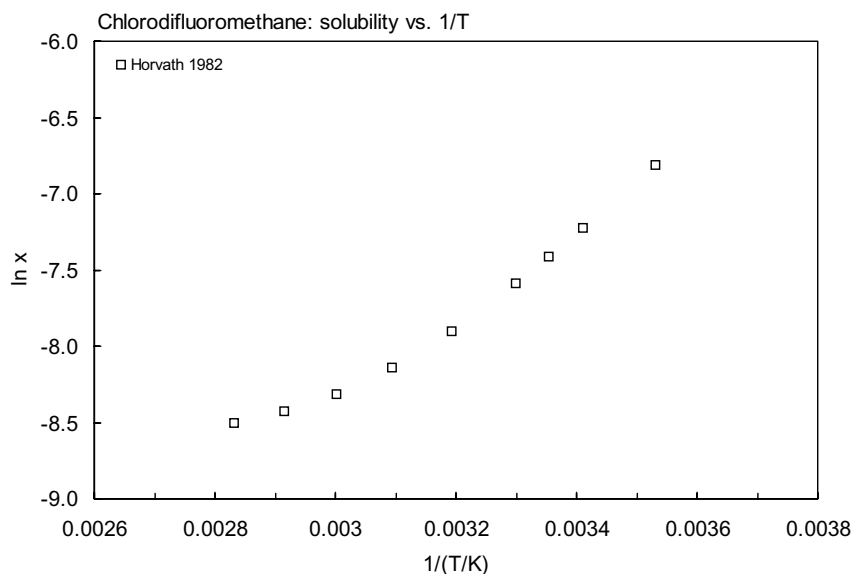
estimated tropospheric lifetime of 4.3 yr as global average for the reaction with hydroxyl radical in air (Bunce et al. 1991);

estimated tropospheric lifetime of 7.5 yr and 15.8 yr by rigorous calculation (Nimitz & Skaggs 1992).

**TABLE 5.1.4.4.1****Reported aqueous solubilities and vapor pressures of chlorodifluoromethane (HCFC-22) at various temperatures**

$$S/(\text{wt}\%) = 0.8171 - 3.5818 \times 10^{-2} \cdot (t/^{\circ}\text{C}) + 8.0081 \times 10^{-4} \cdot (t/^{\circ}\text{C})^2 - 1.0075 \times 10^{-5} \cdot (t/^{\circ}\text{C})^3 + 6.9823 \times 10^{-8} \cdot (t/^{\circ}\text{C})^4 \quad (1)$$

Aqueous solubility		Vapor pressure	
Horvath 1982		Stull 1947	
summary of literature data		summary of literature data	
t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa
10	5296	-122.8	133.3
20	3510	-110.2	666.6
25	2899	-103.7	1333
30	2428	-96.5	2666
40	1783	-88.6	5333
50	1402	-83.4	7999
60	1180	-76.4	13332
70	1052	-65.8	26664
80	972.8	-53.6	53329
		-40.8	101325
eq. 1	S/(wt%)	mp/°C	-160.0

**FIGURE 5.1.4.4.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chlorodifluoromethane.

## 5.1.4.5 Dichlorodifluoromethane (CFC-12)



Common Name: Dichlorodifluoromethane

Synonym: difluorodichloromethane, Freon 12, CFC-12

Chemical Name: dichlorodifluoromethane

CAS Registry No: 75-71-8

Molecular Formula:  $\text{CF}_2\text{Cl}_2$

Molecular Weight: 120.914

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

−158.0 (Weast 1982–83; Dean 1985; Lide 2003)

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

−29.8 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

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

1.3110 ( $25^{\circ}\text{C}$ , Kirk-Othmer 1985)

1.3292, 1.3113 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Riddick et al. 1986)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

92.2 (Stephenson & Malanowski 1987)

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

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

20.112 (bp, Riddick et al. 1986)

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

4.14 (Riddick et al. 1986)

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

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

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

280 (DuPont 1966; quoted, Horvath 1982; Riddick et al. 1986)

276 (Gmelins 1974)

280 (shake flask-GC, Pearson & McConnell 1975)

300 (recommended, Horvath 1982)

280 (Verschuereen 1983; Dean 1985; Kirk-Othmer 1985)

Vapor Pressure (Pa at  $25^{\circ}\text{C}$  and reported temperature dependence equations):

745000, 1031000 ( $20^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , static method, Gilkey et al. 1931)

101325 ( $-29.8^{\circ}\text{C}$ , summary of literature data, temp range  $-118.5$  to  $-29.8^{\circ}\text{C}$ , Stull 1947)

214220 (calculated-Antoine eq., Weast 1975)

$\log(P/\text{mmHg}) = 6.82101 - 839.622/(t/^{\circ}\text{C} + 242.861)$ ; temp range  $-101$  to  $+6^{\circ}\text{C}$  (Antoine eq., Kudchadker et al. 1979)

566500, 769940 ( $20^{\circ}\text{C}$ ,  $30^{\circ}\text{C}$ , Verschuereen 1983)

566600 ( $20^{\circ}\text{C}$ , quoted, Riddick et al. 1986)

$\log(P/\text{kPa}) = 5.94591 - 839.622/(242.861 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

651040 (interpolated-Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 5.94677 - 839.6/(-30.311 + T/\text{K})$ ; temp range 173–244 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 6.0058 - 860.828/(-28.11 + T/\text{K})$ ; temp range 173–240 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 5.92289 - 826.707/(-32.274 + T/\text{K})$ ; temp range 236–285 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 6.30541 - 1035.857/(-1.496 + T/\text{K})$ ; temp range 282–345 K (Antoine eq.-IV, Stephenson & Malanowski 1987)



$\log (P_L/\text{kPa}) = 7.51271 - 2016.711/(132.578 + T/\text{K})$ ; temp range 341–385 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 52.5701 - 2.2537 \times 10^3/(T/\text{K}) - 18.265 \cdot \log (T/\text{K}) + 1.298 \times 10^{-2} \cdot (T/\text{K}) + 2.0286 \times 10^{-13} \cdot (T/\text{K})^2$ ;  
temp range 115–385 K (vapor pressure eq., Yaws 1994)

123390 (248.15 K, selected and summary of literature data, temp range 115.16–249.15 K, Xiang 2002)

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

151960 (calculated-P/C, Mackay & Wolkoff 1973; quoted, Roberts & Dändliker 1983)

43080 (calculated- $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

22800 (estimated, Roberts 1984)

28704 (19.93°C, equilibrium cell-GC, measured range 0–40°C, Warner & Weiss 1985)

$\log K_{AW} = 5.811 - 1399/(T/\text{K})$ ; temp range: 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

304000 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)

39557 (computed value, Yaws et al. 1991)

26566 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

26810 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{AW} = 5.739 - 1380/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

2.16 (shake flask-GC, Hansch et al. 1975)

2.21 (calculated-fragment const., Rekker & de Kort 1979)

2.16 (recommended, Sangster 1993)

2.16 (recommended, Hansch et al. 1995)

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

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

2.05 (soil, selected, Jury et al. 1990)

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

Volatilization: half-life of about few minutes (Mills et al. 1982); loss half-lives in marine mesocosm were estimated to be 20 d in spring at 8–16°C and  $t_{1/2} = 13$  d in winter at 3–7°C (Wakeham et al. 1983).

Photolysis: photolytic dissociation of atmospheric  $\text{CFCl}_3$  and  $\text{CF}_2\text{Cl}_2$  gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).

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:

$k_{OH}^* < 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 297.3 K, measured range 297–423.8 K (flash photolysis-RF, Atkinson et al. 1975)

$k_{OH} < 0.4 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH} < 0.012 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (relative rate method, Cox et al. 1976)

photooxidation  $t_{1/2} = 2118\text{--}21180$  h in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{OH} < 4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson 1985)

$k_{OH} < 4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with estimated tropospheric lifetime of > 50 yr for a global average concentration of OH radical (Bunce et al. 1991).

$k_{OH} < 1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 672\text{--}4320$  h, based on acclimated aerobic screening test data for trichlorofluoromethane (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2688\text{--}16128$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

## Half-Lives in the Environment:

Air: disappearance  $t_{1/2} > 10$  d from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); residence time of about 50 yr in N. troposphere, estimated by one-compartment nonsteady state model (Singh et al. 1978) and

residence time of 60–70 yr by two-compartment nonsteady state model (Singh et al. 1979);

estimated residence time in troposphere about 1 year (Lyman 1982);

$t_{1/2} = 2118$ – $21180$  h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated global average tropospheric lifetime  $\tau > 50$  yr for the reaction with hydroxyl radical in air (Bunce et al. 1991).

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

Ground water:  $t_{1/2} = 1344$ – $8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

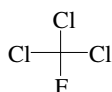
Sediment:

Soil: estimated  $t_{1/2} \sim 10000$  d for volatilization loss from soil (Jury et al. 1990);

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

Biota:

## 5.1.4.6 Trichlorofluoromethane (CFC-11)



Common Name: Trichlorofluoromethane

Synonym: Arcton 11, fluorotrichloromethane, fluorocarbon-11, Freon-11, Frigen 11, R 11, CFC-11

Chemical Name: trichlorofluoromethane, fluorotrichloromethane

CAS Registry No: 75-69-4

Molecular Formula:  $\text{CFCl}_3$

Molecular Weight: 137.368

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

−110.44 (Lide 2003)

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

23.7 (Lide 2003)

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

1.4879, 1.4760 ( $20^{\circ}\text{C}$ ,  $25^{\circ}\text{C}$ , Riddick et al. 1986)

Molar Volume ( $\text{cm}^3/\text{mol}$ ):

93.1 (Stephenson & Malanowski 1987)

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

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

25.02, 25.06 ( $25^{\circ}\text{C}$ , bp, Riddick et al. 1986)

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

6.895 (Riddick et al. 1986)

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  $25^{\circ}\text{C}$ ):

1400 ( $21^{\circ}\text{C}$ , Irmann 1965; Chiou & Freed 1977)

1100 ( $20^{\circ}\text{C}$ , DuPont 1966; quoted, Riddick et al. 1986)

1100 ( $20^{\circ}\text{C}$ , Pearson & McConnell 1975)

1100 (Verschueren 1977, 1983)

1080 (recommended, Horvath 1982)

1080 ( $30^{\circ}\text{C}$ , Horvath 1982)

1400 (Dean 1985)

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

88550\* ( $19.895^{\circ}\text{C}$ , measured range  $-36.673$  to  $19.895^{\circ}\text{C}$ , Osborne et al. 1941)

$\log(P/\text{mmHg}) = 18.54101 - 1841.72/(T/\text{K}) - 3.8423 \cdot \log(T/\text{K})$ ; temp range 236.487–296.822 K (static method-manometry, Osborne et al. 1941)

101325\* ( $23.7^{\circ}\text{C}$ , summary of literature data, temp range  $-84.3$  to  $23.7^{\circ}\text{C}$ , Stull 1947)

95670 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 6424.1/(T/\text{K})] + 7.563786$ ; temp range  $-84.3$  to  $13.1^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)

88500 ( $20^{\circ}\text{C}$ , Pearson & McConnell 1975)

106390 (Antoine eq., Reid et al. 1977)

106349 ( $20^{\circ}\text{C}$ , calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 6.89396 - 1074.04/(t/^{\circ}\text{C} + 237.276)$ ; temp range  $-37$  to  $20^{\circ}\text{C}$  (Antoine eq., Kudchadker et al. 1979)

91580 ( $20^{\circ}\text{C}$ , Verschueren 1983)

$\log(P/\text{kPa}) = 6.01333 - 1044.954/(237.102 + t/^{\circ}\text{C})$ ; temp range  $-36.67$  to  $19.89^{\circ}\text{C}$  (Antoine eq. derived from exptl data of Osborne et al. 1941, Boublik et al. 1984)

107010 (Daubert & Danner 1985)

- 102200 (selected, Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 6.01886 - 1047.04/(237.276 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)  
 106340 (calculated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 5.99210 - 1032.23/(-37.85 + T/\text{K})$ ; temp range 213–249 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 5.99652 - 1034.048/(-37.672 + T/\text{K})$ ; temp range 213–301 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.03083 - 1053.874/(-34.955 + T/\text{K})$ ; temp range 295–363 K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.36472 - 1285.088/(-0.653 + T/\text{K})$ ; temp range 357–429 K (Antoine eq.-IV, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.75501 - 2744.806/(196.225 + T/\text{K})$ ; temp range 424–486 K (Antoine eq.-V, Stephenson & Malanowski 1987)  
 $\log (P/\text{mmHg}) = 44.0884 - 2.5022 \times 10^3/(T/\text{K}) - 14.193 \cdot \log (T/\text{K}) + 7.8086 \times 10^{-3} \cdot (T/\text{K}) + 1.3769 \times 10^{-13} \cdot (T/\text{K})^2$ ;  
 temp range 162–471 K (vapor pressure eq., Yaws 1994)  
 10640 (selected summary of literature data, temp range 162.05–313.15 K, Xiang 2002)

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

- 81200 ( $20^{\circ}\text{C}$ , Pearson & McConnell 1975)  
 11650 (calculated-P/C, Neely 1976)  
 11050 ( $20^{\circ}\text{C}$ , calculated-P/C, Mackay & Shiu 1981)  
 11044 ( $20^{\circ}\text{C}$ , calculated-P/C, Mabey et al. 1982)  
 11754 (estimated-P/C, Lyman 1985)  
 $\ln K_{\text{AW}} = 9.25 - 2372/(T/\text{K})$ ; measured range  $5\text{--}33^{\circ}\text{C}$  (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)  
 $\ln K_{\text{AW}} = 10.50 - 2652/(T/\text{K})$ ; measured range  $5\text{--}33^{\circ}\text{C}$  (seawater, multiply equilibrium-GC, Hunter-Smith 1983)  
 7925 ( $19.93^{\circ}\text{C}$ , equilibrium cell-GC, measured range  $0\text{--}40^{\circ}\text{C}$ , Warner & Weiss 1985)  
 9827 (interpolated data of Warner & Weiss 1985; Howard 1990)  
 5907 (gas stripping-GC, Warner et al. 1987)  
 10234\* (EPICS-GC/FID, measured range  $10\text{--}30^{\circ}\text{C}$ , Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 9.480 - 3513/(T/\text{K})$ ; temp range  $10\text{--}30^{\circ}\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 11144 ( $20\text{--}25^{\circ}\text{C}$  and low ionic strength, Pankow & Rosen 1988; Pankow 1990)  
 12341 (computed value, Yaws et al. 1991)  
 8019 ( $20^{\circ}\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 7824 ( $20^{\circ}\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{\text{AW}} = 5.023 - 1324/(T/\text{K})$  (summary of literature data, Staudinger & Roberts 2001)

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

- 2.53 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)  
 2.53 (recommended, Sangster 1993)  
 2.53 (recommended, Hansch et al. 1995)

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

- 1.92 (microorganisms-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)  
 1.95 (calculated, Klöpffer et al. 1982)

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

- 2.20 (sediment-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)  
 2.31, 2.42, 2.16, 2.21 (estimated- $K_{\text{OW}}$ , Karickhoff 1985)  
 2.13, 2.26 (estimated-S, Karickhoff 1985)  
 2.20 (best estimate, Karickhoff 1985)  
 2.13 (average from estimates of  $K_{\text{OW}}$  and S, Karickhoff 1985; quoted, Neely & Blau 1985)

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

Volatilization: estimated  $t_{1/2} = 3.4$  h from Henry's law constant for a river 1.0 m deep with a 3 m/s wind and 1 m/s current (Lyman et al. 1982; Cadena et al. 1984; quoted, Howard 1990);  
 $t_{1/2} \sim$  few minutes (Mills et al. 1982).

Photolysis: photolytic dissociation of atmospheric  $\text{CFCl}_3$  and  $\text{CF}_2\text{Cl}_2$  gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).

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:

$k_{\text{OH}}^* < 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296.8 K, measured range 297–424 K (flash photolysis-resonance fluorescence, Atkinson et al. 1975)

$k_{\text{OH}} < 0.05 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 2$  K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{\text{OH}} < 0.005 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (relative rate method, Cox et al. 1976)

$k_{\text{OH}} < 1.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

Hydrolysis: estimated exptl. rate constant  $k = 9.5 \times 10^{-7} \text{ d}^{-1}$ , based on carbon tetrachloride (Neely 1985).

Biodegradation: aqueous aerobic  $t_{1/2} = 4032$ –8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 16128$ –34560 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

## Half-Lives in the Environment:

Air: disappearance  $t_{1/2} > 10$  d from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976);  
 estimated residence time about 1000 yr in troposphere for the reaction with OH radical (CEQ 1975);  
 estimated residence time in N. troposphere about 15–20 yr by one-compartment nonsteady state model and  
 40–45 yr in troposphere by two-compartment nonsteady state model (Singh et al. 1979);  
 estimated residence time in troposphere about 1–6 yr (Lyman 1982);  
 $t_{1/2} = 14.7$ –147 yr, based on an measured rate data for the vapor phase reaction with hydroxyl radical in air  
 (Atkinson 1985; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 4032$ –8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 8640$ –17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 4320$ –8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.4.6.1

Reported vapor pressures and Henry's law constants of trichlorofluoromethane (CFC-11) at various temperatures and the coefficients for the vapor pressure equations

Vapor pressure				Henry's law constant	
Osborne et al. 1941		Stull 1947		Ashworth et al. 1988	
static method		summary of literature data		EPICS-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m <sup>3</sup> /mol)
-36.673	6313	-84.3	133.3	10	5431
-21.825	14416	-67.6	666.6	15	6890
-6.887	29811	-59.0	1333	20	8147
-2.352	44611	-49.7	2666	25	10234
-10.362	61790	-39.0	5333	30	12362
15.108	74147	-32.3	7999	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	
19.895	88550	-23.0	13332		
23.662	101325	-9.10	26664		
		6.80	53329		
		23.7	101325	A	9.480
				B	3513
		mp/°C	-		

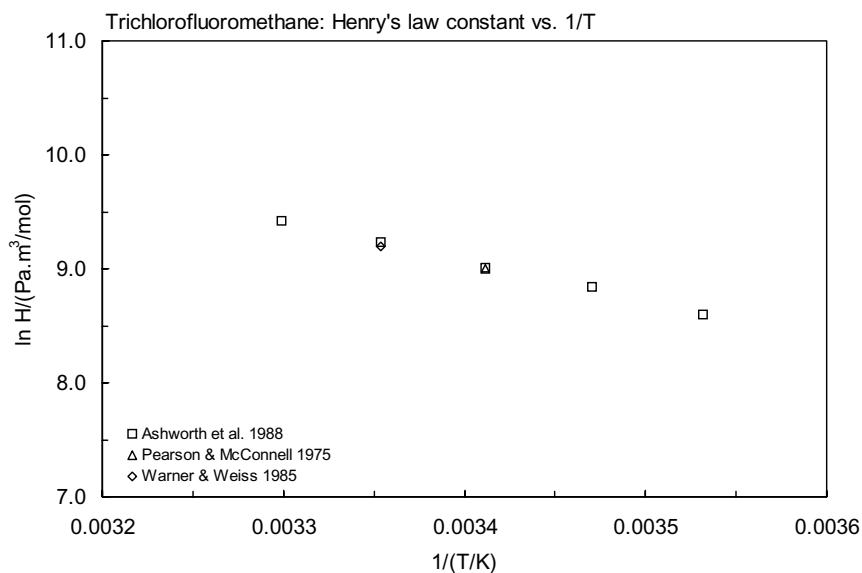


FIGURE 5.1.4.6.1 Logarithm of Henry's law constant versus reciprocal temperature for trichlorofluoromethane.

## 5.1.4.7 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)



Common Name: 1,1,2-Trichloro-1,2,2-trifluoroethane

Synonym: CFC-113, Freon 113, 1,2,2-trifluoro-1,1,2-trichloroethane

Chemical Name: 1,1,2-trichloro-1,2,2-trifluoroethane, Arklone

CAS Registry No: 76-13-1

Molecular Formula:  $C_2Cl_3F_3$ ,  $CClF_2CCl_2F$

Molecular Weight: 187.375

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

−36.22 (Lide 2003)

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

47.7 (Lide 2003)

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

1.5635 ( $25^{\circ}C$ , Dean 1985; Riddick et al. 1986)

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

119.8 ( $20^{\circ}C$ , calculated-density)

129.5 (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  $25^{\circ}C$ , F: 1.0

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

170 (DuPont 1966; quoted, Riddick et al. 1986)

170 (shake flask-GC, Rauws et al. 1973)

170 ( $20^{\circ}C$ , Jones et al. 1977/1978)

166.4\* (summary of literature data, Horvath 1982)

170 (Dean 1985)

170 (recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

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):

53329\* ( $30.2^{\circ}C$ , summary of literature data, temp range  $-68.0$  to  $47.4^{\circ}C$ , Stull 1947)

48476\* (static method-isoteniscope, measured range  $273.35$ – $318.10$  K, Hiraoka & Hildebrand 1963)

39040 (calculated-Antoine eq., Weast 1972–73)

48320 (calculated-Antoine eq., Boublik et al. 1984)

48480 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.6783 - 1499.2/(T/K)$ , temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 5.91657 - 1094.37/(-39.61 + T/K)$ ; temp range  $273$ – $319$  K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.01641 - 1115.812/(-42.515 + T/K)$ ; temp range  $238$ – $364$  K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.53093 - 1500.489/(12.469 + T/K)$ ; temp range  $360$ – $473$  K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.95163 - 1082.588/(-46.427 + T/K)$ ; temp range  $297$ – $317$  K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 33.7911 - 2.5323 \times 10^3/(T/K) - 9.3175 \cdot \log(T/K) + 1.455 \times 10^{-8} \cdot (T/K) + 2.914 \times 10^{-6} \cdot (T/K)^2$ ; temp range  $238$ – $481$  K (vapor pressure eq., Yaws 1994)

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

- 32320\* (EPICS-GC/FID, measured range  $10\text{--}30^\circ\text{C}$ , Ashworth et al. 1988)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.649 - 3243/(T/K)$ ; temp range  $10\text{--}30^\circ\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 53300 (calculated-P/C, Howard 1990)  
 49132 (computed value, Yaws et al. 1991)  
 24616 ( $20^\circ\text{C}$ , selected from reported experimental determined values, Staudinger & Roberts 2001)  
 $\log K_{\text{AW}} = 5.375 - 1281/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

- 3.16 (HPLC- $k'$  correlation, McDuffie 1981; quoted, Howard 1990, Sangster 1993))  
 3.16 (recommended, Hansch et al. 1995)

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

- 1.531, 1.041 (calculated-S, calculated- $K_{\text{OW}}$ , Lyman et al. 1982; quoted, Howard 1990)

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

- 2.28, 2.41 (soil, calculated- $K_{\text{OW}}$ , calculated-S, Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: using Henry's law constant,  $t_{1/2} = 4$  h was estimated for a model river 1 m deep flowing 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: both aqueous and atmospheric photolysis half-lives are infinite (Howard et al. 1991).

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:

$k_{\text{OH}} < 0.3 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (discharge flow-laser magnetic resonance, Howard & Enenson 1976b)

photooxidation  $t_{1/2} = 40\text{--}1000$  yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 4320\text{--}8640$  h, based on a relative resistance of completely halogenated aliphatics to biodegrade; aqueous anaerobic  $t_{1/2} = 17280\text{--}34560$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

degradation rates in microcosms at  $20^\circ\text{C}$ :  $k = 7.6 \times 10^{-3} \text{ d}^{-1}$  by control buffer with  $t_{1/2} = 90$  d,  $k = 9.1 \times 10^{-3} \text{ d}^{-1}$  by redox buffer with  $t_{1/2} = 75$  d,  $k = 1.2 \times 10^{-2} \text{ d}^{-1}$  by 1 mg/L redox-hematin with  $t_{1/2} = 57$  d,  $k = 1.6 \times 10^{-2} \text{ d}^{-1}$  by 2 mg/L redox-hematin with  $t_{1/2} = 43$  d,  $k = 9.9 \times 10^{-2} \text{ d}^{-1}$  by purged leachate with  $t_{1/2} = 7$  d, and  $k = 0.14 \text{ d}^{-1}$  by leachate with  $t_{1/2} = 5$  d (Lesage et al. 1992).

Biotransformation:

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

Half-Lives in the Environment:

Air: disappearance  $t_{1/2} > 10$  d from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 40\text{--}1000$  yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991);

$t_{1/2} = 20$  yr in troposphere (Dilling 1982; quoted, Howard 1990).

Surface water:  $t_{1/2} = 4320\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water:  $t_{1/2} = 1440\text{--}17280$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 4320\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:



TABLE 5.1.4.7.1  
Reported aqueous solubilities, vapor pressures and Henry’s law constants of 1,1,2-trichloro-1,2,2-trifluoroethane (CFC-113) at various temperatures

$$S/(wt\%) = 1.0648 \times 10^{-2} + 3.51135 \times 10^{-4} \cdot (t/^{\circ}C) - 6.1331 \times 10^{-6} \cdot (t/^{\circ}C)^2 + 6.70235 \times 10^{-8} \cdot (t/^{\circ}C)^3$$
(1)

$$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$$
(2)

Aqueous solubility		Vapor pressure				Henry’s law constant	
Horvath 1982		Stull 1947		Hiraoka & Hildebrand 1963		Ashworth et al. 1988	
summary of literature data		summary of literature data		static method isoteniscope		EPICS-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m <sup>3</sup> /mol)
0	106.5	−68.0	133.3	0.20	17252	10	15604
10	136.1	−49.4	666.6	5.0	21278	15	21785
20	157.5	−40.3	1333	10.3	26731	20	24825
25	166.4	−30.0	2666	10.45	26891	25	32323
30	174.7	−18.5	5333	15.1	32597	30	32525
40	191.7	−11.2	7999	20.0	39970		
50	212.5	−1.70	13332	25.05	48476	eq. 2	H/(atm m <sup>3</sup> /mol)
60	241.1	13.5	26664	30.1	58528	A	9.649
70	281.6	30.2	53329	35.1	69887	B	3243
80	338.0	47.4	101325	40.1	82286		
				44.95	96898		
eq.1	S/wt%	mp/°C	−35				

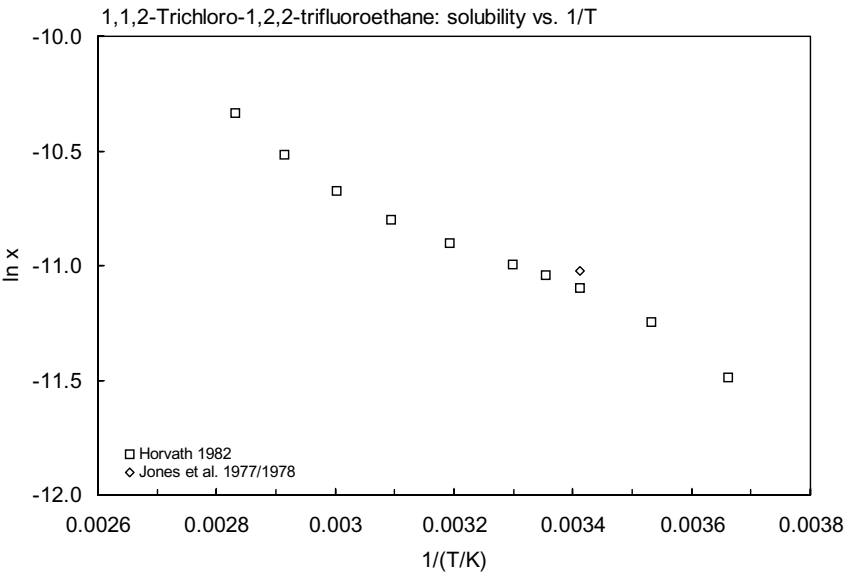
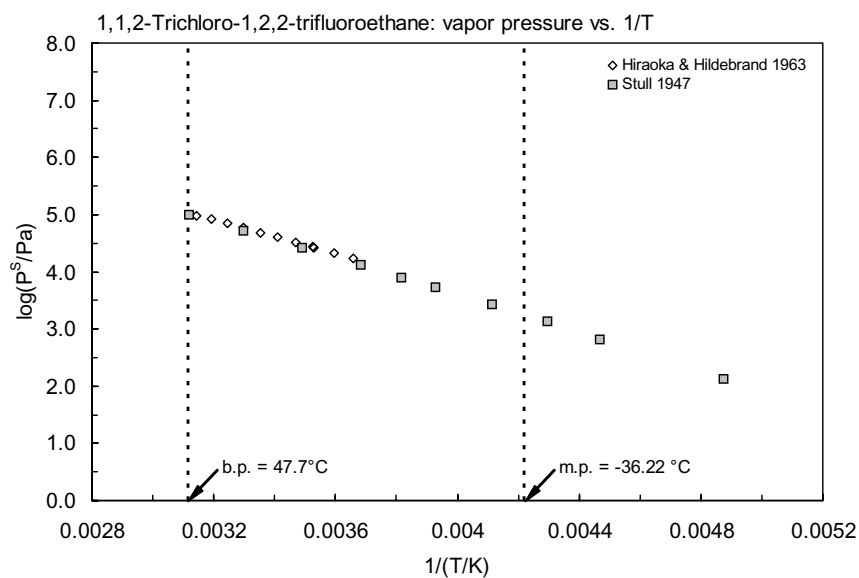
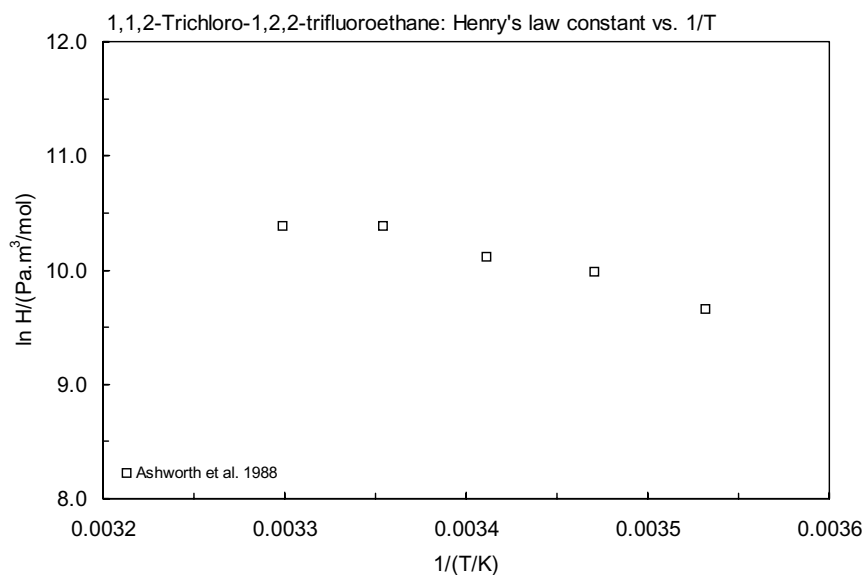


FIGURE 5.1.4.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

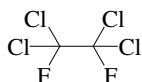


**FIGURE 5.1.4.7.2** Logarithm of vapor pressure versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.



**FIGURE 5.1.4.7.3** Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

## 5.1.4.8 1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)



Common Name: 1,1,2,2-Tetrachloro-1,2-difluoroethane

Synonym: Freon-112, CFC-112

Chemical Name: 1,2-difluorotetrachloroethane

CAS Registry No: 76-12-0

Molecular Formula:  $C_2F_2Cl_4$ ,  $Cl_2FCCl_2$

Molecular Weight: 203.830

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

26.55 (Riddick et al. 1986)

24.9 (Lide 2003)

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

92.80 (Riddick et al. 1986; Lide 2003)

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

1.6447 ( $25^{\circ}C$ , Riddick et al. 1986)

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

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

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

35 (Riddick et al. 1986)

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

3.666 (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  $25^{\circ}C$ ):

120 (DuPont 1966; quoted, Riddick et al. 1986)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

6106 ( $20^{\circ}C$ , measured range  $10$ – $91.5^{\circ}C$ , Hovorka & Geiger 1933)

7609 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 9.94341 - 4259.092/(444.991 + t/^{\circ}C)$ , temp range  $10$ – $91.5^{\circ}C$  (Antoine eq. derived from exptl. data of Hovorka & Geiger 1933, Boublik et al. 1984)

8770 (selected, Riddick et al. 1986)

$\log(P/kPa) = 7.2972 - 1929.27/(T/K)$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_s/kPa) = 6.50788 - 1526.24/(-28.93 + T/K)$ ; temp range  $235$ – $293 K$  (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.67780 - 1567.8/(-29.58 + T/K)$ ; temp range  $301$ – $365 K$  (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.97313 - 1239.993/(-53.468 + T/K)$ ; temp range  $312$ – $362 K$  (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -38.1282 - 1.2604 \times 10^3/(T/K) + 23.347 \cdot \log(T/K) - 3.4436 \times 10^{-2} \cdot (T/K) + 1.7407 \times 10^{-5} \cdot (T/K)^2$ ; temp range  $299$ – $551 K$  (vapor pressure eq., Yaws 1994)

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

9869 (calculated- $1/K_{AW}$ ,  $C_W/C_A$ , reported as exptl., Hine & Mookerjee 1975)

248, 1426 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

161419 (computed value, Yaws et al. 1991)

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

2.82 (shake flask, Log P Database, Hansch & Leo 1987)

3.73 (Howard 1990)

2.82 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:

1.62 (estimated-S, Lyman et al. 1982)

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

2.50 (soil, estimated-linear regression with S, Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: volatilization  $t_{1/2} \sim 4.0$  h from a model river 1 m deep flowing 1 m/s with a wind velocity of 3 m/s, based on estimated Henry's law constant (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Photolysis: will not undergo direct photolysis in the troposphere (quoted, Howard 1990).

Oxidation: inert to react with photochemically produced radicals and ozone molecules (Dilling 1982; Atkinson 1985,1987; quoted, Howard 1990).

Hydrolysis: not an environmentally significant fate process (DuPont 1980; quoted, Howard 1990).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: by analogy to other Freon compounds, Freon-112 is predicted to have a stratospheric lifetime on the order of several decades (Chou et al. 1978; quoted, Howard 1990).

Surface water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Ground water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Sediment: will volatilize very rapidly from soil surfaces (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Soil:

Biota:

### 5.1.5 FLUOROALKANES AND FLUOROALKENES

A large number of stable and volatile fluorinated and chlorinated alkanes and alkenes have been synthesized and used, primarily as refrigerants. These “freons” have been implicated as the cause of observed reductions in stratospheric ozone levels, thus permitting greater penetration of ultraviolet radiation to the Earth’s surface. Their high vapor pressures and relatively low solubilities in water result in high Henry’s law constants or air-water partition coefficients. Fate calculations show that when released into the environment virtually the total mass of these substances will partition to the atmospheric compartment. Levels in water, soil, sediments and biota are likely to be very low and of little concern. Accordingly, there is little merit in compiling detailed data on these substances in a format comparable to that, for example, the chlorobenzenes or PCBs.

In the interest of conserving space in this handbook, a compact tabular presentation format has been adopted. [Table 5.1.5.1](#) lists the chemical name, and its freon number (if applicable), molecular formula, molar weight and melting and boiling points. These data are available for virtually all substances in this group. Also shown in this table is the availability, expressed as a tick mark, of data on vapor pressure, solubility in water, octanol-water partition coefficient ( $K_{OW}$ ) and the second order reaction rate constant with hydroxyl radicals. This rate constant is the critical determinant of persistence in the atmosphere. [Tables 5.1.5.2](#) to [Table 5.1.5.5](#) list the compounds and give the available property data with citations.

**TABLE 5.1.5.1**  
**Summary of physical constants for fluoroalkanes and fluoroalkenes**

Compound	Freon no.	CAS no.	Molecular formula	Molecular weight g/mol	mp°C	bp°C	LeBas molar volume, V <sub>M</sub> cm <sup>3</sup> /mol	Properties**			
								S	P	K <sub>OW</sub>	k <sub>OH</sub>
Fluoroalkanes											
Fluoromethane	HFC-41	593-53-3	CH <sub>3</sub> F	34.05	−141.8	−79.1	34.6	✓	✓	✓	✓
Difluoromethane	HFC-32	75-10-5	CH <sub>2</sub> F <sub>2</sub>	52.02	−136	−51.6	39.6	✓	✓	✓	✓
Trifluoromethane	HFC-23	75-46-7	CHF <sub>3</sub>	70.01	−155.2	−82.16	44.6	✓	✓	✓	✓
Tetrafluoromethane	FC-14	75-73-0	CF <sub>4</sub>	88.005	−183.60	−128.0	49.6	✓	✓	✓	✓
Chlorofluoromethane	HCFC-31	593-70-4	CH <sub>2</sub> ClF	68.48	−133	−9.1	55.5	✓	✓		✓
Dichlorofluoromethane	HCFC-21	75-43-4	CHCl <sub>2</sub> F	102.92	−135	8.92	76.4	✓	✓	✓	✓
Chlorodifluoromethane	HCFC-22*	75-45-6	CHClF <sub>2</sub>	86.47	−160	−40.7	60.5	✓	✓	✓	✓
Chlorotrifluoromethane	CFC-13	75-72-9	CF <sub>3</sub> Cl	104.46	−181	−82	65.5	✓	✓	✓	✓
Dichlorodifluoromethane	CFC-12*	75-71-8	CCl <sub>2</sub> F <sub>2</sub>	120.91	−155	−29.8	81.4	✓	✓	✓	✓
Trichlorofluoromethane	CFC-11*	75-69-4	CFCl <sub>3</sub>	137.37	−111	23.82	97.3	✓	✓	✓	✓
Fluoroethane	HFC-161	353-36-6	CH <sub>3</sub> CH <sub>2</sub> F	48.06	−143	−37.7	56.8	✓	✓		✓
1,1-Difluoroethane	HFC-152a	75-37-6	CH <sub>3</sub> CHF <sub>2</sub>	66.05	−117	−24.7	61.8	✓	✓	✓	✓
1,2-Difluoroethane	HFC-152	624-72-6	CH <sub>2</sub> FCH <sub>2</sub> F	66.05		26	61.8	✓			✓
1,1,1-Trifluoroethane	HFC-143a	420-46-2	CF <sub>3</sub> CH <sub>3</sub>	84.04	−111.3	−47.4	66.8	✓	✓		✓
1,1,2-Trifluoroethane	HFC-143b	430-66-0	CH <sub>2</sub> FCHF <sub>2</sub>	84.04	−84	3.7	66.8	✓			✓
1,1,2,2-Tetrafluoroethane	HFC-134	359-35-3	CHF <sub>2</sub> CHF <sub>2</sub>	102.03	−89	−19.9	71.8	✓	✓		✓
1,1,1,2-Tetrafluoroethane	HFC-134a	811-97-2	CH <sub>2</sub> FCF <sub>3</sub>	102.03	−103.3	−26.08	71.8	✓	✓	✓	✓
Pentafluoroethane	HFC-125	354-33-6	CF <sub>3</sub> CHF <sub>2</sub>	120.02	−103	−48.5	76.8	✓	✓		✓
Hexafluoroethane	FC-116	76-16-4	CF <sub>3</sub> CF <sub>3</sub>	138.01	−100.6	−79	81.8	✓	✓	✓	
1-Chloro-2-fluoroethane	HCFC-151	762-50-5	CH <sub>2</sub> FCH <sub>2</sub> Cl	82.5	<−50	52.8	77.7	✓			
1-Chloro-1,1-difluoroethane	HCFC 142b	75-68-3	CH <sub>3</sub> CClF <sub>2</sub>	100.5	−130.8	−9.5	82.7	✓	✓	✓	✓
1-Chloro-1,1,2-trifluoroethane	HCFC-133a	421-04-5	CH <sub>2</sub> ClCF <sub>3</sub>	118.49		12	87.7				✓
1-Chloro-1,2,2,2-tetrafluoroethane	HCFC-124	2837-89-0	CHClF <sub>2</sub> CF <sub>3</sub>	136.5		−11.0	92.7	✓	✓	✓	✓
1-Chloropentafluoroethane	CFC-115	76-15-3	CClF <sub>2</sub> CF <sub>3</sub>	154.47	−99.4	−39.1	97.7	✓	✓	✓	
1,1-Dichloro-1-fluoroethane	HCFC-141b	1717-00-6	CCl <sub>2</sub> FCH <sub>3</sub>	116.95	−103.5	32.0	98.6	✓	✓	✓	✓
1,2-Dichloro-1,1-difluoroethane	HCFC-132b	1649-08-7	CClF <sub>2</sub> CH <sub>2</sub> Cl	134.97	−101.2	46.8	103.6				✓
1,1-Dichlorotrifluoroethane	HCFC-123	306-83-2	CHCl <sub>2</sub> CF <sub>3</sub>	152.93	−107	27.6	108.6	✓	✓		✓
1,2-Dichloro-1,1,2,2-tetrafluoroethane	CFC-114	76-14-2	CClF <sub>2</sub> CClF <sub>2</sub>	170.92	−93.9	3.8	113.6	✓	✓	✓	
1,1-Dichloro-1,2,2,2-tetrafluoroethane	CFC-114a	374-07-2	CCl <sub>2</sub> FCF <sub>3</sub>	170.92	−56.6	3.4	113.6	✓		✓	
1,1,1-Trichloro-2,2,2-trifluoroethane	CFC-113a	354-58-5	CCl <sub>3</sub> CF <sub>3</sub>	187.38	14.2	47.57	129.5		✓		
1,1,2-Trichloro-1,2,2-trifluoroethane	CFC-113*	76-13-1	CCl <sub>2</sub> FCClF <sub>2</sub>	187.38	−36.4	47.7	129.5	✓	✓	✓	

1,1-Difluorotetrachloroethane			CClF <sub>2</sub> CCl <sub>3</sub>	203.83	38	91	145.4			✓	
1,1,2,2-tetrachloro-1,2-difluoroethane	CFC-112*	76-12-0	CCl <sub>2</sub> FCCL <sub>2</sub> F	203.83	25	93	145.4	✓	✓	✓	
2-Fluoropropane	HFC-281ea	420-26-8	CH <sub>3</sub> CHFCH <sub>3</sub>	62.09	-133.4	-10	79.0	✓	✓		
1,1,2,2,3-Pentafluoropropane	HFC-245ca	679-86-7	CH <sub>2</sub> FCF <sub>2</sub> CHF <sub>2</sub>	134.05			99.0		✓		✓
1,1,1,3,3-Pentafluoropropane	HFC-245fa	460-73-1	CF <sub>3</sub> CH <sub>2</sub> CHF <sub>2</sub>	134.05			99.0		✓		
1,1,1,2,2-Pentafluoropropane	HFC-245cb	1814-88-6	C <sub>3</sub> H <sub>3</sub> F <sub>5</sub>	134.05		-17.4	99.0		✓		✓
1,1,1,2,3,3-Hexafluoropropane	HFC-236ea	431-63-0	CHF <sub>2</sub> CHFCF <sub>3</sub>	152.04		6.1	104.0		✓		✓
1,1,1,3,3,3-Hexafluoropropane	HFC-236fa	690-39-1	CF <sub>3</sub> CH <sub>2</sub> CF <sub>3</sub>	152.04	-93.6	-1.0	104.0		✓		✓
1,1,1,2,3,3,3-Heptafluoropropane	HFC-227ea	431-89-0	CF <sub>3</sub> CHFCF <sub>3</sub>	170.03	-131	-16.4	109.0		✓		✓
Octafluoropropane	FC-218	76-19-7	CF <sub>3</sub> CF <sub>2</sub> CF <sub>3</sub>	188.02	-183	-38	114.0	✓	✓		
Trichlorotrifluoropropane									✓		
1-Chloro-2,2,2-trifluoropropane			CH <sub>2</sub> ClCH <sub>2</sub> CF <sub>3</sub>	132.51	-106.2	45.1	109.9	✓	✓		
Perfluorobutane	FC-3110	355-25-9	C <sub>4</sub> F <sub>10</sub>	238.03	-129.1	-1.9	146.2		✓		
Perfluorocyclobutane	FC-118	115-25-3	C <sub>4</sub> F <sub>8</sub>	200.03	-40.19	-5.9	120.3	✓	✓		
Perfluoropentane	FC-87	678-26-2	C <sub>5</sub> F <sub>12</sub>	288	-10	29.2	178.4		✓		
Perfluorocyclopentane		376-77-2							✓		
Perfluoro-2-methylcyclopentane									✓		
Perfluoro-3-methylcyclopentane									✓		
Perfluorocyclohexane		355-68-0	C <sub>6</sub> F <sub>12</sub>	300.05	48	52	178.2		✓		
Perfluorohexane	FC-72	355-42-0	C <sub>6</sub> F <sub>14</sub>	338.04	-88.2	56.6	210.6		✓		
<b>Fluoroalkenes</b>											
Fluoroethene	HFC-1141	75-02-5	CHF=CH <sub>2</sub>	46.05	-160	-72.2	49.4	✓			
1,1-Difluoroethene	HFC-1132a	75-38-7	CF <sub>2</sub> =CH <sub>2</sub>	64.04	-144	-82	54.4	✓			✓
Tetrafluoroethene	FC-1114	116-14-3	CF <sub>2</sub> =CF <sub>2</sub>	100.02	-131.15	-75.9	64.4	✓	✓		
Chlorotrifluoroethene	CFC-1113	79-38-9	CClF=CF <sub>2</sub>	116.47	-158.2	-26.2	80.3		✓		
1,2-Dichloro-1,2-difluoroethene	CFC-1112	311-81-9	CClF=CClF	132.92	-119.6	21.1	96.2		✓		
1,1-Dichloro-2,2-difluoroethene	CFC-1112a	79-35-6	CCl <sub>2</sub> =CF <sub>2</sub>	132.925	-115	19	96.2		✓		
3-Fluoropropene		818-92-8	CH <sub>2</sub> FCH=CH <sub>2</sub>	60.07		-3.0	71.6	✓			
Hexafluoropropene	FC-1216	116-15-4	C <sub>3</sub> F <sub>6</sub>	150.002	-156.5	-29.6		✓	✓		

\* See [Section 5.1.4. Mixed halogenated hydrocarbons](#).

\*\* S = water solubility; P = vapor pressure; K<sub>OW</sub> = octanol-water partition coefficient; k<sub>OH</sub> = second order reaction rate constant with hydroxyl radicals.

**TABLE 5.1.5.2**  
**Aqueous solubilities for fluoroalkanes and fluoroalkenes**

Compound	Temp.°C	Solubility	Unit	Range, wt %	Mole fraction $x$	Temp./pressure range	Reference
Fluoroalkanes							
Fluoromethane	25	0.2001	wt %	0.4227–0.08005	0.001061	0–80°C, 1 atm partial pressure	1
	25	2390	ppm (wt)				2
Difluoromethane	25	4390	ppm (wt)				2
Trifluoromethane	25 at 1 atm	0.09	g/100 mL	0.09–0.02		25–75°C, pressure 1–20.41 atm	1
	25	0.4087	wt %		0.001056	1 atm partial pressure	1
	25	900	ppm (wt)				2
Tetrafluoromethane	25	0.0733	g/100 mL			from Hine & Mookerjee (1975)	3
	25	0.001877	wt %	0.003892–0.001300	3.84×10 <sup>-6</sup>	0–50°C, 1 atm partial pressure	1
	25 at 1 atm	0.00160	g/100 mL	0.00160–0.0005		25–75°C, 1–10.2 atm	1
	25	16.0	ppm (wt)				2
Chlorofluoromethane	25	0.4592	10 <sup>3</sup> L <sub>2,1</sub> , Ostwald coefficient			288–303 K, 1atm partial pressure	4
	25	1.0522	wt %	1.6840–0.3285	0.002790	10–50°C, 1 atm partial pressure	1
	25	10500	ppm (wt)			1 atm partial pressure	2
Dichlorofluoromethane	25 at 1 atm	1.880	g/100 mL	1.88–0.418		25–75°C, 0.068–3.40 atm	1
	25	0.95	wt %			DuPont	5
	25	18800	ppm (wt)				2
Chlorodifluoromethane	25	0.2899	wt %	0.5296–0.09728	6.055×10 <sup>-4</sup>	10–50°C, 1 atm partial pressure	1
	25 at 1 atm	0.277	g/100 mL	0.792–0.089		5–76.7°C, 1–33.34 atm	1
	25	0.30	wt %				5
	25	27.7	ppm (wt)				2
Chlorotrifluoromethane	25 at 1 atm	0.2899	g/100 mL			from Horvath (1982)	3
	25 at 1 atm	0.009	g/100 mL	0.009–0.004		25–75°C, 1–23.81 atm	1
	25	0.009	wt %				5
	25	90	ppm (wt)				
	25	2.253	10 <sup>3</sup> L <sub>2,1</sub> , Ostwald coefficient			288–303 K, 1 atm partial pressure	4
Dichlorodifluoromethane	25 at 1 atm	0.030	g/100 mL	0.030–0.008		25–76.7°C, 1–6.80 atm	1
	25	0.028	wt %				5
	25 at 1 atm	0.028	g/100 mL			quoted Riddick (1986)	6
	25	300	ppm (wt)				2
	25	7.110	10 <sup>3</sup> L <sub>2,1</sub> , Ostwald coefficient			288–303 K, 1 atm partial pressure	4
Trichlorofluoromethane	30 at 1 atm	0.1080	g/100 mL	0.108–0.031		30–75°C, 1–3.4 atm	1
	25	0.11	wt %			DuPont	5
	25	1080	ppm (wt)				1



	25	0.108	g/100 mL			from Horvath (1982)	9
Fluoroethane	25	0.2158	wt %	0.4022–0.2158	$8.10 \times 10^{-4}$	14–25°C, 1 atm partial pressure	1
	25	2160	ppm (wt)			1 atm partial pressure	
1,1-Difluoroethane	21	0.32	wt %	0.54–0.25	$8.748 \times 10^{-4}$	0–27.5°C, 1 atm partial pressure	1
	25	2500	ppm (wt)			1 atm partial pressure	2
	25 at 1 atm	0.280	g/100 mL			from Horvath (1982)	3
1,2-Difluoroethane	25	0.0157	wt %	0.012–0.02660	$1.342 \times 10^{-5}$	25–80°C, saturation pressure	1
1,1,2-Trifluoroethane	25	0.01664	wt %	0.01065–0.03380	$1.60 \times 10^{-5}$	0–80°C, saturated pressure	1
	30	0.011	g/100 mL	0.011–0.026		30–75°C, 0.34–2.04 atm	1
1,1,1,2-Tetrafluoroethane	37	0.0550	wt %		$9.71 \times 10^{-5}$	37°C, 1 atm partial pressure	1
1,1,2,2-Tetrafluoroethane	25	0.2962	wt %	0.3299–0.4199	$3.187 \times 10^{-4}$	1 atm	1
Pentafluoroethane	25	0.04995	wt %	0.05411–0.07783	$4.45 \times 10^{-5}$	0–80°C, saturated pressure	1
	25	58.0	ppm (wt)				2
	25	0.0039	g/100 mL			estimated from $K_{OW}$	6
Hexafluoroethane	22.3	0.0050	wt %		$3.805 \times 10^{-6}$	22.3°C, 0.0050 atm	1
	25	7.90	ppm (wt)				2
	25.314				$9.975 \times 10^{-7}$	287–328 K, 96.6–120.5 kPa	7
1-Chloro-2-fluoroethane	25	2.4390	wt %		0.005429	saturated pressure	1
1-Chloro-1,1-difluoro-	21 at 1 atm	0.140	wt %	0.214–0.140	$2.512 \times 10^{-4}$	13–21°C, 1 atm partial pressure	1
1-Chloro-1,2,2,2-tetrafluoro-	25	0.0404	g/100 mL			estimated from $K_{OW}$	6
1-Chloropentafluoro-	25 at 1 atm	0.0058	g/100 mL	0.0058–0.0013		25–75°C, 1–6.80 atm	1
	25	0.006	wt %				5
1,1-Dichloro-1-fluoro	25	0.066	wt %				
1,1-Dichlorotrifluoroethane	25	0.0046	wt %				8
	25	0.01857	g/100 mL			estimated from $K_{OW}$	6
1,2-Dichloro-1,1,2,2-tetra-	25	0.0120	wt %	0.0120–0.02662	$1.061 \times 10^{-5}$	25–80°C, saturated pressure	1
	25	0.1792	wt %	0.1792–0.03487	$1.586 \times 10^{-6}$	25–80°C, 1 atm partial pressure	1
	30 at 1 atm	0.009	g/100 mL	0.009–0.020		30–75°C, 0.068–0.612 atm	1
	25	0.013	wt %				5
	25	137	ppm (wt)				2
	25	0.013	g/100 mL			from Riddick (1986)	9
1,1-Dichloro-1,2,2,2-tetra-	25	0.1100	wt %	0.1197–0.1848	$11.82 \times 10^{-6}$	0–80°C, saturation pressure	1
	21	0.0060	g/100 mL			from Horvath (1982)	3
1,1,2-Trichloro-1,2,2-tri-	25	0.01664	wt %	0.01065–0.003380	$1.60 \times 10^{-5}$	0–80°C, saturated pressure	8
	30 at 0.34 atm	0.011	g/100 mL			30–75°C, 0.34–2.04 atm	1
	25	0.017	wt %				5
	25	170	ppm (wt)				2
	25	0.017	g/100 mL			from Riddick (1986)	9

(Continued)

TABLE 5.1.5.2 (Continued)

Compound	Temp.°C	Solubility	Unit	Range, wt %	Mole fraction $x$	Temp./pressure range	Reference
1,2-Difluorotetrachloro-	25	0.012	wt %				5
	25	0.012	g/100 mL			from Riddick (1986)	9
2-Fluoropropane	15	0.3663	wt %		0.001066	1 atm partial pressure	1
	15	3660	ppm (wt)			1 atm partial pressure	2
Octafluoropropane	15	0.001495	wt %		$1.432 \times 10^{-6}$	15°C, saturated pressure	1
Perfluorocyclobutane	21	0.014	wt %		$1.259 \times 10^{-5}$	21°C, 1 atm partial pressure	1
	26 at 1 atm	0.005	g/100 mL			0–37.8°C, 1–2.72 atm	1
	26	50.0	ppm (wt)				2
<b>Fluoroalkenes</b>							
1-Fluoroethene	80 at 34 atm	0.9312	wt %		0.003664	34 atm	1
	80 at 68 atm	1.5166	wt %		0.005988	68 atm	1
1,1-Difluoroethene	25	0.01649	wt %		$4.638 \times 10^{-5}$	1 atm partial pressure	1
	25	165	ppm (wt)			1 atm partial pressure	2
Tetrafluoroethene	25	0.01585	wt %	0.04062–0.008782	$2.856 \times 10^{-5}$	0–70°C, 1 atm partial pressure	1
	23 at 4.4 atm	0.001	wt %	0.001–1.274	$1.78 \times 10^{-6}$	23°C, total pressure 4.4–13.45 atm	1
	25	158	ppm (wt)				2
3-Fluoropropene	13	0.007167	wt %		$2.149 \times 10^{-5}$	1 atm partial pressure	1
Hexafluoropropene	25	0.01691	wt %	0.04164–0.007132	$2.327 \times 10^{-5}$	0–70°C, 1 atm partial pressure	1

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**TABLE 5.1.5.3**  
**Vapor pressures for fluoroalkanes and fluoroalkenes**

Compound	Temp. °C or K	P° kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
<b>Fluoroalkanes</b>						
Fluoromethane				−103 – −76°C	20–116	Moles and Batuecas 1919 <sup>#</sup>
			static	−133.1 – −78.5°C	1.33–101	Grosse et al. 1940
			literature summary	−147.3 – −78.2°C	0.1333–101.325	Stull 1947
	15.28°C	3045.3	manometer	−109–15°C	13–3045	Michels and Wassenaar 1948
Difluoromethane	298.15 K	3824.9	literature summary	131–317 K	0.43–5880	Xiang 2002
	298.16 K	1689	static	191–352 K	16.36–5828	Malbrunot et al. 1968
			comparative ebulliometry	208–237 K	49–214	Weber and Goodwin 1993
	298.174 K	1690.81	Burnett	268–348 K	690–5409	Defibaugh et al. 1994
			apparatus/densimeter			
			isochoric	320–351 K	2919–5783.6	Sato et al. 1994
			ebulliometry (metal)	236–266 K	200–650	Weber and Silva 1994
	299.985 K	1774	manometer/densimeter	220–325 K	95–3278	Widiatmo et al. 1994
	297.15 K	1645.1	Burnett apparatus	233–351 K	177–5767.9	Fu et al. 1995
	298.15 K	1689.7	literature summary	137–351 K	5.69×10 <sup>−2</sup> – 5780	Xiang 2002
Trifluoromethane	308.15 K	2191	VLE			Horstmann et al. 2004
			calorimetry static	145–192 K	2.72–102.51	Valentine et al. 1962
Tetrafluoromethane	298.15 K	4714.9	literature summary	118–299 K	5.71×10 <sup>−2</sup> – 4800	Xiang 2002
			literature summary	−184.6 – −127.7°C	0.1333–101.325	Stull 1947
			calorimetry static	115–146 K	7–106	Smith and Pace 1969
						Bonifácio et al. 2001
Chlorofluoromethane			literature summary	90–228 K	1.04×10 <sup>−1</sup> –3740	Xiang 2002
	298.15 K	343.82	literature summary	138–427 K	2.28×10 <sup>−3</sup> –5700	Xiang 2002
Dichlorofluoromethane			isoteniscopic	−29.65–174.6°C	17.31–4894	Benning and McHarness 1940
			literature summary	−91.3–8.90°C	0.1333–101.325	Stull 1947
	298.15 K	181.67	literature summary	138–452 K	2.94×10 <sup>−4</sup> – 5183	Xiang 2002
Chlorodifluoromethane	22.6°C	951	manometer	22.6–96.4°C	951–4912	Booth and Swinehart 1935
	25.15°C	1050.74	isoteniscopic	−61.26–92.6°C	35.12–4652.84	Benning and McHarness 1940
			literature summary	−122.8 – −40.8°C	0.1333–101.325	Stull 1947
	50°C	1955	VLE			Leu and Robinson 1992
	65°C	2710	VLE			Leu and Robinson 1992
	70°C	3003	VLE			Leu and Robinson 1992
	75°C	3843	VLE			Leu and Robinson 1992

(Continued)

TABLE 5.1.5.3 (Continued)

Compound	Temp. °C or K	P° kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
Chlorotrifluoromethane	289.10 K	811.7	isochoric	245–328 K	180–2195	Giuliani et al. 1995a
	298.15 K	1044.2	literature summary	115–369 K	4.26×10 <sup>-4</sup> –4988	Xiang 2002
			literature summary	–149.5 – –81.2°C	0.1333–101.325	Stull 1947
Dichlorodifluoromethane	298.15 K	3578.3	literature summary	92–302 K	4.40×10 <sup>-4</sup> –3890	Xiang 2002
			literature summary	–118.5 – –29.8°C	0.1333–101.325	Stull 1947
Trichlorofluoromethane	25.338°C	656		25–111°C	656–4062	Michels et al. 1966
	298.15 K	650.91	literature summary	115–385 K	2.33×10 <sup>-4</sup> –4100	Xiang 2002
	24.02°C	102.24	isoteniscopic	–29.65–195.65°C	1.05–4273.89	Benning and McHarness 1940
	293.055 K	88.55	calorimetry static	236–293 K	6.31–88.55	Osborne et al. 1941
	23.7°C	101.325	literature summary	–84.3–23.7°C	0.1333–101.325	Stull 1947
Fluoroethane	298.15 K	106.4	literature summary	162–471 K	6.26×10 <sup>-3</sup> –4408	Xiang 2002
	25.65°C	932	manometer	25.65–102.16°C	932–5028	Booth and Swinehart 1935
			static	–103.6 – –37.1°C	1.33–101	Grosse et al. 1940
	295.82 K	865.9	static	228–322 K	70–1699	Vidaauri 1975
1,1-Difluoroethane	20°C	833.3		16–78°C	738–3197	Beyerlein et al. 1998
	290.76 K	22	mercury manometer	234–291 K	0.858–22	Li and Pitzer 1956
	298.15 K	596	isochoric	239–368 K	59–3334	Zhao et al. 1992
			ebulliometry	220–273 K	23–264	Silva and Weber 1993
1,1,1-Trifluoroethane	295.452 K	550.01	ebulliometry	281–335 K	352–1550	Defibaugh and Morrison 1996
	298.15 K	597	strain gauge	243–333 K	73–1499	Takagi et al. 2004
			mercury manometer	174–226 K	3.49–101.01	Russell et al. 1944
	299.995 K	1331	manometer/densimeter	278–340 K	769–3337	Widiatmo et al. 1994
	298.22 K	1265.1	isochoric	244–345 K	226–3717	Giuliani et al. 1995b
	300 K	1327.0	Burnett apparatus	295–342 K	1164–3474	Zhang et al. 1995a
	279.484 K	751.294	ebulliometry	236–279 K	160–751	Weber and Defibaugh 1996b
	298.165 K	1262.0	PVT apparatus	279–343 K	744–3556	Weber and Defibaugh 1996b
	293.149 K	1104.8		263–346 K	447–3763	Fujiwara et al. 1998
	283.11 K	834.8	VLE			Bobbo et al. 2000b
1,1,2,2-Tetrafluoroethane	298.16 K	1260.7	VLE			Bobbo et al. 2000b
	313.21 K	1832.5	VLE			Bobbo et al. 2000b
	300 K	1325.3	isochoric	300–345 K	1325–3748	Widiatmo et al. 2001
	298.16 K	1262.62	Burnett apparatus	251–343 K	292–3554	Duan et al. 2004
	299.994 K	546		200–390 K	15–4465	Maezawa et al. 1991b
	299.976 K	699		280–350 K	38–2459	Maezawa et al. 1990

	297.15 K	645.53		279–363 K	363–3236	Zhu et al. 1992
	298.21 K	666.7	isochoric	250–347 K	116–2316	Giuliani et al. 1995a
	298.13 K	666	acoustic interferometer	243–333 K	83–1673	Takagi 1996a
	293.66 K	580	VLE			Bobbo et al. 1998
	303.68 K	780.9	VLE			Bobbo et al. 1998
	283.62 K	420.7	VLE			Bobbo et al. 1998
	293.14 K	571.5		263–373 K	200–3973	Fujiwara et al. 1998
	293.15 K	571.3	VLE			Bobbo et al. 2001
	303.15 K	769.4	VLE			Bobbo et al. 2001
	313.15 K	1014.6	VLE			Bobbo et al. 2001
Pentafluoroethane			isochoric	195–339 K	20–100 bars	Wilson et al. 1992
			ebulliometry (glass)	219–247 K	74–262	Weber and Silva 1994
	284.714 K	951.5741	ebulliometry (metal)	240–285 K	200–952	Weber and Silva 1994
	299.985 K	1444	manometer/densimeter	220–335 K	79–3303	Widiatmo et al. 1994
	300 K	1446.6	Burnett apparatus	290–339 K	1107–3606	Ye et al. 1995
	298.21 K	1380	acoustic interferometer	242–333 K	221–3171	Takagi 1996b
	299.998 K	1447.57	isochoric	220–338 K	79–3529	Duarte-Garza et al. 1997b
	303.19 K	1568.5	VLE			Bobbo et al. 1999
	323.26 K	2539.3	VLE			Bobbo et al. 1999
	308.15 K	1778.8	VLE			Horstmann et al. 2004
Hexafluoroethane			calorimetry static	180–195 K	42–103	Pace and Aston 1948
	291.2 K	2902.1		177–291 K	35–2902	Kao and Miller 2000
1-Chloro-1,1-difluoroethane				320–400 K	632–3388	Maezawa et al. 1991a
	284.688 K	218.216	ebulliometry	225–285 K	15–218	Silva and Weber 1993
1-Chloro-1,2,2,2-tetrafluoroethane	286.098 K	258.829	ebulliometry (glass)	222–286 K	14–259	Weber and Silva 1994
1-Chloropentafluoroethane			calorimetry static	178–234 K	3–101	Aston et al. 1955
				178–346 K	3–2696	Mears et al. 1966
1,1-Dichloro-1-fluoroethane	300 K	84.20	Burnett apparatus	250–450 K	9–2791	Duarte-Garza et al. 1997a
	299.968 K	86		200–400 K	4–1177	Maezawa et al. 1991b
	299.795 K	83.43	comparative ebulliometry	271–313 K	25–129	Weber 1992
1,1-Dichlorotrifluoroethane	289.988 K	67		280–350 K	46–440	Maezawa et al. 1990
	308.26 K	131	isochoric	308–457 K	131–3658	Piao et al. 1991
	293.143 K	76.6	isochoric	243–448 K	7–3172	Oguchi et al. 1992
	299.950 K	97.45	comparative ebulliometry	272–308 K	30–130	Weber 1992
1,2-Dichloro-1,1,2,2-tetrafluoroethane			literature summary	–95.4–3.50°C	0.133–101.325	Stull 1947
1,1,1-Trichloro-2,2,2-trifluoroethane	298.2 K	48.143	isoteniscopic	287–309 K	31–72	Hiraoka and Hildebrand 1963
1,1,2-Trichloro-1,2,2-trifluoroethane	20.19°C	36.64	isoteniscopic	–8.4–210.62°C	10.08–3266.72	Benning and McHarness 1940
	30.2°C	53.329	literature summary	–68.0–47.6°C	0.133–101.325	Stull 1947

(Continued)

TABLE 5.1.5.3 (Continued)

Compound	Temp. °C or K	P <sup>s</sup> kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
1,1,2,2-Tetrachloro-1,2-difluoroethane	298.2 K	48.476	isoteniscopic	273–318 K	17–97	Hiraoka and Hildebrand 1963
	20°C	6.106		10–92°C	4–101	Hovorka and Geiger 1933
	19.8°C	5.333	literature summary	–37.5–92.0°C	0.1333–101.325	Stull 1947
2-Fluoropropane	30°C	407	VLE			Parrish and Sitton 1982
	50°C	700	VLE			Parrish and Sitton 1982
1,1,2,2,3-Pentafluoropropane	298.98 K	100.7	isochoric	258–353 K	16–573	Di Nicola and Passerini 2002
1,1,1,3,3-Pentafluoropropane	298.17 K	151.9	isochoric	293–426 K	127–3595	Sotani & Kubota 1999
	298.21 K	149.04	Burnett apparatus	255–393 K	21–1951	Wang and Duan 2004
	293.15 K	122.8	VLE			Bobbo et al. 2001
	303.15 K	178.4	VLE			Bobbo et al. 2001
	313.15 K	250.8	VLE			Bobbo et al. 2001
	293.15 K	123.1	VLE			Bobbo et al. 2001
	303.15 K	178.1	VLE			Bobbo et al. 2001
	313.15 K	250.6	VLE			Bobbo et al. 2001
	297.97 K	147.1	isochoric	266–352 K	35–762	Di Nicola 2001
	30°C	535.05	mercury piston gauge	–5.34–106.96°C	33.33–3137.4	Shank 1967
	292.955 K	397.36	comparative ebulliometry	248–326 K	74–995	Weber and Defibaugh 1996a
	300 K	219.6	Burnett apparatus	300–410 K	220–3264	Zhang et al. 1995b
1,1,1,2,3,3-Hexafluoropropane	283.12 K	118.6	VLE			Bobbo et al. 2000c
	298.16 K	205.8	VLE			Bobbo et al. 2000c
	313.21 K	340.4	VLE			Bobbo et al. 2000c
	283.12 K	118.4	VLE			Bobbo et al. 2000c
	298.17 K	207.0	VLE			Bobbo et al. 2000c
	313.22 K	338.5	VLE			Bobbo et al. 2000c
	298.41 K	208.1	isochoric	255–363 K	35–1266	Di Nicola and Giuliani 2000
	299.15 K	281.15	Burnett apparatus	253–396 K	44–3064	Duan et al. 2004
	283.62 K	162.6	VLE			Bobbo et al. 1998
	303.68 K	325.8	VLE			Bobbo et al. 1998
1,1,1,3,3,3-Hexafluoropropane	303.2 K	322.2	VLE			Bobbo et al. 1999
	323.26 K	584.2	VLE			Bobbo et al. 1999
	323.26 K	585.7	VLE			Bobbo et al. 1999
	298.27 K	272.5	isochoric	248–360 K	34–1472	Di Nicola et al. 1999
	283.13 K	160.0	VLE			Bobbo et al. 2000a
	303.19 K	322.3	VLE			Bobbo et al. 2000a

	323.26 K	586.3	VLE			Bobbo et al. 2000a
	283.11 K	160.9	VLE			Bobbo et al. 2000b
	298.16 K	272.5	VLE			Bobbo et al. 2000b
	313.21 K	439.3	VLE			Bobbo et al. 2000b
	283.12 K	159.1	VLE			Bobbo et al. 2000c
1,1,1,2,3,3,3-Heptafluoropropane				238–373 K	41–2831	Salvi-Narkhede et al. 1992
	299.06 K	467.35	Burnett apparatus	243–375 K	54–2936	Shi et al. 1999
				273–373 K	192–2818	Gruzdev et al. 2002
	298.152 K	441.234		233–375 K	32–2937	Hu et al. 2002
	295.27 K	416.1	isochoric	235–365 K	36–2402	Di Nicola 2003
	297.22 K	441.61	Burnett apparatus	253–373 K	87–2825	Wang and Duan 2004
Octafluoropropane	29.17°C	9.69 atm		–60.15 – 67.65°C	0.306–24.13 atm	Brown 1963
				182–237 K	3.29–106.47	Crowder et al. 1967
	50°C	1652	VLE			Leu and Robinson 1992
	65°C	2304	VLE			Leu and Robinson 1992
	70°C	2554	VLE			Leu and Robinson 1992
Trichlorotrifluoropropane				48 – 90°C	19–88	Varuschenko & Druzhinina 1972#
1-Chloro-2,2,2-trifluoropropane				29 – 68°C	19–88	Varuschenko & Druzhinina 1972#
Perfluorobutane	20°C	232.033	isoteniscopic recirculating still	–28–90°C	35–1388	Fowler et al. 1947
				233–260 K	16–64	Simons and Mausteller 1952
	31.73°C	330.3		–40–110°C	17–2178	Brown and Mears 1958
Perfluorocyclobutane	17.70°C	249		–36–18°C	26–249	Whipple 1952
				–32–0°C	30–131	Furukava et al. 1954#
	22.53°C	288.76		–40–115°C	19–2778	Martin 1962
	293.21 K	265.2		234–387 K	20–2697	Kao and Miller 2000
Perfluoropentane	24.10°C	83.23	equilibrium still	10–65°C	46.34–318.84	Barber and Cady 1956
	297.59 K	84.71		221–303 K	1–104	Crowder et al. 1967
Perfluorocyclopentane	22.57°C	101.53	equilibrium still	17–56°C	82–307	Barber and Cady 1956
	296.83 K	105.72		230–297 K	2.60–105.72	Crowder et al. 1967
Perfluoro-2-methylcyclopentane	23.82°C	27.464	equilibrium still	4–68°C	11–143	Stiles and Cady 1952
	298.86 K	30.15		254–451 K	2.71–1763.46	Crowder et al. 1967
Perfluoro-3-methylcyclopentane	300.78 K	32.13		255–450 K	2.99–1674.8	Crowder et al. 1967
Perfluorocyclohexane				63–121°C	152–709	Rowlinson and Thacker 1957#
	300.74 K	33.75		253–451 K	2.11–2006.54	Crowder et al. 1967
Perfluorohexane	24.9°C	29.051	equilibrium still	11–69°C	15–149	Stiles and Cady 1952
	30.06°C	36.461	equilibrium still	30–57°C	36–102	Dunlap et al. 1958

(Continued)

TABLE 5.1.5.3 (Continued)

Compound	Temp. °C or K	P <sup>s</sup> kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
	291.52 K	21.85		256–447 K	3.28–1701.14	Crowder et al. 1967
<b>Fluoroalkenes</b>						
Tetrafluoroethene				–131 – –65°C	1–177	Furukava et al. 1953 <sup>#</sup>
Chlorotrifluoroethene			manometer	195–250 K	6–123	Booth et al. 1933
	21.9°C	577.55	manometer	21.9–107°C	577.55–3951.68	Booth and Swinehart 1935
			literature summary	–116 – –27.9°C	0.1333–101.325	Stull 1947
			calorimetry static	–67 – –11°C	13–205	Oliver et al. 1951
1,2-Dichloro-1,2-difluoroethene	295 K	105.8	manometer	240–295 K	8–106	Booth et al. 1933
	20.9°C	101.325	literature summary	–82.0–20.9°C	0.1333–101.325	Stull 1947
1,1-Dichloro-2,2-difluoroethene	295 K	105.8	manometer	240–295 K	8–106	Booth et al. 1933
Hexafluoropropene	19.75°C	652.7		–41–20°C	62–653	Whipple 1952

\* VLE – vapor-liquid equilibrium.

\*\* For temperature dependence equation, see [reference](#).<sup>#</sup> Boublik et al. 1984.



TABLE 5.1.5.4

Henry's law constants and octanol-water partition coefficients for fluoroalkanes and fluoroalkenes

Compound	Henry's law constant Pa•m <sup>3</sup> /mol	Temp. °C	Method/temp. range	Reference	K <sub>OW</sub>	Reference
<b>Fluoroalkanes</b>						
Fluoromethane	1418	25	calculated	Yaws et al. 1991	0.51	Sangster 1993
	1948	20		Glew & Moelwyn-Hughes 1953	0.51	Hansch et al. 1995
	1717	25	calculated C <sub>A</sub> /C <sub>W</sub>	Hine & Mookerjee 1975		
	1742	20T		Staudinger & Roberts 2001		
Difluoromethane	1160	25		Yaws et al. 1991	0.20	Sangster 1993, Hansch et al. 1995
Trifluoromethane	5907	25	gas stripping-GC	Warner et al. 1987	0.64	Hansch & Leo 1985
	9211	25		Hine & Mookerjee 1975	0.64	Sangster 1993
	7794	25		Yaws et al. 1991	0.64	Hansch et al. 1995
	9626	25	calculated-P/C	Howard 1993	0.64	Howard 1993, Hansch et al. 1995
Tetrafluoromethane	539961	25		Yaws et al. 1991	1.18	Sangster 1993, Hansch et al. 1995
Chlorofluoromethane	654.4	25		Yaws et al. 1991		
Dichlorofluoromethane	529.1	25		Yaws et al. 1991	1.55	Hansch et al. 1995
Chlorodifluoromethane	3058	25		Yaws et al. 1991	1.08	Hansch et al. 1995
	2979	25		Howard 1993	1.08	Howard 1993
Chlorotrifluoromethane	113889	25		Yaws et al. 1991	1.65	Hansch et al. 1995
Dichlorodifluoromethane	28704	19.93	0–40°C	Warner & Weiss 1985	2.16	Hansch et al. 1996
	39557	25		Yaws et al. 1991	2.16	Howard 1997
	27976	25		Howard 1997		
	26810	20T		Staudinger & Roberts 2001		
Trichlorofluoromethane	7925	19.93	0–40°C	Warner & Weiss 1985	2.53	Hansch et al. 1995
	10234	25T		Ashworth et al. 1988	2.53	Howard 1990
	9827	25		Howard 1990		
	12341	25		Yaws et al. 1991		
	7824	20T		Staudinger & Roberts 2001		
Fluoroethane	2253	25		Yaws et al. 1991		
1,1-Difluoroethane	2672	25		Yaws et al. 1991	0.75	Hansch et al. 1995
	2203	25		Hine & Mookerjee 1975	0.75	Sangster 1993
	2061			Howard 1993	0.75	Howard 1993

(Continued)

TABLE 5.1.5.4 (Continued)

Compound	Henry's law constant Pa•m³/mol	Temp. °C	Method/temp. range	Reference	K <sub>OW</sub>	Reference
1,1,2-Trifluoroethane	1876	25	EPICS-GC	Zheng et al. 1997		
	32323	25T		Ashworth et al.1988		
	24616	20T		Staudinger & Roberts 2001		
1,1,1,2-Tetrafluoroethane	5629	25	calc-bond contribution	Zheng et al. 1997	1.06	Franklin 1993
Hexafluoroethane	1715432	25		Yaws et al. 1991	2.00	Sangster 1993
1-Chloro-1,1-difluoroethane	1652940	25T		Bonifacio et al. 2001	2.00	Hansch et al. 1995
	24217	25		Howard 1990	1.60	Howard 1990
1-Chloro-1,2,2,2-tetrafluoro-	54716	25		Howard 1997	1.867	estimated, Howard 1997
1-Chloropentafluoroethane	261418	25		Yaws et al. 1991	2.30	Howard 1997
	309041	25		Howard 1997		
1,1-Dichloro-1-fluoroethane	2442	25		Howard 1997	2.04	Howard 1997
1,2-Dichlorotetrafluoroethane	122502	25		Yaws et al. 1991	2.82	Sangster 1993, Hansch et al. 1995
1,1-Dichlorotetrafluoroethane					2.85	Sangster 1993, Hansch et al. 1995
1,1,2-Trichloro-1,2,2-trifluoro-	49132	25	calculated-P/C	Yaws et al. 1991	3.16	McDuffie 1981, Sangster 1993
	53297			Howard 1990	3.16	Howard 1990, Hansch 1995
1,1-Difluorotetrachloroethane	171239		calculated-P/C	Howard 1993	2.85	estimated, Howard 1993
1,2-Difluoro-1,1,2,2-tetrafluoro-	283710			Howard 1990	2.82	Howard 1990, Sangster 1993, Hansch et al. 1995
1,1,2,2-Tetrachloro-1,2-difluoro-	9869		calculated-C <sub>A</sub> /C <sub>w</sub>	Hine & Mookerjee 1975	3.73	Howard 1990
1-Fluoropropane	1627	14		Yaws et al. 1991		
2-Fluoropropane	1713	15		Yaws et al. 1991		
Perfluorocyclobutane	391925	25		Yaws et al. 1991		
Fluoroalkenes						
1,1-Difluoroethene	39344	25		Yaws et al. 1991	1.24	Hansch et al. 1995
Tetrafluoroethene	61981	25		Yaws et al. 1991		
Chlorotrifluoroethene	63328	25		Yaws et al. 1991		
Hexafluoropropene	349397	25		Wilhelm et al. 1977		

TABLE 5.1.5.5  
Atmospheric fate rates for fluoroalkanes

Compound	Atmospheric fate rate (photooxidation in air)			Lifetime, $\tau$	Reference
	T/K	$k_{OH}^*/(\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$	Temp. range**		
<b>Fluoroalkanes</b>					
Fluoromethane	296	$16 \times 10^{-15}$	294–480 K	2–4.1 yr	Howard & Evenson 1976a
	298	$1.68 \times 10^{-14}$			Atkinson 1989
Difluoromethane	296	$7.8 \times 10^{-15}$	293–425 K	7.1–7.7 yr 4–7.3 yr	Cooper et al. 1992
	298	$7.2 \times 10^{-15}$			Howard & Evenson 1976a
	298	$1.09 \times 10^{-14}$			Clyne et al.1978
	298	$1.13 \times 10^{-14}$			Atkinson 1989
Trifluoromethane	296	$0.2 \times 10^{-15}$	387–1445		Talukdar et al. 1991
	298	$2.4 \times 10^{-16}$			Cooper et al. 1992
Tetrafluoromethane	298	$<4 \times 10^{-16}$			Howard & Evenson 1976a
Chlorofluoromethane	296	$37 \times 10^{-15}$	245–486 K		Atkinson 1989
	298	$4.41 \times 10^{-14}$			Howard & Evenson 1976a
Dichlorofluoromethane	296	$26 \times 10^{-15}$	293–425 K		Atkinson 1989
	298	$3.9 \times 10^{-14}$			Howard & Evenson 1976a
	298	$3.03 \times 10^{-14}$			Clyne et al. 1978
Chlorodifluoromethane	296	$3.4 \times 10^{-15}$	241–483 K		Atkinson 1989
	298	$4.1 \times 10^{-15}$			Howard & Evenson 1976a
	298	$4.68 \times 10^{-15}$			Clyne et al. 1978
Chlorotrifluoromethane	296	$<0.7 \times 10^{-15}$	293–425 K	17.2 yr	Atkinson 1989
	298	$<7 \times 10^{-16}$			Brown et al. 1990
Dichlorodifluoromethane	296	$<1.0 \times 10^{-15}$	250–482 K	>330 yr	Howard & Evenson 1976a
	296	$<0.4 \times 10^{-15}$			Atkinson 1989
	293	$<10^{-16}$			Atkinson et al.1975
	298	$<1.0 \times 10^{-17}$			Howard & Evenson 1976a
Trichlorofluoromethane	296	$<1.0 \times 10^{-15}$		105 yr	Cox et al. 1976
	296	$<0.5 \times 10^{-15}$			Atkinson 1989
	293	$<10^{-17}$			Brown et al. 1990
	298	$<1.0 \times 10^{-17}$			Atkinson et al. 1975
				1000 yr	Howard & Evenson 1976a
					Cox et al. 1976
					Atkinson 1989

(Continued)

TABLE 5.1.5.5 (Continued)

Compound	Atmospheric fate rate (photooxidation in air)			Lifetime, $\tau$	Reference
	T/K	$k_{OH}^*/(\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$	Temp. range**		
Fluoroethane				60 yr	Brown et al. 1990
				182–635 yr	Cooper et al. 1992
				0.2–1 yr	Cooper et al. 1992
	298	$5.1 \times 10^{-14}$	293–425 K		Clyne et al. 1978
	295	$3.4 \times 10^{-14}$			Atkinson 1989
1,1-Difluoroethane	303	$5.6 \times 10^{-14}$	230–423 K	1.5 yr	Brown et al. 1990
	298	$4.2 \times 10^{-14}$	243–400 K	1.5 yr	Liu et al. 1990
				1–1.68 yr	Cooper et al. 1992
				0.58–0.8 yr	Cooper et al. 1992
1,2-Difluoroethane					Clyne et al. 1978
1,1,1-Trifluoroethane	298	$1.5 \times 10^{-15}$	293–425 K		Talukdar et al. 1991
	298	$1.35 \times 10^{-15}$	223–374	72–74 yr	Brown et al. 1990
1,1,2-Trifluoroethane				6.3 yr	Cooper et al. 1992
				20–45 yr	Clyne et al. 1978
	298	$4.9 \times 10^{-14}$	293–425		Cooper et al. 1992
				1–3.8 yr	Clyne et al. 1978
1,1,2,2-Tetrafluoroethane	298	$6.9 \times 10^{-15}$	293–425		Atkinson 1989
	298	$8.54 \times 10^{-15}$	249–473 K		Cooper et al. 1992
1,1,1,2-Tetrafluoroethane				2–12.3 yr	Clyne et al. 1978
	298	$6.9 \times 10^{-15}$	293–425		Brown et al. 1990
	301	$6.9 \times 10^{-15}$	231–423 K	10.7 yr	Liu et al. 1990
	298	$5.18 \times 10^{-15}$	243–400 K	14.4 yr	Franklin 1993
Pentafluoroethane				13.1–15.5 yr	Cooper et al. 1992
	298	$5.0 \times 10^{-15}$	293–425 K		Clyne et al. 1978
	303	$2.9 \times 10^{-15}$	226–423 K	22.1 yr	
	298	$1.9 \times 10^{-15}$	220–364 K	47–48 yr	Talukdar et al. 1991
1-Chloro-1,1-difluoroethane				17–28.1 yr	Cooper et al. 1992
	298	$6.74 \times 10^{-15}$	293–425 K		Clyne et al. 1978
	298	$3.58 \times 10^{-15}$	273–375 K		Atkinson 1989
	303	$3.7 \times 10^{-15}$	231–423 K	15.4 yr	Brown et al. 1990
1-Chloro-1,1,2-trifluoroethane	298	$4.02 \times 10^{-15}$	243–400 K	17.8 yr	Liu et al. 1990
	298	$1.5 \times 10^{-14}$	293–425 K		Clyne et al. 1978
	298	$1.61 \times 10^{-14}$	263–373 K		Atkinson 1989

1-Chloro-1,2,2,2-tetrafluoroethane	298	$1.02 \times 10^{-14}$	250–375 K		Atkinson 1989
1,1-Dichloro-1-fluoroethane	298	$7.1 \times 10^{-15}$	243–400 K	6.7 yr	Liu et al. 1990
	297	$1.61 \times 10^{-14}$	238–426 K	4.3 yr	Brown et al. 1990
	298	$5.92 \times 10^{-15}$	233–393 K	13–14 yr	Talukdar et al. 1991
	298	$2.61 \times 10^{-14}$	249–473 K		Atkinson 1989
1,1-Dichlorotrifluoroethane	298	$4.2 \times 10^{-14}$	293–425 K		Clyne et al. 1978
	298	$3.34 \times 10^{-14}$	245–375 K		Atkinson 1989
	303	$5.9 \times 10^{-14}$	232–425 K	1.0 yr	Brown et al. 1990
	298	$3.52 \times 10^{-14}$	270–400 K	1.4 yr	Liu et al. 1990
1,1,2,2,3-Pentafluoropropane	298	$2 \times 10^{-14}$ , $4 \times 10^{-14}$		2, 1.3 yr	Cooper et al. 1993
1,1,1,2,2-Pentafluoropropane	298	$7 \times 10^{-15}$ , $8 \times 10^{-15}$		7 yr	Cooper et al. 1993
1,1,1,2,3,3-Hexafluoropropane	298	$4 \times 10^{-15}$ , $6 \times 10^{-15}$		10, 9 yr	Cooper et al. 1993
1,1,1,3,3,3-Hexafluoropropane	298	$5 \times 10^{-16}$ , $2 \times 10^{-16}$		77, 218 yr	Cooper et al. 1993
1,1,1,2,3,3,3-Heptafluoropropane	298	$7 \times 10^{-16}$		63, 72 yr	Cooper et al. 1993

\*  $k_{OH}$  = second order reaction rate constant with hydroxyl radicals

\*\* For temperature dependence equation, see [reference](#).

## 5.1.5 FLUOROALKANES AND FLUOROALKENES

TABLE 5.2.1

Summary of physical properties of halogenated hydrocarbons

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V <sub>M</sub>	
							cm <sup>3</sup> /mol	
							MW/ρ at 20°C	Le Bas
Chloroalkanes:								
Chloromethane (Methyl chloride)	74-87-3	CH <sub>3</sub> Cl	50.488	−97.7	−24.09	1	54.79	50.5
Dichloromethane	75-09-2	CH <sub>2</sub> Cl <sub>2</sub>	84.933	−97.2	40	1	64.07	71.4
Trichloromethane (Chloroform)	67-66-3	CHCl <sub>3</sub>	119.378	−63.41	61.17	1	79.67	92.3
Tetrachloromethane (Carbon tetrachloride)	56-23-5	CCl <sub>4</sub>	153.823	−22.62	76.8	1	96.50	113.2
Chloroethane (Ethyl chloride)	75-00-3	C <sub>2</sub> H <sub>5</sub> Cl	64.514	−138.4	12.3	1	72.00	72.7
1,1-Dichloroethane	75-34-3	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	98.959	−96.9	57.3	1	84.18	93.6
1,2-Dichloroethane	107-06-2	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	98.959	−35.7	85.3	1	79.04	93.6
1,1,1-Trichloroethane	71-55-6	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	133.404	−30.01	74.09	1	99.70	114.5
1,1,2-Trichloroethane	79-00-5	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	133.404	−36.3	113.8	1	92.69	114.5
1,1,1,2-Tetrachloroethane	630-20-6	C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>	167.849	−70.2	130.2	1	108.95	135.4
1,1,2,2-Tetrachloroethane	79-34-5	C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>	167.849	−42.4	145.2	1	105.27	135.4
Pentachloroethane	76-01-7	C <sub>2</sub> HCl <sub>5</sub>	202.294	−28.78	162.0	1	120.36	156.3
Hexachloroethane	67-72-1	C <sub>2</sub> Cl <sub>6</sub>	236.739				113.22	177.2
1-Chloropropane ( <i>n</i> -Propyl chloride)	540-54-5	C <sub>3</sub> H <sub>7</sub> Cl	78.541	−122.9	46.5	1	88.26	94.9
2-Chloropropane	75-29-6	C <sub>3</sub> H <sub>7</sub> Cl	78.541	−117.18	35.7	1	91.15	94.9
1,2-Dichloropropane	78-87-5	C <sub>3</sub> H <sub>6</sub> CL <sub>2</sub>	112.986	−100.53	96.4	1	97.74	115.8
1,2,3-Trichloropropane	96-18-4	C <sub>3</sub> H <sub>5</sub> Cl <sub>3</sub>	147.431	−14.7	157	1	106.59	136.7
1-Chlorobutane ( <i>n</i> -Butyl chloride)	109-69-3	C <sub>4</sub> H <sub>9</sub> Cl	92.567	−123.1	78.4	1	104.51	117.1
2-Chlorobutane	78-86-4	C <sub>4</sub> H <sub>9</sub> Cl	92.567	−131.3	68.2	1	106.01	117.1
1-Chloropentane ( <i>n</i> -Amyl chloride)	543-59-6	C <sub>5</sub> H <sub>11</sub> Cl	106.594	−99.0	108.4	1	120.85	139.3
1-Chlorohexane	544–10–5	C <sub>6</sub> H <sub>13</sub> Cl	120.620	−94.0	135.1	1	137.30	161.5
1-Chloroheptane	629–06–1	C <sub>7</sub> H <sub>15</sub> Cl	134.647	−69.5	160.4	1	153.74	183.7
1-Chlorooctane	111–85–3	C <sub>8</sub> H <sub>17</sub> Cl	148.674	−57.8	183.5	1	170.15	205.9
1-Chlorononane	2473–01–0	C <sub>9</sub> H <sub>19</sub> Cl	162.700	−39.4	205.2	1	206.31	228.1
1-Chlorodecane	1002–69–3	C <sub>10</sub> H <sub>21</sub> Cl	176.727	−31.3	225.9	1	203.02	250.3

**Chloroalkenes:**

Chloroethene (Vinyl chloride)	75-01-4	C <sub>2</sub> H <sub>3</sub> Cl	62.498	-153.84	-13.8	1	68.63	65.3
1,1-Dichloroethene	75-35-4	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.943	-122.56	31.6	1	79.91	86.2
<i>cis</i> -1,2-Dichloroethene	156-59-2	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.943	-80.0	60.1	1	75.52	86.2
<i>trans</i> -1,2-Dichloroethene	156-60-5	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.943	-49.8	48.7	1	77.15	86.2
Trichloroethylene	79-01-6	C <sub>2</sub> HCl <sub>3</sub>	131.388	-84.7	87.21	1	89.73	107.1
Tetrachloroethylene	127-18-4	C <sub>2</sub> Cl <sub>4</sub>	165.833	-22.3	121.3	1	120.19	128.0
<i>cis</i> -1,3-Dichloropropene	10061-01-5	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub>	110.970		104.3		91.18	108.4
<i>trans</i> -1,3-Dichloropropene	10061-02-6	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub>	110.970		112		90.66	108.4
Chloroprene	126-99-8	C <sub>4</sub> H <sub>5</sub> Cl	88.536	-130	59.4	1	92.39	102.3
Hexachloro-1,3-butadiene	87-68-3	C <sub>4</sub> Cl <sub>6</sub>	260.761	-21	215	1	155.03	206.8
Hexachlorocyclopentadiene	77-47-4	C <sub>5</sub> H <sub>6</sub>	272.772	-9	239	1	160.27	210.1

**Bromoalkanes and bromoalkenes:**

Bromomethane	74-83-9	CH <sub>3</sub> Br	94.939	-93.68	3.5	1	56.66	52.9
Dibromomethane	74-95-3	CH <sub>2</sub> Br <sub>2</sub>	173.835	-52.5	97	1	69.62	76.2
Tribromomethane	75-25-2	CHBr <sub>3</sub>	252.731	8.69	149.1	1	87.42	99.5
Bromoethane (Ethyl bromide)	74-96-4	C <sub>2</sub> H <sub>5</sub> Br	108.965	-118.6	38.5	1	75.12	75.1
1,2-Dibromoethane	106-93-4	C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>	187.861	9.84	131.6	1	86.21	98.4
1-Bromopropane ( <i>n</i> -Propyl bromide)	106-94-5	C <sub>3</sub> H <sub>7</sub> Br	122.992	-110.3	71.1	1	90.86	97.3
2-Bromopropane	75-26-3	C <sub>3</sub> H <sub>7</sub> Br	122.992	-89.0	59.5	1	93.60	97.3
1,2-Dibromopropane	78-75-1	C <sub>3</sub> H <sub>6</sub> Br <sub>2</sub>	201.888	-55.49	141.9	1	104.48	120.6
1-Bromobutane ( <i>n</i> -Butyl bromide)	109-65-9	C <sub>4</sub> H <sub>9</sub> Br	137.018	-112.6	101.6	1	107.40	119.5
1-Bromopentane ( <i>n</i> -Amyl bromide)	110-53-2	C <sub>5</sub> H <sub>11</sub> Br	151.045	-88.0	129.8	1	123.99	141.7
1-Bromohexane	111-25-1	C <sub>6</sub> H <sub>13</sub> Br	165.071	-83.7	155.3	1	140.56	163.9
1-Bromoheptane	629-04-9	C <sub>7</sub> H <sub>15</sub> Br	179.098	-56.1	178.9	1	157.10	186.1
1-Bromooctane	111-83-1	C <sub>8</sub> H <sub>17</sub> Br	193.125	-55.0	200.8	1	173.64	208.3
1-Bromodecane	112-29-8	C <sub>10</sub> H <sub>21</sub> Br	221.178	-29.2	240.6	1	206.67	252.7
1-Bromododecane	143-15-7	C <sub>12</sub> H <sub>25</sub> Br	249.231	-9.5	276	1	239.67	297.1
Bromocyclohexane	108-85-0	C <sub>6</sub> H <sub>11</sub> Br	163.055	-56.5	166.2	1	122.06	141.5
Vinyl bromide	593-60-2	C <sub>2</sub> H <sub>3</sub> Br	106.949	-139.54	15.8	1	71.62	67.7

(Continued)

TABLE 5.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V <sub>M</sub>	
							cm <sup>3</sup> /mol	
							MW/ρ at 20°C	Le Bas
<b>Iodoalkanes:</b>								
Iodomethane (Methyl iodide)	74-88-4	CH <sub>3</sub> I	141.939	−66.4	42.43	1	62.28	62.9
Iodoethane (Ethyl iodide)	75-03-6	C <sub>2</sub> H <sub>5</sub> I	155.965	−111.1	72.3	1	80.57	85.1
1-Iodopropane ( <i>n</i> -Propyl iodide)	107-08-4	C <sub>3</sub> H <sub>7</sub> I	169.992	−101.3	102.5	1	97.20	107.3
2-Iodopropane	75−30−9	C <sub>3</sub> H <sub>7</sub> I	169.992	−90	89.5	1	99.75	107.3
1-Iodobutane ( <i>n</i> -Butyl iodide)	542-69-8	C <sub>4</sub> H <sub>9</sub> I	184.018	−103	130.5	1	113.91	129.5
1-Iodopentane	628−17−1	C <sub>5</sub> H <sub>11</sub> I	198.045	−85.6	157.0	1	130.63	151.7
<b>Mixed halogenated hydrocarbons:</b>								
Bromochloromethane	74-97-5	CH <sub>2</sub> BrCl	129.384	−87.9	68.0	1	66.89	73.8
Bromodichloromethane	75-27-4	CHBrCl <sub>2</sub>	163.829	−57	90	1	83.12	94.7
Dibromochloromethane	124-48-1	CHBr <sub>2</sub> Cl	208.280	−20	120	1	84.98	97.1
Chlorodifluoromethane (HCFC-22)	75-45-6	CHClF <sub>2</sub>	86.469	−157.42	−40.7	1	71.25	60.5
Dichlorodifluoromethane (CFC-12)	75-71-8	CCl <sub>2</sub> F <sub>2</sub>	120.914	−158	−29.8	1	90.97	81.4
Trichlorofluoromethane (CFC-11)	75-69-4	CCl <sub>3</sub> F	137.368	−110.44	23.7	1	92.32	97.3
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	76-13-1	C <sub>2</sub> F <sub>3</sub> Cl <sub>3</sub>	187.375	−36.22	47.7	1	119.84	129.5
1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)	76−12−0	C <sub>2</sub> F <sub>2</sub> Cl <sub>4</sub>	203.830	24.8	92.8	1		145.4

\* Assuming ΔS<sub>fus</sub> = 56 J/mol K.



TABLE 5.2.2

Summary of selected physical-chemical properties of halogenated hydrocarbons at 25°C

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility				H/(Pa·m <sup>3</sup> /mol)	
	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> )	log K <sub>OW</sub>	calcd P/C	exptl
<b>Chloroalkanes:</b>								
Chloromethane	570000	570000	5325	105.5	105.5	0.91	960.7*	894
Dichloromethane	58000	58000	13200	155.4	155.4	1.25	373.2	300
Trichloromethane	26200	26200	8200	68.69	68.69	1.97	381.4	427
Tetrachloromethane	15250	15250	800	5.200	5.200	2.83	2932	2989
Chloroethane	16000	16000	5700	88.35	88.35	1.43	181.1	1023
1,1-Dichloroethane	30260	30260	5040	50.93	50.93	1.79	594.1	569
1,2-Dichloroethane	10540	10540	8600	86.90	86.90	1.48	121.3	143
1,1,1-Trichloroethane	16500	16500	1290	9.670	9.670	2.49	1706	1763
1,1,2-Trichloroethane	3220	3220	4590	34.41	34.41	2.38	93.59	92.2
1,1,1,2-Tetrachloroethane	1580	1580	1070	6.375	6.375		247.8	
1,1,2,2-Tetrachloroethane	793	793	2830	16.86	16.86	2.39	47.03	25.7
Pentachloroethane	590	590	490	2.422	2.422	3.22	243.6	
Hexachloroethane	50	1923	50	0.2112	8.123	4.14	236.7	846
1-Chloropropane	46000	46000	2500	31.83	31.83	2.04	1445	
2-Chloropropane	68700	68700	3000	38.20	38.20	1.90	1798	
1,2-Dichloropropane	6620	6620	2740	24.25	24.25	2.00	273.0	287
1,2,3-Trichloropropane	492	492	1896	12.86	12.86		38.26	
1-Chlorobutane	13700	13700	615	6.644	6.644	2.64	2062	1537
2-Chlorobutane	20210	20210	1000	10.80	10.80		1871	2267
1-Chloropentane	4142	4142	198	1.858	1.858		2230	2375
<b>Chloroalkenes:</b>								
Chloroethene	354600	354600	2763	44.21	44.21	1.38	8021	2685
1,1-Dichloroethene	80500	80500	3344	34.49	34.49	2.13	2334	2624
<i>cis</i> -1,2-Dichloroethene	27000	27000	3500	36.10	36.10	1.86	747.8	460
<i>trans</i> -1,2-Dichloroethene	44400	44400	6260	64.57	64.57	1.93	687.6	958
Trichloroethylene	9900	9900	1100	8.372	8.372	2.53	1182	1034
Tetrachloroethylene	2415	2415	150	0.904	0.904	2.88	2670	1733

(Continued)

TABLE 5.2.2 (Continued)

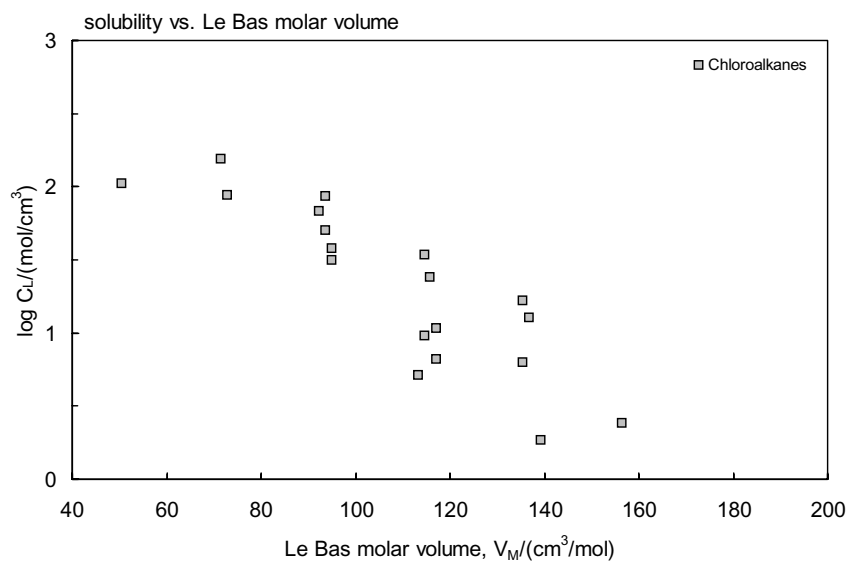
Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility			log K <sub>ow</sub>	H/(Pa·m <sup>3</sup> /mol)	
	P <sup>S</sup> /Pa	P <sub>L</sub> /Pa	S/(g/m <sup>3</sup> )	C <sup>S</sup> /(mol/m <sup>3</sup> )	C <sub>L</sub> /(mol/m <sup>3</sup> )		calcd P/C	exptl
1,3-Dichloropropene						1.98		
Chloroprene	23194	23194				2.03		
Hexachloro-1,3-butadiene	20.0	20.0	3.2	0.013	0.013	4.70	1630	
Hexachlorocyclopentadiene	10.9	10.9	1.80	0.0066	0.0066	5.04	1652	
<b>Bromoalkanes and bromoalkenes:</b>								
Bromomethane	217700	217700	15223	160.3	160.3	1.19	631.9*	
Dibromomethane	6034	6034	11442	65.82	65.82	2.50	91.67	86.13
Tribromomethane	727	727	3100	12.27	12.27	2.38	59.27	46.61
Bromoethane	62500	62500	8939	82.04	82.04	1.6	1235*	
1,2-Dibromoethane	1500	1500	4152	22.10	22.10		67.87	65.86
1-Bromopropane	18440	18440	598	4.862	4.862	2.1	3792	
2-Bromopropane	31940	31940	3086	25.09	25.09	1.9	1273	
1,2-Dibromopropane	1040	1040	1428	7.073	7.073		147.0	
1-Bromobutane	5500	5500				2.6		
Vinyl bromide	140476	140476						
<b>Iodoalkanes:</b>								
Iodomethane	54000	54000	13894	97.89	97.89	1.5	551.6	541
Iodoethane	18160	18160	4041	25.91	25.91	2	700.9	
1-Iodopropane	5745	5745	1051	6.183	6.183	2.5	929.2	
1-Iodobutane	1848	1848	182	0.989	0.989	3	1868	
<b>Mixed halogenated hydrocarbons:</b>								
Bromochloromethane	19600	19600	14778	114.2	114.2	1.41	171.6	
Bromodichloromethane	6670	6670	4500	27.47	27.47	2.1	242.8	162
Dibromochloromethane			4000	19.20	19.20	2.24		86.13
Chlorodifluoromethane (HCFC-22)	1044000	1044000	2899	33.53	33.53		3022*	
Dichlorodifluoromethane (CFC-12)	651000	651000	300	2.481	2.481	2.16	40840*	
Trichlorofluoromethane (CFC-11)	102200	102200	1080	7.862	7.862	2.53	12890*	10243
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	48320	48320	166	0.886	0.886	3.16	114375*	32323

\* Vapor pressure exceeds atmospheric pressure, Henry's law constant H (Pa·m<sup>3</sup>/mol) = 101325 Pa/C<sup>S</sup> mol/m<sup>3</sup>.

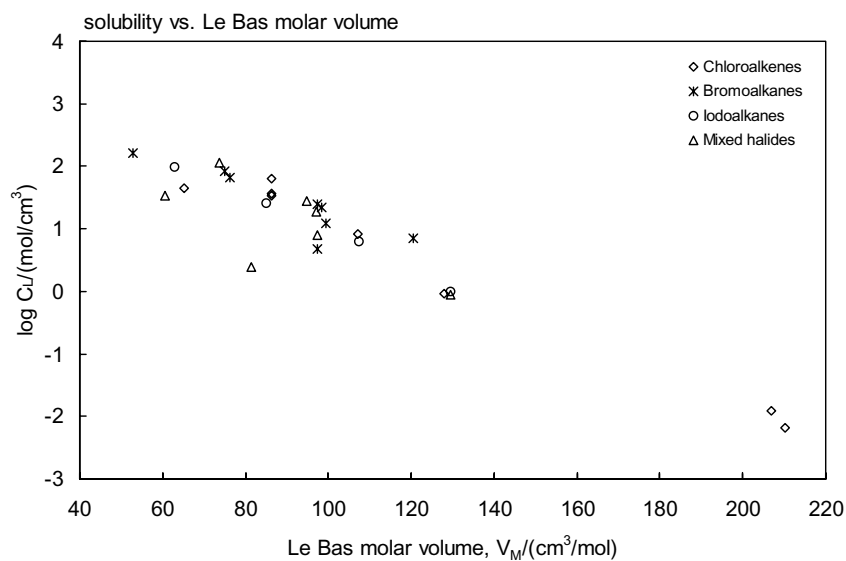
TABLE 5.2.3

Suggested half-life classes of halogenated hydrocarbons in various environmental compartments at 25°C

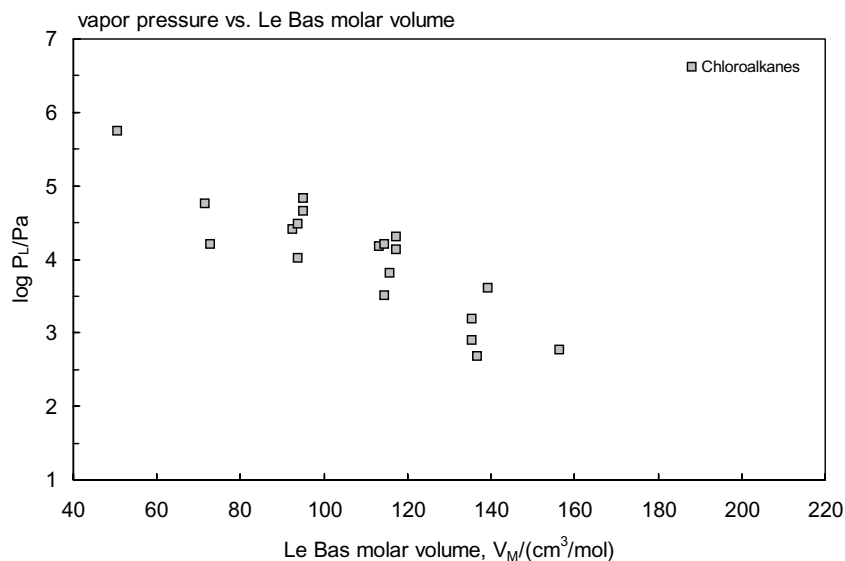
Compound	Air class	Water class	Soil class	Sediment class
Cycloalkanes and cycloalkenes:				
Dichloromethane	6	6	7	8
Trichloromethane	6	6	7	8
Tetrachloroethane	8	6	7	8
Chloroethane	6	6	7	8
1,2-Dichloroethane	6	6	7	8
1,1,2,2-Tetrachloroethane	8	6	7	8
Pentachloroethane	8	6	7	8
Hexachloroethane	8	6	7	8
1,2-Dichloropropane	5	6	7	8
1,2,3-Trichloropropane	5	6	7	8
Chloroethene (Vinyl chloride)	3	5	6	7
Trichloroethylene	4	6	7	8
Tetrachloroethylene	5	6	7	8
Chloroprene	3	5	6	7
Bromoalkanes and bromoalkenes:				
Tribromomethane	6	6	7	8
Mixed halogenated hydrocarbons:	5	5	6	7
Bromodichloromethane	5	5	6	7
Trichlorofluoromethane (CFC-11)	8	8	9	9
<b>Class</b>	<b>Mean half-life (h)</b>		<b>Range (h)</b>	
1	5		< 10	
2	17 (~ 1 d)		10–30	
3	55 (~ 2 d)		30–100	
4	170 (~ 1 week)		100–300	
5	550 (~ 3 weeks)		300–1,000	
6	1700 (~ 2 months)		1,000–3,000	
7	5500 (~ 8 months)		3,000–10,000	
8	17000 (~ 2 yr)		10,000–30,000	
9	55000 (~ 6 yr)		> 30,000	



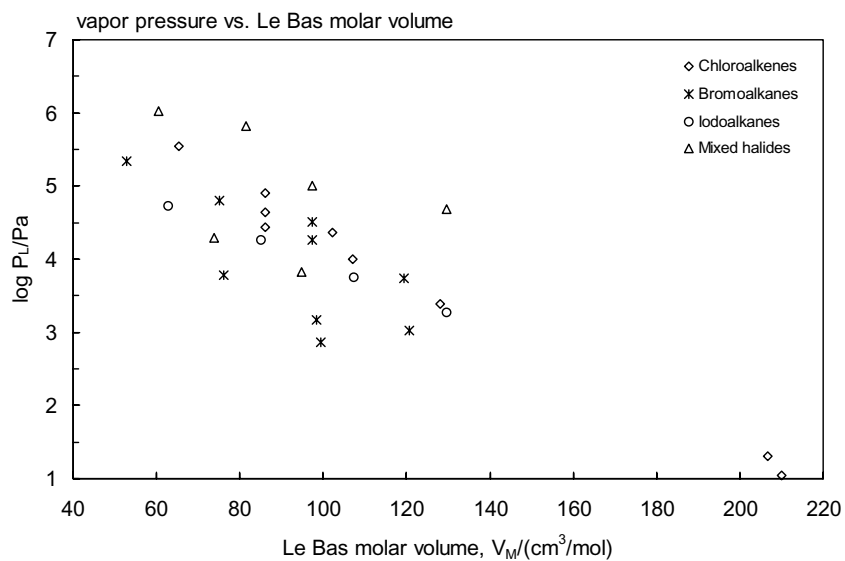
**FIGURE 5.2.1** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.



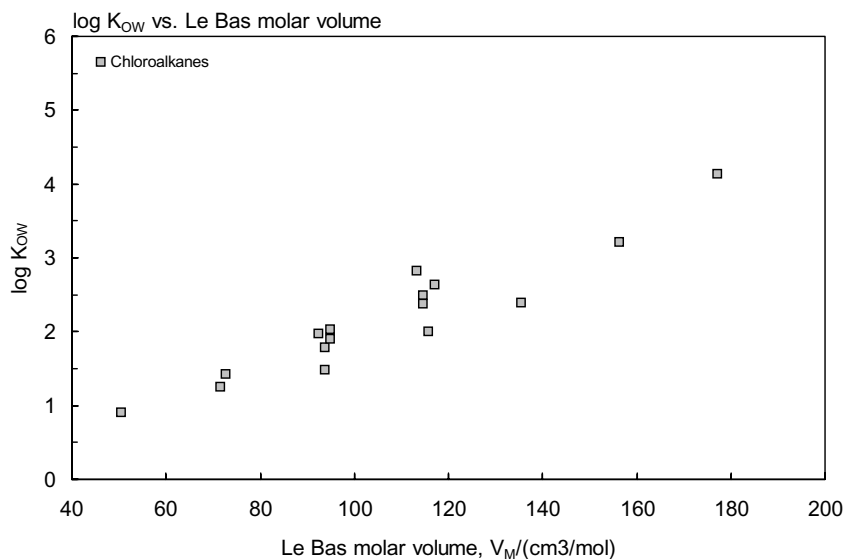
**FIGURE 5.2.2** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.



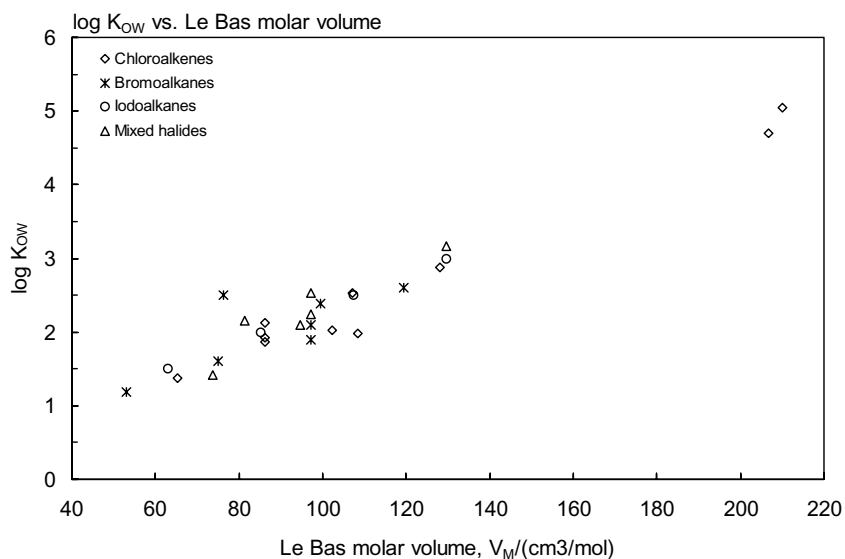
**FIGURE 5.2.3** Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.



**FIGURE 5.2.4** Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.



**FIGURE 5.2.5** Octanol-water partition coefficient versus Le Bas molar volume for chloroalkanes.



**FIGURE 5.2.6** Octanol-water partition coefficient versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

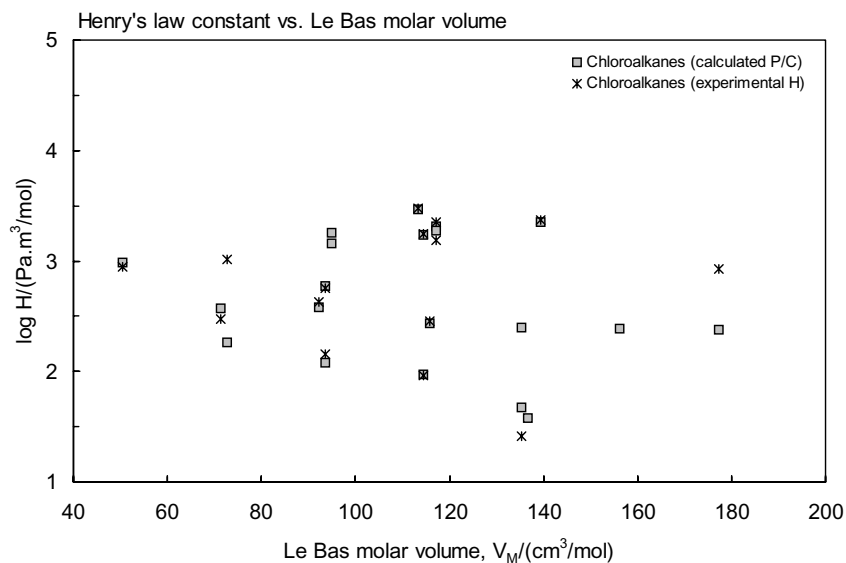


FIGURE 5.2.7 Henry's law constant versus Le Bas molar volume for chloroalkanes.

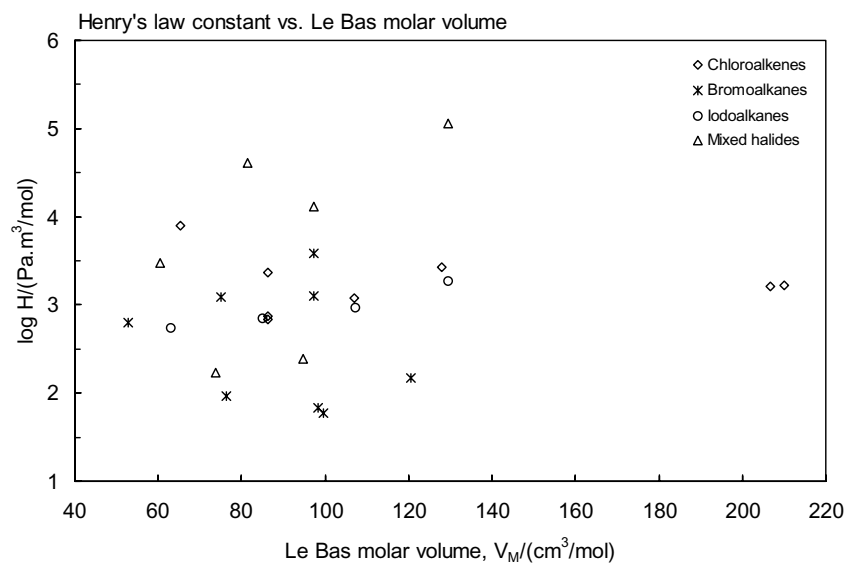
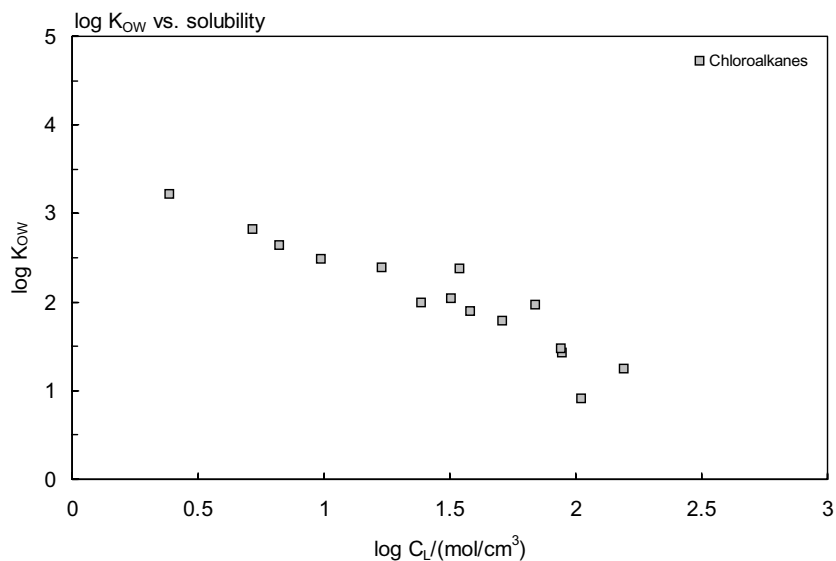
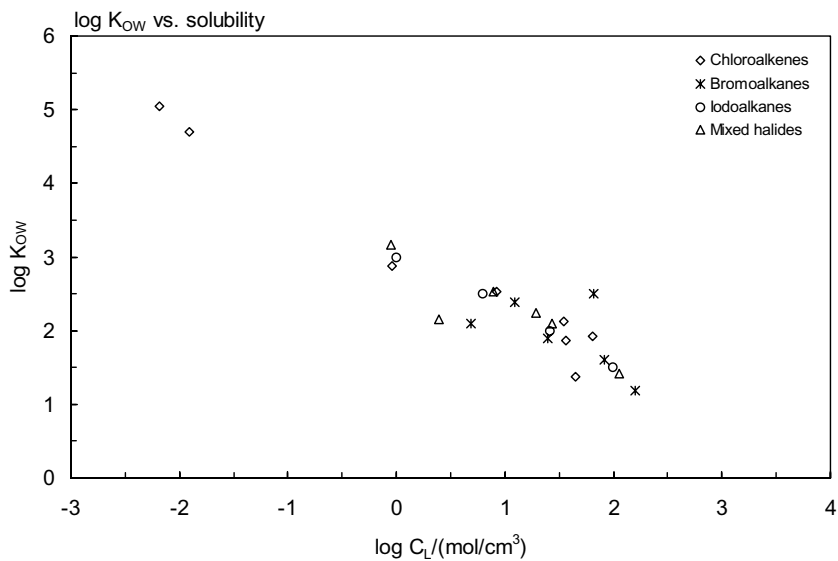


FIGURE 5.2.8 Henry's law constant versus Le Bas molar volume for halogenated aliphatic hydrocarbons.



**FIGURE 5.2.9** Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for chloroalkanes.



**FIGURE 5.2.10** Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for halogenated aliphatic hydrocarbons.



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