
16 Nitrogen and Sulfur Compounds

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16.1 LIST OF CHEMICALS AND DATA COMPILATIONS

16.1.1 NITRILES (ORGANIC CYANIDES)

16.1.1.1 Acetonitrile



Common Name: Acetonitrile

Synonym: cyanomethane, ethanenitrile, methyl cyanide

Chemical Name: acetonitrile

CAS Registry No: 75-05-8

Molecular Formula: $\text{C}_2\text{H}_3\text{N}$, CH_3CN

Molecular Weight: 41.052

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

−43.82 (Lide 2003)

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

81.65 (Lide 2003)

Density (g/cm^3 at 20°C):

0.7857 (Dreisbach 1961; Weast 1982–83; Dean 1985)

0.7803 (25°C , Dreisbach 1961)

Molar Volume (cm^3/mol):

52.7 (calculated-density, Rohrschneider 1973)

57.4 (exptl. at normal bp, Lee et al. 1972)

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

Dissociation Constant, pK :

29.1 (pK_a , Riddick et al. 1986; Howard 1993)

32.2 (pK_s , Riddick et al. 1986)

−10.12 (pK_{BH^+} , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.01, 31.51 (25°C , bp, Dreisbach 1961)

32.94, 29.82 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.167 (Riddick et al. 1986)

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

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

$> 3.1 \times 10^6$ (Booth & Everson 1948)

miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990; Howard 1993)

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):

11870* (interpolated-regression of tabulated data, temp range -47 – 81.8°C , Stull 1947)

$\log (P/\text{mmHg}) = 7.12257 - 1315.2/(230 + t/^{\circ}\text{C})$, (Antoine eq., Dreisbach & Martin 1949)

11240 (calculated by formula, Dreisbach 1961)

$\log (P/\text{mmHg}) = 7.07354 - 1279.2/(224.0 + t/^{\circ}\text{C})$, temp range 5 – 119°C , (Antoine eq. for liquid state, Dreisbach 1961)

12156* (25.56°C , measured range 7.3 – 27.38°C , Putnam et al. 1965)

$\log (P/\text{mmHg}) = 7.89511 - 1773.06/(T/\text{K})$; temp range 280 – 300.5 K (Antoine eq., Putnam et al. 1965)

11510 (Hoy 1970)

24459* (41.82°C , ebulliometry, measured range 41 – 82°C , Meyer et al. 1971)

$\log (P/\text{mmHg}) = 6.23655 - 1397.9228/(239.275 + t/^{\circ}\text{C})$; temp range 41 – 82°C (ebulliometry, Meyer et al. 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 8173.2/(T/\text{K})] + 7.938662$; temp range: -47.0 to 81.8°C , (Antoine eq., Weast 1972–73)

11919* (25.3°C , measured range 15.1 – 89.2°C , Dojcanske & Heinrich 1974)

- 8306* (saturated-vapor volume, extrapolated from fitted Antoine eq., Mousa 1981)
 $\log(P/\text{kPa}) = 6.4914 - 1420.8649/(T/K - 42.15)$; temp range 438.9–530.1 K (ebulliometry, Mousa 1981)
 9864, 15330 (20°C, 30°C, Verschueren 1983)
 11790, 11830 (interpolated values-Antoine equations, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.39532 - 1420.682/(241.852 + t/^\circ\text{C})$, temp range: 15.1–89.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 7.54606 - 2093.145/(298.369 + t/^\circ\text{C})$, temp range: 7.26–27.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 12310 (calculated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 7.11988 - 1314.4/(230 + t/^\circ\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
 11840 (Riddick et al. 1986; Howard et al. 1986; quoted, Banerjee et al. 1990; Howard 1993)
 $\log(P/\text{kPa}) = 6.24747 - 1315.2/(230.0 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 11800 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.34522 - 1388.446/(-34.856 + T/K)$, temp range: 314–355 K, (Antoine eq., Stephenson & Malanowski 1987)
 11840 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.24724 - 1315.2/(230 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P/\text{mmHg}) = 23.1953 - 2.3389 \times 10^3/(T/K) - 5.4954 \cdot \log(T/K) + 7.9894 \times 10^{-10} \cdot (T/K) + 2.3293 \times 10^{-6} \cdot (T/K)^2$; temp range 229–546 K (vapor pressure eq., Yaws 1994)
 10604* (22.634°C, comparative ebulliometry, measured range 278–373 K, Ewing & Sanchez Ochoa 2004)
 $\ln(P/\text{kPa}) = 14.7340 - 3268.53/(T/K - 31.615)$, for temp range 290–362 K (comparative ebulliometry, Ewing & Sanchez Ochoa 2004)

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

- 3.50, 2.78 (exptl., calculated-bond contribution, Hine & Mookerjee 1975)
 2.07* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 2.033 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 1.474* (20°C, headspace-GC, measured range 6.0–30°C, Benkelberg et al. 1995)
 1.474, 1.477, 1.685 (20°C, headspace-GC, deionized water, rain water, artificial seawater, Benkelberg et al. 1995)
 $\ln(k_H/\text{atm}) = (13.8 \pm 0.3) - (4106 \pm 101)/T/K$, temp range: 6–30°C (headspace-GC measurement, Benkelberg et al. 1995)
 1.55 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 2.353 - 1627/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 2.05 (Ostwald concentration coefficient-concn ratio-GC/FID, Bebahani et al. 2002)

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

- 0.34 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1969, 1971; Hansch & Leo 1985)
 –0.54 (shake flask-GC, Tani & Hashimoto 1984)
 –0.34 (recommended, Sangster 1989, 1993)
 –0.34 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, $\log BCF$:

- 0.523 (estimated- K_{OW} as per regression eq of Bysshe 1982, Howard 1993)

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

- 0.523 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
 –0.714 (calculated- K_{OW} , Kollig 1993)

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

- Volatilization: $t_{1/2} \sim 21$ h from a model river of 1-m deep flowing at 1 m/s with a wind velocity of 3 m/s based on Henry's law constant (Lyman et al. 1982; quoted, Howard 1993)

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:

photooxidation $t_{1/2} = 314 - 12559$ yr in water, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)

$k_{\text{OH}}^* = (4.94 \pm 0.6) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297.2 K, measured range 297–424 K (flash photolysis-resonance fluorescence, Harris et al. 1981; quoted, Howard 1993)

$k_{\text{OH}}^* = (1.94 \pm 0.37) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 250–363 K (flash photolysis-resonance fluorescence, Kurylo & Knable 1984)

$k_{\text{OH}}^* = (2.1 \pm 0.3) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–393 K (discharge flow-EPR, Poulet et al. 1984)

$k_{\text{OH}}(\text{exptl}) = 2.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 2.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985)

$k_{\text{OH}} = 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993)

$k_{\text{OH}} = 1.90 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k(\text{soln}) = 3.70 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}}^* = 2.14 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

$k = 5.8 \times 10^{-3} \text{ M}^{-1} \text{ h}^{-1}$ at pH 7 and 25°C with $t_{1/2} > 150000$ yr (Ellington et al. 1987)

$k_{\text{O}_3}(\text{aq.}) \leq 6 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 18$ yr at pH 7 (Yao & Haag 1991).

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 168 - 672$ h, based on aerobic river die-away test data (Ludzack et al. 1958; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 672 - 2688$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1299 - 12991$ h, based on measured rate constant $k = 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 168 - 672$ h, based on aerobic river die-away test data (Howard et al. 1991);

photooxidation $t_{1/2} = 314 - 12559$ yr, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991);

$t_{1/2} \geq 18$ yr for direct reaction with ozone in water at pH 7 and 22°C (Yao & Haag 1991).

Groundwater: $t_{1/2} = 336 - 8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

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

Biota:

TABLE 16.1.1.1

Reported vapor pressures of acetonitrile 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)		

(Continued)

TABLE 16.1.1.1.1 (Continued)

1.

Stull 1947		Putnam et al. 1965		Meyer et al. 1971		Dojcanske & Heinrich 1974	
summary of literature data		manometer		ebulliometry		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−47.0	133.3	7.259	4997	41.82	24459	15.1	7359
−26.6	666.6	10.47	5861	46.09	29026	20.1	9413
−16.3	1333	13.791	6914	46.11	29032	25.3	11919
−5.0	2666	18.701	8809	50.36	34288	30.7	15252
7.7	5333	21.905	10244	55.37	41393	35	18292
15.9	7999	23.401	11031	60.64	50155	39.95	22465
27	13332	25.563	12156	65.91	60390	40	22625
43.7	26664	27.38	13187	70.74	71145	44.9	27638
62.5	53329			76.31	85512	50.1	33797
81.8	101325	eq. 1	P/mmHg	81.87	101990	54.9	40517
		A	7.89511	81.89	102010	60	49022
mp/°C	−41.0	B	1773.06			64.4	57182
				bp/°C	81.66	64.95	58102
				eq. 2	P/mmHg	70	68967
				A	6.23655	73.05	76713
				B	1397.923	75.1	81380
				C	239.275	77.2	87952
						81.1	99431
						85.2	112364
						88.2	123189
						89.2	124776

2.

Mousa 1981		Ewing & Sanchez Ochoa 2004			
ebulliometry-pressure gauge		comparative ebulliometry			
T/K	P/kPa	t/°C	P/Pa	t/°C	P/kPa
		set A		set B	
438.9	784.4	4.772	4323#	81.4	100.745
440.9	842.8	5.475	4490#	87.792	122.631
442.6	862.3	8.417	5247#	98.589	168.122
444.5	876.9	12.226	6385#	105.665	204.592
447.9	960.3	14.517	7165#	110.961	235.792
450.5	999.2	17.497	8296	121.144	306.279
455.7	1116.5	19.596	9182	132.086	399.5
460.2	1234.6	22.634	10604	142.063	502.665
505.3	2604.9	27.674	13366	150.533	605.601
508.1	1704.6	30.661	15271	157.974	708.993
512.1	1924.0	36.486	19639	164.152	804.861
519.7	3243.3	42.283	24972	170.346	910.819
521.6	3303.1	47.968	31311	176.446	1025.47
524.8	3482.8	51.872	36387	182.586	1151.97
530.1	3722.1	58.125	45907	188.724	1290.2
		63.263	55169	195.22	1450.28
bp/K	354.8	68.029	65092	200.902	1602.63
		72.425	75440	206.004	1749.88

TABLE 16.1.1.1.1 (Continued)

Mousa 1981		Ewing & Sanchez Ochoa 2004			
ebulliometry-pressure gauge		comparative ebulliometry			
T/K	P/kPa	t/°C	P/Pa	t/°C	P/kPa
eq.3	P/kPa	76.178	85311	211.619	2110.77
A	6.4914	79.929	95589	217.22	2303.51
B	1420.8649	81.515	101120	222.602	2523.66
C	−42.15	84.406	110614	228.33	2747.95
		88.462	125129	233.771	2999.22
		95.816	155329	339.66	3254.08
		100.02	175036	244.858	3512.89
				254.64	3760.37
		for temp range 290–373 K		258.929	4001.46
		eq. 2a	P/mmHg	261.882	4174.61
		A	14.734		
		B	3268.53	data fitted to Wagner eq.	
		C	−31.615	for temp range 354.5–535 K	
		# data not used in regression			

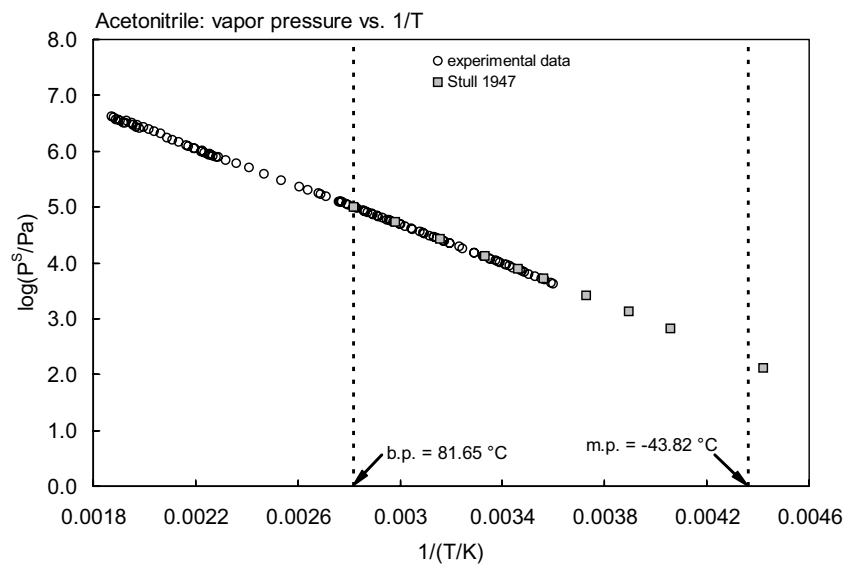


FIGURE 16.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for acetonitrile.

TABLE 16.1.1.2

Reported Henry's law constants of acetonitrile 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)		
$\ln [H/(\text{Pa} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$	(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)		

Snider & Dawson 1985		Benkelberg et al. 1995	
gas stripping-GC		equil. vapor phase concn-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
			deionized water
0	0.614	6	0.72
25	2.066	10	1.0706
		20	1.474
		30	2.356
enthalpy of transfer:			rain water
$\Delta H/(\text{kJ mol}^{-1}) = 30.54$		20	1.477
			artificial
		20	1.685
		eq. 3	H/atm
		A	13.8 ± 0.3
		B	4106 ± 101

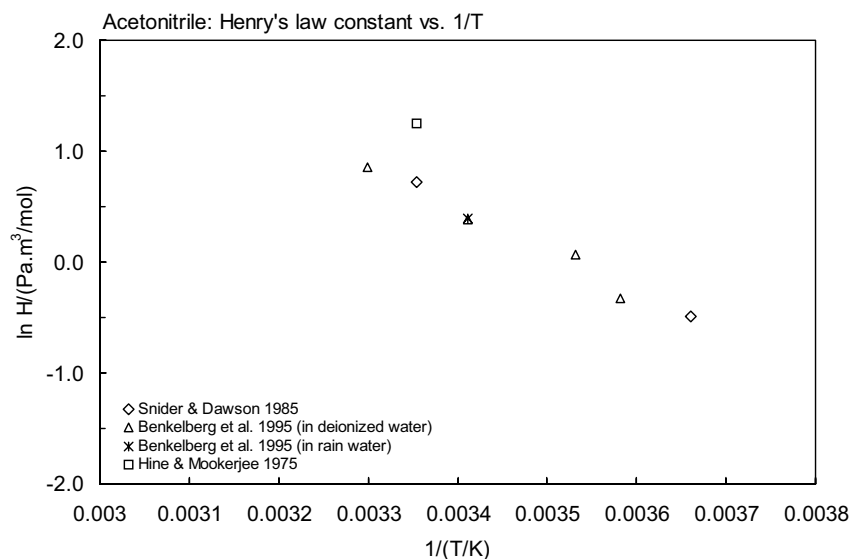
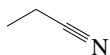


FIGURE 16.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for acetonitrile.

16.1.1.2 Propionitrile



Common Name: Propionitrile

Synonym: propanenitrile, ethyl cyanide, cyanoethane, propyl nitrile

Chemical Name: propionitrile

CAS Registry No: 107-12-0

Molecular Formula: C_3H_5N , CH_3CH_2CN

Molecular Weight: 55.079

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

−92.78 (Lide 2003)

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

97.14 (Lide 2003)

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

0.7818 (Weast 1982–83; Dean 1985)

0.78182, 0.77682 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

70.4 (calculated-density, Taft et al. 1985; Leahy 1986; Kamlet et al. 1986, 1987)

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

Dissociation Constant:

33.54 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_{vap} (kJ/mol):

37.41, 32.77 ($25^{\circ}C$, bp, Dreisbach 1961)

36.03, 30.96 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.045 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

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

104950 (Seidell 1941)

105200 (Hansch et al. 1968)

103000 (Dean 1985; Riddick et al. 1986; Howard 1990)

55000, 65000 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC, measured range 0 – $90^{\circ}C$, Stephenson 1994)

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):

6005* (interpolated-regression of tabulated data, temp range -35 – $97.1^{\circ}C$, Stull 1947)

10114* ($35.5^{\circ}C$, ebulliometry, measured range 35.5 – $97.35^{\circ}C$, Dreisbach & Shrader 1949)

$\log(P/mmHg) = 7.15217 - 1398.2/(230 + t/^{\circ}C)$; temp range 35.5 – $97.35^{\circ}C$, (Antoine eq., Dreisbach & Martin 1949)

5333* ($22.05^{\circ}C$, measured range -84.66 – $22.05^{\circ}C$, Milazzo 1956)

5950 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.05846 - 1327.9/(221.0 + t/^{\circ}C)$, temp range: 17 – $137^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 8769.0/(T/K)] + 8.079473$; temp range: -35 to $97.1^{\circ}C$, (Antoine eq., Weast 1972–73)

6140 ($22.05^{\circ}C$, quoted exptl., Boublik et al. 1973, 1984)

6163, 6143 (extrapolated values-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.89149 - 1181.562/(206.603 + t/^{\circ}C)$, temp range: 35.5 – $97.39^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 4.43918 - 677.415/(160.551 + t/^{\circ}C)$, temp range: -84.7 to $22.05^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6140 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 5.2782 - 665.52/(159.0 + t/^{\circ}\text{C})$, temp range: -84 to 22°C (Antoine eq., Dean 1985, 1992)
 5950 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.27702 - 1398.2/(230 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 7.15190 - 1894.10/(T/\text{K})$; temp range: 9 – 25°C , (Antoine eq., Riddick et al. 1986)
 6306 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.395 - 3213/(T/\text{K})$, temp range: 357 – 413 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 10.31055 - 3994.667/(T/\text{K})$, temp range: 373 – 413 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 33.7908 - 2.9113 \times 10^3/(T/\text{K}) - 9.1506 \cdot \log(T/\text{K}) + 1.1173 \times 10^{-11} \cdot (T/\text{K}) + 3.2756 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 180 – 564 K (vapor pressure eq., Yaws 1994)

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

3.800 (partial pressure, Butler & Ramchandani 1935)
 3.748 (partial vapor pressure-GC, Buttery et al. 1969)
 3.752, 3.752, 4.114 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 5.947 (Howard 1990)

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

0.041 (shake flask, Collander 1951)
 0.16 (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)
 -0.10 (shake flask-GC, Tanii & Hashimoto 1984)
 0.16 (recommended, Sangster 1989, 1993)
 0.16 (recommended, Hansch et al. 1995)

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

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

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

-0.108 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

0.079 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: using Henry's law constant, $t_{1/2} = 13.3$ h was estimated for a model river 1 m deep flowing 1 m/s with wind speed 3 m/s (Lyman et al. 1982; 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 and/or the Arrhenius expression see reference:

$k_{\text{OH}}^* = (1.94 \pm 0.20) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.2 K, measured range 298 – 423 K (flash photolysis-resonance fluorescence, Harris et al. 1981)

$k_{\text{OH}} = 1.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985)

$k_{\text{OH}} = 1.94 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.2 K, $k(\text{soln}) = 1.60 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

photooxidation $t_{1/2} = 83$ d in air, based on experimental rate constant assuming $t_{1/2} = 12$ h of sunlight for the vapor-phase reaction with hydroxyl radical in air and $t_{1/2} > 100$ d for the reaction with ozone in the atmosphere (Howard 1990)

$k_{\text{OH}} = 0.194 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.2 K (review, Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

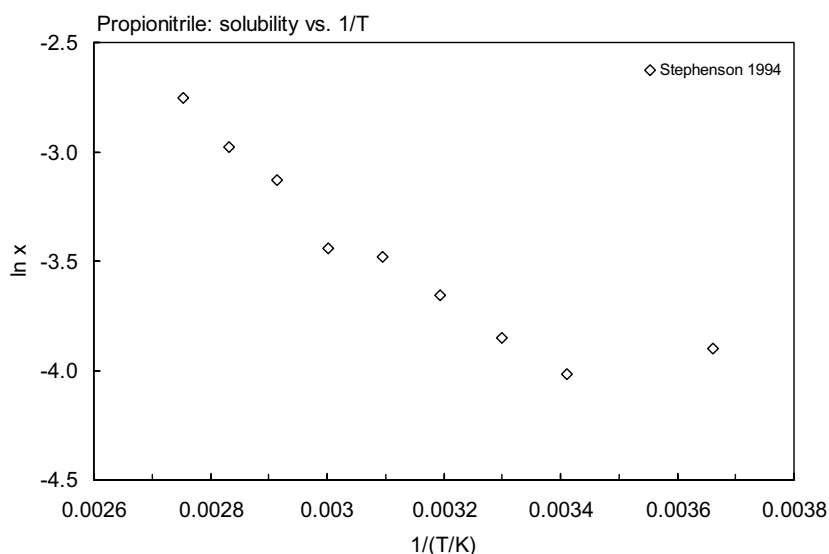
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 83$ d, based on experimental rate constant assuming 12 h of sunlight for the vapor-phase reaction with hydroxyl radical in air and $t_{1/2} > 100$ d for the reaction with ozone in the atmosphere (Harris et al. 1981; quoted, Howard 1990).

TABLE 16.1.1.2.1**Reported aqueous solubilities and vapor pressures of propionitrile at various temperatures**

$\log P = A - B/(T/K)$	(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						
Stephenson 1994	Stull 1947	Dreisbach & Shrader 1949	Milazzo 1956				
shake flask-GC	summary of literature data	ebulliometry					
t/^{\circ}C	S/g\cdot m^{-3}	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa
0	62000	-35.0	133.3	35.5	10114	-84.66	1
20	55000	-13.8	666.6	43.76	16500	-77.01	2
30	65000	-3.0	1333	70.45	42066	-67.42	6
40	79000	8.8	2666	84.44	67661	-65.49	7
50	94000	22	5333	97.35	101325	-59.72	13
60	98000	30.1	7999			-52.96	17
70	134000	41.4	13332			-46.19	49
80	156000	58.2	26664			-34.95	133
90	195000	77.7	53329			-22.85	356
		97.1	101325			-13.08	707
						-2.95	1347
		mp/^{\circ}C	-91.9			6.36	2400
						16.42	4146
						22.05	5333

**FIGURE 16.1.1.2.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for propionitrile.

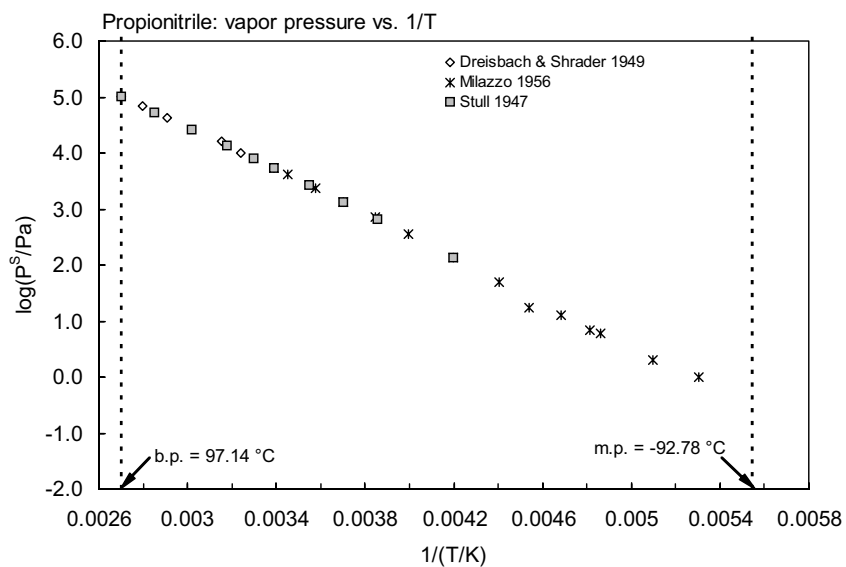
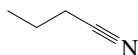


FIGURE 16.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for propionitrile.

16.1.1.3 Butyronitrile



Common Name: *n*-Butyronitrile

Synonym: butanenitrile

Chemical Name: butyronitrile

CAS Registry No: 109-74-0

Molecular Formula: C_4H_7N , $CH_3CH_2CH_2CN$

Molecular Weight: 69.106

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

-111.9 (Lide 2003)

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

117.6 (Lide 2003)

Density (g/cm^3):

0.7911, 0.7865 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

88.4 ($30^{\circ}C$, Stephenson & Malanowski 1987)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.33, 34.43 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.021 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

33000 (selected, Riddick et al. 1986)

33500* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90^{\circ}C$, Stephenson 1994)

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

1333* ($25.7^{\circ}C$, summary of literature data, temp range -20 to $117.5^{\circ}C$, Stull 1947)

3592* ($30.64^{\circ}C$, ebulliometry, measured range 30.64 – $120.223^{\circ}C$, Meyer et al. 1971)

$\log (P/mmHg) = 6.771124 - 1444.5851/(t/^{\circ}C + 223.275)$; temp range 30.64 – $120.223^{\circ}C$ (Antoine eq., ebulliometric measurements, Meyer et al. 1971)

13831* ($59.807^{\circ}C$, ebulliometry, measured range 59.807 – $127.707^{\circ}C$, Meyer & Hotz 1976)

2546 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.25390 - 1452.076/(t/^{\circ}C + 224.1855)$; temp range not specified (Riddick et al. 1986)

$\log (P_L/kPa) = 6.25397 - 1452.076/(-46.9645 + T/K)$; temp range 332 – $401 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 4.8780 - 2.5505 \times 10^3/(T/K) + 3.6306 \cdot \log (T/K) - 1.663 \times 10^{-2} \cdot (T/K) + 1.0604 \times 10^{-5} \cdot (T/K)^2$; temp range 161 – $582 K$ (vapor pressure eq., Yaws 1994)

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

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

0.53 (shake flask-GC, Tani & Hashimoto 1984)

0.53 (recommended, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

TABLE 16.1.1.3.1

Reported aqueous solubilities and vapor pressures of butyronitrile at various temperatures

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)					
Aqueous solubility		Vapor pressure					
Stephenson 1994		Stull 1947		Meyer et al. 1971		Meyer & Hotz 1976	
shake flask-GC		summary of literature data		ebulliometry		ebulliometry	
t/°C	S/g·m ^{–3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	37500	–20.0	133.3	30.64	3592	59.807	13831
20	33500	2.10	666.6	39.03	5459	65.615	17513
30	33100	13.4	1333	49.913	9041	71.638	22151
40	32500	25.7	2666	59.226	13527	77.023	27111
50	32300	38.4	5333	67.536	18888	83.599	34366
60	32100	47.3	7999	77.313	27448	89.462	42109
70	31900	59.0	13332	86.71	39316	96.022	52382
80	34000	76.7	26664	93.675	48525	102.279	63984
90	36100	96.8	53329	100.638	60811	109.175	79081
		117.5	101325	100.701	60928	115.651	95737
		mp/°C		107.041	74214	121.838	114148
				112.04	88451	127.707	134135
				117.254	100344		
				120.223	109170		
				bp/°C	117.583		
			log P = A – B/(C + t/°C)				
				P/mmHg			
				A	6.771124		
				B	1444.5851		
				C	223.275		

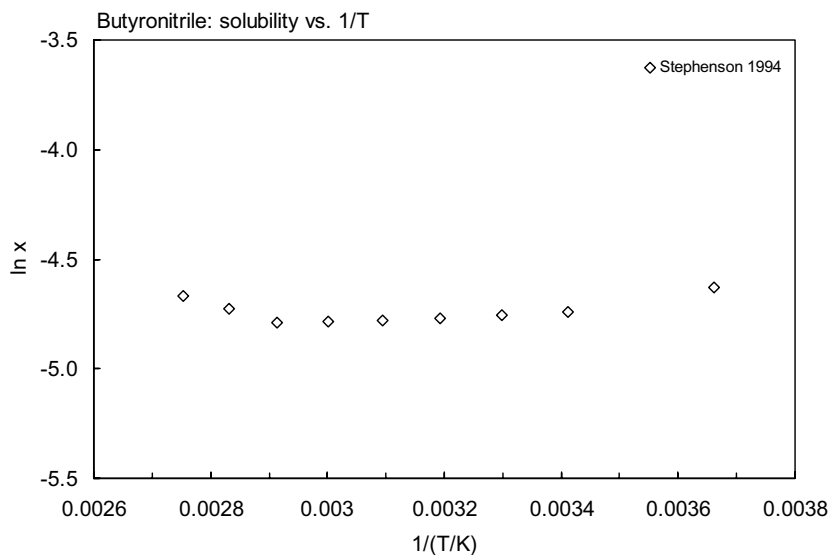


FIGURE 16.1.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for butyronitrile.

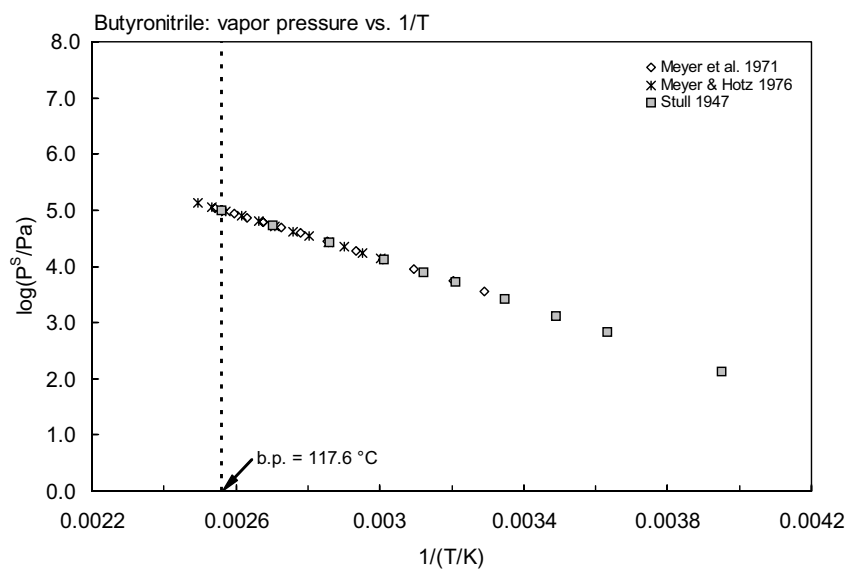
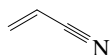


FIGURE 16.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for butyronitrile.

16.1.1.4 Acrylonitrile (2-Propenenitrile)



Common Name: Acrylonitrile

Synonym: cyanoethylene, propenenitrile, 2-propenenitrile, vinyl cyanide

Chemical Name: acrylonitrile, cyanoethylene

CAS Registry No: 107-13-1

Molecular Formula: C_3H_3N , $CH_2=CHCN$

Molecular Weight: 53.063

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

-83.48 (Lide 2003)

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

77.30 (Riddick et al. 1986; Howard 1989; Lide 2003)

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

0.8060, 0.8004 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

65.8 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.230 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

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

79000 (Klein et al. 1957)

75000 (Günther et al. 1968)

73500 ($20^{\circ}C$, Windholz 1976)

73240 (shake flask-LSC, Veith et al. 1980)

7.35 wt%* ($20^{\circ}C$, Kirk-Othmer Encyclopedia 3rd ed., measured range $0-60^{\circ}C$, quoted, Basu et al. 1983)

73500 ($20^{\circ}C$, Riddick et al. 1986)

69000*, 66400 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC, measured range $0-70^{\circ}C$, Stephenson 1994)

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):

14340* (interpolated-regression of tabulated data, temp range -51 to $78.5^{\circ}C$, Stull 1947)

11732* ($20^{\circ}C$, temp range $20-77^{\circ}C$, Gudkov et al. 1964; quoted, Boublik et al. 1984)

14100 (Hoy 1970)

$\log(P/mmHg) = [-0.2185 \times 7941.4/(T/K)] + 7.851016$; temp range: -51 to $78.5^{\circ}C$, (Antoine eq., Weast 1972-73)

14720 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 4.77668 - 649.583/(155.006 + t/^{\circ}C)$, temp range $20-70^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

14370 (Daubert & Danner 1985)

15240 (calculated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.03855 - 1232.53/(222.47 + t/^{\circ}C)$, temp range -20 to $140^{\circ}C$ (Antoine eq., Dean 1985, 1992)

11000 ($20^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 6.643 - 11644.7/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

14560 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.12021 - 1288.9/(-38.74 + T/K)$; temp range $257-352 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.4811 - 1518.381/(-12.003 + T/K)$; temp range $283-343 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

15600 (calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 35.921 - 2.7763 \times 10^3/(T/K) - 10.101 \cdot \log(T/K) - 3.1547 \times 10^{-10} \cdot (T/K) + 4.7299 \times 10^{-6} \cdot (T/K)^2$;
temp range 190–535 K (vapor pressure eq., Yaws 1994)

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

11.14 (Bocek 1976; quoted, Basu et al. 1983; Howard 1989)

8.918 (calculated-P/C, Mabey et al. 1982)

9.420 (quoted, WERL Treatability Database, Ryan et al. 1988)

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

0.25 (shake flask-HPLC, Pratesi et al. 1979)

0.00 (shake flask, Fujisawa & Masuhara 1980, 1981)

0.09 (shake flask-GC, Tani & Hashimoto 1984)

0.25 (Hansch & Leo 1985)

0.25 (recommended, Sangster 1989)

0.25 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

1.68 (bluegill sunfish, Barrows et al. 1978)

0.00 (estimated-S, Kenaga 1980)

1.68, 0.32 (bluegill sunfish, calculated- K_{OW} , Veith et al. 1980)

0.017 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

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

0.954 (soil, calculated-S, Kenaga 1980)

−0.071 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.101, 1.006; 1.09 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

−0.0899 (calculated- K_{OW} , Walton et al. 1992)

−0.0890 (calculated- K_{OW} , Kolig 1993)

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

Volatilization: $t_{1/2} = 6, 1.2, 4.8$ d in a typical pond, river and lake are 6, 1.2, and 4.8 d, respectively, with the reaeration for oxygen in typical bodies of water (Lyman et al. 1982; quoted, Howard 1989)

evaporation $t_{1/2} = 795$ min from water with an assumed 1-m depth (Basu et al. 1983).

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:

$k < 1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, and $36 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$t_{1/2} = 4.0$ h for photooxidation in the troposphere (Callahan et al. 1979)

$k_{OH} = (40.6 \pm 4.1) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (flash photolysis-resonance fluorescence technique, Harris et al. 1981)

$k_{O_3} < 1 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K, and tropospheric lifetimes, $\tau > 115$ d and $\tau = 3$ d due to reactions with O_3 and OH radical, respectively (Atkinson et al. 1982)

$k_{O_3} < 1 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Atkinson et al. 1983; quoted, Atkinson & Carter 1984)

$t_{1/2} = 3.5$ d for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989)

$k_{OH} = 4.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.7 K, and $k_{OH} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (review, flash photolysis-resonance fluorescence technique Atkinson 1985)

photooxidation $t_{1/2} = 3.4$ –189 h, based on measured rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)

$k_{OH} = (3.4 - 4.80) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296–298.2 K (review, Atkinson 1989)

Hydrolysis: $k(\text{acid}) = 4.2 \times 10^{-2} \text{ M}^{-1} \text{ h}^{-1}$ at pH 5.0 with $t_{1/2} = 188 \text{ yr}$ and $k(\text{base}) = 6.1 \times 10^{-2} \text{ M}^{-1} \text{ h}^{-1}$ at pH 9.0 with $t_{1/2} = 13 \text{ yr}$ (Ellington et al. 1987; quoted, Howard et al. 1991, Kollig 1993);
 $t_{1/2} = 1210 \text{ yr}$ at pH 7.0, based on measured acid and base catalyzed hydrolysis constants (Ellington et al. 1987; quoted, Howard et al. 1991)
 $t_{1/2} = 69 \text{ d}$ at pH 2, $t_{1/2} = 440000 \text{ d}$ at pH 7 and $t_{1/2} = 4.7 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995).
 Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 30\text{--}552 \text{ h}$, based on river die-away test data (Going et al. 1979; Ludzack et al. 1958; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 120\text{--}2208 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
 ^{14}C labeled acrylonitrile at concentrations up to 100 ppm was completely degraded within 2.0 d in a London soil under aerobic conditions (Donberg et al. 1992)
 $t_{1/2}(\text{aerobic}) = 1.3 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 5 \text{ d}$ in natural waters (Capel & Larson 1995)
 Biotransformation: $k = \text{of } 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982).
 Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 4.0 \text{ h}$ for photooxidation in the troposphere (Callahan et al. 1979);
 $t_{1/2} = 3.5 \text{ d}$ for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989);
 photooxidation $t_{1/2} = 13.4\text{--}189 \text{ h}$, based on measured rate constant for the reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991);
 atmospheric transformation lifetime was estimated to be 1 – 5 to > 5 d (Kelly et al. 1994).
 Surface water: $t_{1/2} = 30\text{--}552 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
 Biodegradation $t_{1/2}(\text{aerobic}) = 100 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 400 \text{ d}$; hydrolysis $t_{1/2} = 69 \text{ d}$ at pH 2, $t_{1/2} = 440000 \text{ d}$ at pH 7 and $t_{1/2} = 4.7 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995).
 Groundwater: $t_{1/2} = 60\text{--}1104 \text{ h}$ based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
 Sediment:
 Soil: $t_{1/2} < 10 \text{ d}$ in soil (USEPA 1979; quoted, Ryan et al. 1988);
 $t_{1/2} = 30\text{--}552 \text{ h}$ based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
 Biota:

TABLE 16.1.1.4.1

Reported aqueous solubilities and vapor pressures of acrylonitrile at various temperatures

Aqueous solubility				Vapor pressure			
Othmer Encyclopedia		Stephenson 1994		Stull 1947		Gudkov et al. 1964	
Basu et al. 1983		shake flask-GC		summary of literature data		in Boublik et al. 1984	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
0	72000	0	65800	–51.0	133.3	20	11732
20	73500	10	66800	–30.7	666.6	30	18932
40	79000	20	69000	–20.3	1333	40	27998
60	91000	30	66400	–9.0	2666	50	38530
		40	68800	3.8	5333	60	57328
		50	73600	11.8	7999	70	78660
		60	73900	22.8	13332		
		70	85600	38.7	26664		
				58.3	53329		
				78.5	101325		
				mp/°C	–82.0		

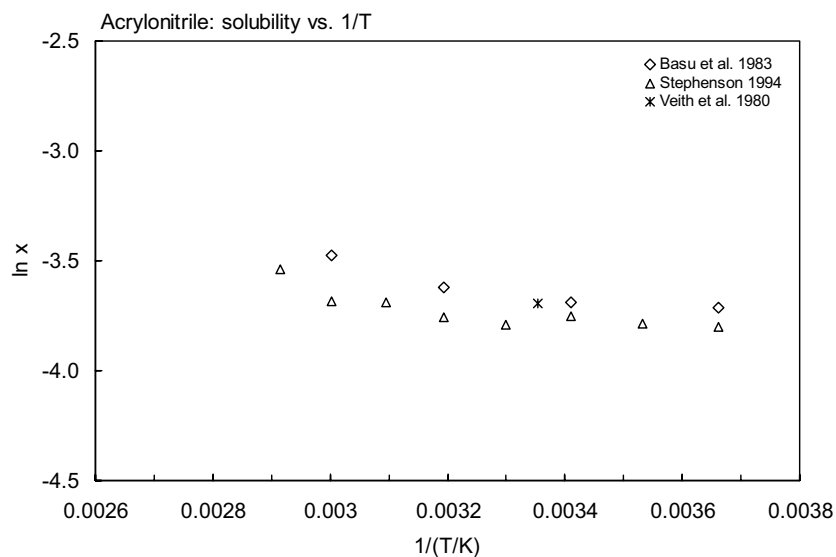


FIGURE 16.1.1.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for acrylonitrile.

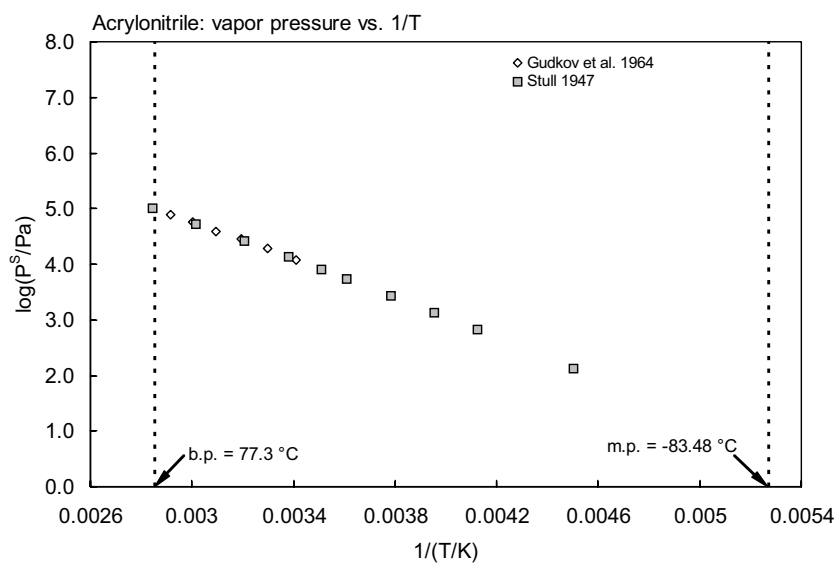
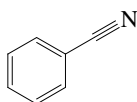


FIGURE 16.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for acrylonitrile.

16.1.1.5 Benzonitrile



Common Name: Benzonitrile

Synonym: benzenecarbonitrile, cyanobenzene, phenyl cyanide

Chemical Name: benzonitrile, benzoic acid nitrile

CAS Registry No: 100-47-0

Molecular Formula: C_6H_5CN

Molecular Weight: 103.122

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

-13.99 (Lide 2003)

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

191.1 (Lide 2003)

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

1.0006 ($25^{\circ}C$, Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.1 ($25^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

55.48, 45.94 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.88 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

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

4330 (shake flask-UV, McGowan et al. 1966)

2000 (Dean 1985; Riddick et al. 1986)

10000 (selected, Yaws et al. 1990)

4000* (shake flask-GC/TC, measured range $0-90^{\circ}C$, Stephenson 1994)

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

133.3* ($38.4^{\circ}C$, static method, measured range $38.4-190.6^{\circ}C$, Kahlbaum 1898)

133.3* ($28.2^{\circ}C$, summary of literature data, temp range $28.2-190.6^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11341.0/(T/K)] + 8.239760$; temp range: $28.2-190.6^{\circ}C$ (Antoine eq., Weast 1972-73)

78.86 (calculated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.74631 - 1436.72/(181 + t/^{\circ}C)$, temp range: liquid (Antoine eq., Dean 1985, 1992)

100.0 (Riddick et al. 1986)

$\log(P/kPa) = 5.87121 - 1436.72/(181.0 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

106.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.79506 - 2066.71/(-32.19 + T/K)$, temp range $301-464 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

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

55.32 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

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

1.56 (shake flask-UV spectrophotometry, Fujita et al. 1964; quoted, Leo et al. 1969; Hansch & Leo 1979)

1.56 (shake flask-UV, Holmes & Lough 1976)

1.67	(calculated-fragment const., Rekker 1977)
1.56	(shake flask at pH 7, Unger et al. 1978)
1.66	(RP-HPLC- k' correlation, Miyake & Terada 1982)
1.65 \pm 0.01	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.50	(HPLC- k' correlation, Haky & Young 1984)
1.56	(shake flask-GC, Tanii & Hashimoto 1984)
1.56	(RP-HPLC-capacity ratio, Minick et al. 1988)
1.45	(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
1.56	(recommended, Sangster 1989, 1993)
1.56	(shake flask-GC, Alcorn et al. 1993)
1.56	(recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis:

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

$k_{OH} = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Zetzsch 1982; Atkinson 1989)

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

$k_{OH}(\text{calc}) = 3.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{OH}(\text{calc}) = 3.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs}) = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(\text{calc}) = 4.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Surface water: an estimated $t_{1/2} = 1.3 \text{ d}$ in Rhine River in case of first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.1.5.1

Reported aqueous solubilities and vapor pressures of butyronitrile at various temperatures

Aqueous solubility		Vapor pressure					
Stephenson 1994		Kahlbaum 1898*				Stull 1947	
shake flask-GC		static-manometer				summary of literature data	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
0	3500	38.4	133.3	141.4	26664	28.2	133.3
10	3300	45.3	266.6	155.8	39997	55.3	666.6
20	4000	50.0	400.0	165.8	53329	69.2	1333
40	4500	53.8	533.3	174.4	66661	83.4	2666
50	3800	56.9	666.6	181.6	79993	99.6	5333
60	4200	69.1	1333.2	187.7	93326	109.8	7999

(Continued)

TABLE 16.1.1.5.1 (Continued)

Aqueous solubility		Vapor pressure					
Stephenson 1994		Stull 1947		Meyer et al. 1971		Meyer & Hotz 1976	
shake flask-GC		summary of literature data		ebulliometry		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70	6000	83.0	2666.4	190.6	101325	123.5	13332
80	9500	92.1	3999.7			144.1	26664
90	9100	98.5	5332.9	*complete list see ref.		156.7	53329
		103.9	6666.1			190.6	101325
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$		113.7	9999.2				
25 °C		121.3	13332			mp/°C	-12.9

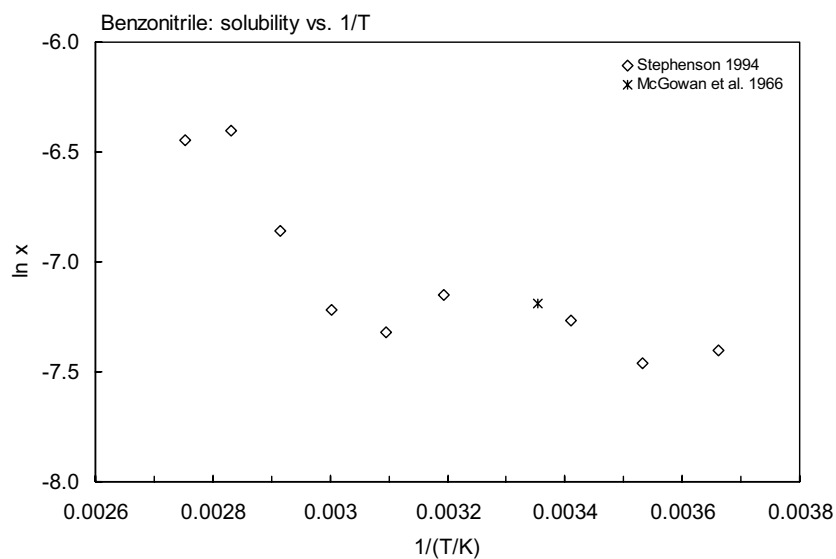


FIGURE 16.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzonitrile.

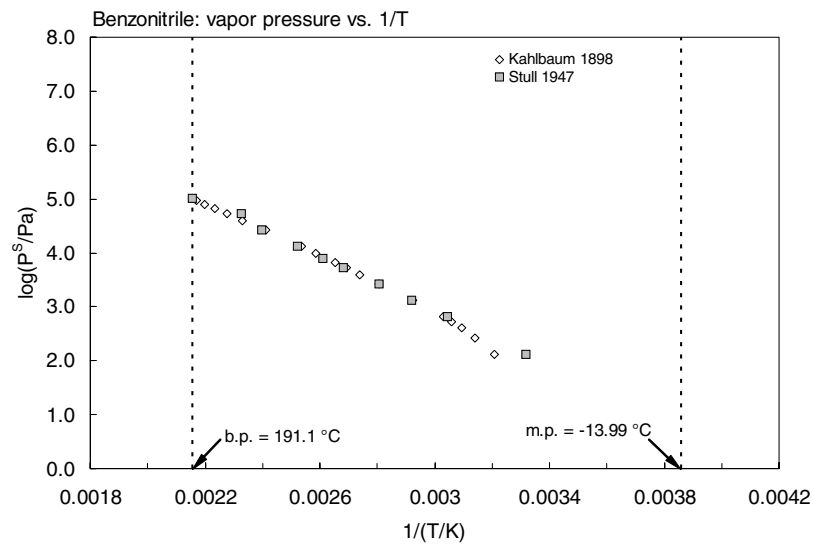


FIGURE 16.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for benzonitrile.

16.1.2 ALIPHATIC AMINES

16.1.2.1 Dimethylamine



Common Name: Dimethylamine

Synonym: aminomethylmethane, N-methylmethanamine

Chemical Name: aminomethylmethane, dimethylamine

CAS Registry No: 124-40-3

Molecular Formula: C_2H_7N , CH_3NHCH_3

Molecular Weight: 45.084

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

-92.18 (Lide 2003)

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

6.88 (Lide 2003)

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

0.6804 ($0^{\circ}C$, Weast 1982-83)

0.6556, 0.6496 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.8 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

10.732 (Perrin 1965; Weast 1982-83; Howard 1990)

10.77 (protonated cation + 1, Dean 1985)

10.77 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

23.84, 24.61 ($25^{\circ}C$, bp, Dreisbach 1961)

23.65, 24.61 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.941 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

very soluble (Dean 1985)

620000 (selected, Yaws et al. 1990)

miscible (Stephenson 1993b)

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

101141* ($280.018 K$, static method, measured range 201.387 – $280.018 K$, Ashton et al. 1939)

236420* (extrapolated-regression of tabulated data, temp range -87.2 to $+7.4^{\circ}C$, Stull 1947)

196800 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 7.06396 - 1024.4/(238.0 + t/^{\circ}C)$, temp range -55 to $37^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = [-0.2185 \times 6660.0/(T/K)] + 7.995166$; temp range -87.7 to $162.6^{\circ}C$, (Antoine eq., Weast 1972-73)

172220 ($20^{\circ}C$, Verschueren 1983)

206180 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.21132 - 962.001/(221.852 + t/^{\circ}C)$, temp range -71.77 to $6.858^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

202620 (Daubert & Danner 1985)

206000 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.08212 - 960.242/(221.67 + t/^{\circ}C)$, temp range -72 to $6^{\circ}C$ (Antoine eq., Dean 1985, 1992)

196800 (quoted lit., Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.18886 - 1.024.40/(238.0 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

205300 (interpolated-Antoine eq.-II., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.29031 - 993.586/(-48.12 + T/\text{K})$, temp range 201–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.20646 - 965.728/(-50.151 + T/\text{K})$, temp range 277–360 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 7.81489 - 2369.425/(141.433 + T/\text{K})$, temp range 358–438 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 36.9182 - 2.4965 \times 10^3/(T/\text{K}) - 10.417 \cdot \log(T/\text{K}) - 1.6287 \times 10^{-9} \cdot (T/\text{K}) + 4.6496 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 181–438 K (vapor pressure eq., Yaws 1994)

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

1.796 (exptl., Hine & Mookerjee 1975; quoted, Howard 1990)

1.796, 1.03 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.718 (calculated-molecular structure, Russell et al. 1992)

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

−0.38 (shake flask-RC at pH 13, Wolfenden 1978)

−0.38 (Hansch & Leo 1985)

−0.38 (recommended, Sangster 1989; 1993)

−0.38 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, $\log BCF$:

−0.523 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

2.638 (adsorption isotherm average for five soils, Rao & Davidson 1982; quoted, Howard 1990)

0.602; 2.212; 2.706 (Podzol soil; Alfisol soil; sediment, von Oepen et al. 1991)

2.63 (soil, calculated-MCI, Sabljic et al. 1995)

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

Volatilization: using Henry's law constant, $t_{1/2} = 35.1$ h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; selected, 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:

$k_{OH} = 6.54 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Atkinson et al. 1977; quoted, Carlier et al. 1986; Atkinson 1989)

photooxidation $t_{1/2} = 5.9$ h in air was estimated for the vapor phase reaction with hydroxyl radical of 5×10^5 radicals/ cm^3 in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990);

$k_{O_3} = (2.61 \pm 0.30) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Atkinson & Carter 1984; quoted, Atkinson 1985)

$k_{OH} = 6.5 \times 10^{-11} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with 5×10^5 OH radicals/ cm^3 at room temp. having a loss rate of 2.8 d^{-1} (Atkinson 1985)

$k_{OH}(\text{calc}) = 63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1987).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 2\text{--}79$ h, based on river die-away test data (Digeronimo et al. 1979; Dojlido 1979; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 8\text{--}316$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 5.9$ h was estimated for the vapor phase reaction with hydroxyl radical of 5×10^5 radicals/cm³ in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990);

photooxidation $t_{1/2} = 0.892\text{--}9.20$ h, based on measured rate constant for the gas-phase reaction with OH radical (Atkinson 1985; quoted, Howard et al. 1991) and ozone (Tuazon et al. 1978; selected, Howard et al. 1991).

Surface water: $t_{1/2} = 2\text{--}79$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 4\text{--}158$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 86\text{--}336$ h, based on soil die-away test data (Tate & Alexander 1976; Greene et al. 1981; selected, Howard et al. 1991).

Biota:

TABLE 16.1.2.1.1

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

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

$$\log P = A - B/(T/K) - C \log (T/K) + D \cdot (T/K) - E \cdot (T/K)^2 + F \cdot (T/K)^3 \quad (5)$$

Ashton et al. 1939				Stull 1947	
static method				summary of literature data	
T/K	P/Pa			t/°C	P/Pa
201.387	648	bp/K	280.04	-87.7	133.3
213.802	1959	mp/K	180.97	-72.2	666.6
222.078	3780	$\Delta H_v/(\text{kJ mol}^{-1}) = 26.48$ (bp)		-64.6	1333
232.137	7775	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 5.94$ (mp)		-56.0	2666
242.078	14743			-46.7	5333
249.640	22949	eq. 5	P/mmHg	-40.7	7999
256.449	33269	A	32.26370	-32.6	13332
262.977	46404	B	2460.10	-20.4	26664
270.182	65491	C	8.6390	-7.1	53329
275.934	84860	D	7.6055×10^{-3}	7.4	101325
279.980	100974	E	3.51389×10^{-5}		
277.680	91519	F	5.3241×10^{-8}	mp/°C	-96.0
280.018	101141				

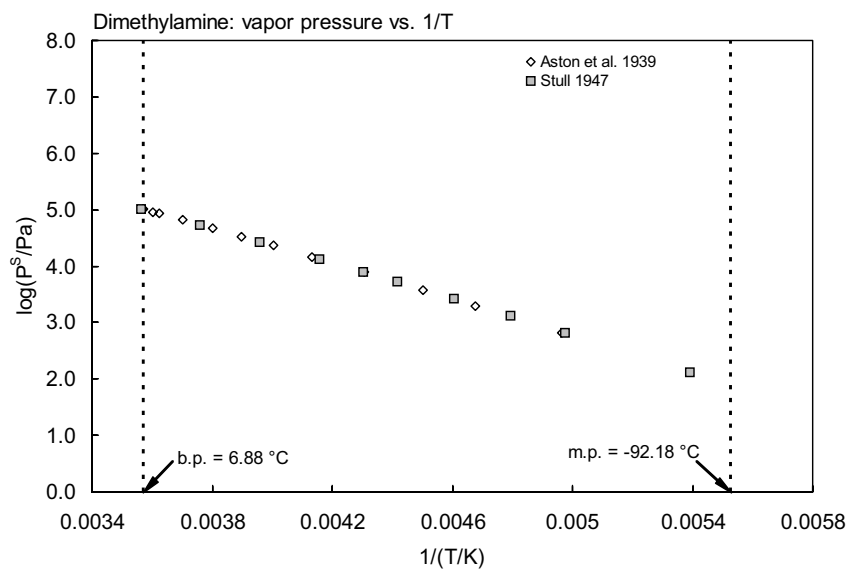


FIGURE 16.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethylamine.

16.1.2.2 Trimethylamine



Common Name: Trimethylamine

Synonym: dimethylamino methane, TMA

Chemical Name: trimethylamine

CAS Registry No: 75-50-3

Molecular Formula: C_3H_9N , $CH_3N(CH_3)_2$

Molecular Weight: 59.110

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

-117.1 (Lide 2003)

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

2.87 (Lide 2003)

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

0.6356 (Weast 1982–83)

Molar Volume (cm^3/mol):

93 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

9.801, 9.987 (Perrin 1972; quoted, Howard 1990)

9.80 (pK_a , protonated cation + 1, Dean 1985)

9.79 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

22.85, 24.13 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

410000 (Dean 1985)

890000 ($30^{\circ}C$, Howard 1990)

291000 (selected, Yaws et al. 1990)

miscible (Stephenson 1993b)

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 chapter):

221715* (isoteniscope, measured range 0 – $40^{\circ}C$, Swift & Hochanadel 1945)

$\log (P/mmHg) = 24.91300 - 2018.37/(T/K) - 6.0303 \cdot \log (T/K)$; temp range 0 – $40^{\circ}C$ (isoteniscope method, Swift & Hochanadel 1945)

265200* (extrapolated-regression of tabulated data, temp range -97.1 to $+2.9^{\circ}C$, Stull 1947)

226540 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 6.97038 - 968.7/(234.0 + t/^{\circ}C)$, temp range -58 to $32^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = [-0.2185 \times 6361.7/(T/K)] + 7.952370$; temp range -97.1 to $2.9^{\circ}C$ (Antoine eq., Weast 1972–73)

192500 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

219300, 221800 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.98554 - 1957.276/(237.664 + t/^{\circ}C)$, temp range -80.3 to $3.45^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 5.87712 - 894.366/(228.276 + t/^{\circ}C)$, temp range 0 – $40^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

214200 (Daubert & Danner 1985)

219000 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.85755 - 955.94/(237.52 + t/^{\circ}C)$, temp range -80 to $3^{\circ}C$ (Antoine eq., Dean 1985, 1992)

219900 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.01402 - 968.978/(-34.253 + T/\text{K})$, temp range 192–277 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 58.6807 - 2.686 \times 10^3/(T/\text{K}) - 20.36 \cdot \log (T/\text{K}) + 1.3131 \times 10^{-2} \cdot (T/\text{K}) - 6.563 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 156–433 K (vapor pressure eq., Yaws 1994)

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

6.672 (exptl., Hine & Mookerjee 1975)

12.71, 2.16 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

15.64 (calculated-molecular structure, Russell et al. 1992)

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

0.27 (shake flask-TN, Sandell 1962; quoted, Leo et al. 1971)

0.27; 0.20 (calculated-f const., calculated- π const., Rekker 1977)

0.16 (shake flask, Hansch & Leo 1985)

0.16 (recommended, Sangster 1989)

0.16 (recommended, Hansch et al. 1995)

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

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

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

1.462 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

0.602 (soil, estimated-solubility, Lyman et al. 1982; quoted, Howard 1990)

0.778; 2.365; 2.831 (Podzol soil; Alfisol soil; sediments von Oepen et al. 1991)

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

Volatilization: using Henry's law constant, $t_{1/2} = 11$ h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Hydrolysis:

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:

$k_{OH} = 6.09 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Atkinson et al. 1977; Atkinson 1989)

photooxidation $t_{1/2} = 62$ d in water, based on rate constant $k = 1.3 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with photochemically produced hydroxyl radicals of $1 \times 10^{-17} \text{ mol} \cdot \text{L}^{-1}$ in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)

$k_{OH} = 6.10 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with 1×10^6 OH radicals/ cm^3 with a loss rate of 5.0 d^{-1} and rate constant $k_{O_3} = 9.70 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with $7 \times 10^{11} \text{ O}_3$ molecules/ cm^3 with a loss rate of 0.6 d^{-1} both at room temp. (Atkinson & Carter 1984)

calculated $k_{OH} = 64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 4.0$ h, based on rate constant $k = 6.09 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radical of 8×10^5 radicals/ cm^3 in air at 25.5°C and $t_{1/2} = 1.4$ d, based on rate constant $k = 9.73 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with ozone of 6×10^{11} molecules/ cm^3 in air at 24.4°C (Atkinson 1985; GEMS 1986; quoted, Howard 1990).

Surface water: $t_{1/2} = 62$ d, based on rate constant $k = 1.3 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with photochemically produced hydroxyl radicals of $1 \times 10^{-17} \text{ mol L}^{-1}$ in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).

TABLE 16.1.2.2.1

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

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

Aston et al. 1944		Swift & Hochanadel 1945		Stull 1947	
static method		isoteniscope		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-80.315	805	0	91059	-97.1	133.3
-74.081	1367	15	158520	-81.7	666.6
-62.339	3354	20	188651	-73.8	1333
-51.938	6777	25	221715	-65.0	2666
-46.842	9305	30	259444	-55.2	5333
-41.774	12548	35	302107	-48.8	7999
-35.617	17684	40	349437	-40.3	13332
-28.507	25624			-27.0	26664
-24.155	31772	bp/K	276.03	-12.5	53329
-23.067	33494			2.90	101325
-20.164	38401	eq. 4	P/mmHg		
-15.974	46505	A	24.91300	mp/°C	-117.1
-11.422	56802	B	2018.37		
-8.985	63039	C	6.0303		
-7.399	67346				
-3.113	80208	$\Delta H_v/(\text{kJ mol}^{-1}) = 23.93$			
0.780	93495	at bp			
2.928	101526				
3.454	103611				

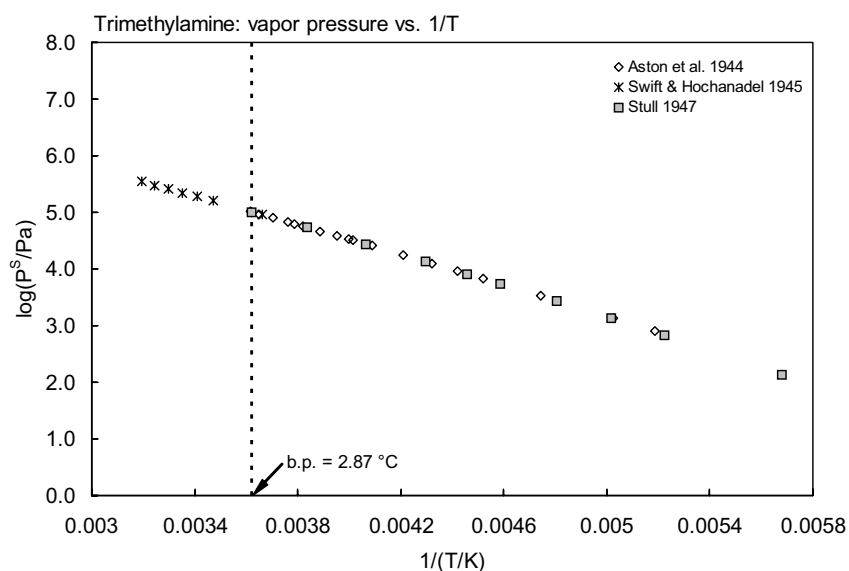
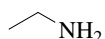


FIGURE 16.1.2.2.1 Logarithm of vapor pressure versus reciprocal temperature for trimethylamine.

16.1.2.3 Ethylamine



Common Name: Ethylamine

Synonym: aminoethane, ethanamine, monoethylamine

Chemical Name: aminoethane, ethylamine

CAS Registry No: 75-04-7

Molecular Formula: C_2H_7N , $CH_3CH_2NH_2$

Molecular Weight: 45.084

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

−80.5 (Lide 2003)

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

16.5 (Lide 2003)

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

0.6829 (Dreisbach 1961; Weast 1982–83)

0.6769 ($25^{\circ}C$, Dreisbach 1961)

Molar Volume (cm^3/mol):

65.4 ($5^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

10.79 (Perrin 1972)

10.81 ($20^{\circ}C$, Weast 1982–83)

10.63 (protonated cation + 1, Dean 1985)

10.70 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.08, 27.57 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

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

miscible (Dean 1985; Howard 1990; Stephenson 1993b)

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):

156200* (extrapolated-regression of tabulated data, temp range -82.3 to $16.6^{\circ}C$, Stull 1947)

141620 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.3862 - 1137.30/(235.85 + t/^{\circ}C)$; temp range -43 to $47^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

93325* ($20^{\circ}C$, temp range 1.95 to $20^{\circ}C$, Bittrich et al. 1962)

$\log(P/mmHg) = [-0.2185 \times 6845.1/(T/K)] + 7.973674$; temp range -82.3 to $176^{\circ}C$, (Antoine eq., Weast 1972–73)

121570, 172220 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

139100 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.12561 - 559.427/(162.579 + t/^{\circ}C)$; temp range 1.95 – $14.65^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

139700 (Daubert & Danner 1985)

141000 (calculated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.05413 - 987.31/(220.0 + t/^{\circ}C)$; temp range -20 to $90^{\circ}C$ (Antoine eq., Dean 1985, 1992)

137500, 141200 (calculated-Antoine eq.-II, III, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.57462 - 1167.57/(-34.18 + T/K)$; temp range 213 – $297\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.43082 - 1140.62/(-32.433 + T/K)$; temp range 290 – $449\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.21526 - 1009.66/(-49.804 + T/\text{K})$; temp range 291–367 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.48782 - 1176.995/(-26.674 + T/\text{K})$; temp range 377–456 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

140900 (calculated-Cox eq., Chao et al. 1990)

$\log (P/\text{mmHg}) = 33.2962 - 2.4307 \times 10^3/(T/\text{K}) - 9.0779 \cdot \log (T/\text{K}) - 1.3848 \times 10^{-9} \cdot (T/\text{K}) + 3.8183 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 192–456 K (vapor pressure eq., Yaws 1994)

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

1.012 (partial pressure, Butler & Ramchandani 1935)

0.683 (exptl., Hine & Mookerjee 1975)

0.859, 0.730 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.421 (calculated-molecular structure, Russell et al. 1992)

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

−0.30 (shake flask-titration with ion correction, Korenman et al. 1973)

−0.16, −0.14; −0.19 (calculated-fragment const.; calculated- π const., Rekker 1977)

−0.13 (Hansch & Leo 1985)

−0.13 (recommended, Sangster 1989)

−0.14 (calculated-CLOGP, Jäkel & Klein 1991)

−0.13 (recommended, Hansch et al. 1995)

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

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

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

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

Volatilization: using Henry's law constant, $t_{1/2} = 2.0$ d was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (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 $t_{1/2} > 9.9$ d for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = 2.77 \times 10^{-11} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$ at 299 K (Atkinson et al. 1977; quoted, Carlier et al. 1986)

photooxidation $t_{1/2} = 321$ d in water, based on a rate constant $k = 2.5 \times 10^9 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$ for the aqueous-phase reaction with photochemically produced OH radical of $1 \times 10^{-17} \text{ mol} \cdot \text{L}^{-1}$ (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)

$k_{O_3} = (2.76 \pm 0.34) \times 10^{-20} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$ at 296 ± 2 K under atmospheric conditions (Atkinson & Carter 1984)

$k_{OH} = 27.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.6 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 8.6$ h, based on rate constant $k = 6.54 \times 10^{-11} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$ for the vapor-phase reaction with an average hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ at 25.5°C (Atkinson 1985; quoted, Howard 1990).

Surface water: $t_{1/2} = 321$ d, based on a rate constant $k = 2.5 \times 10^9 \text{ L}\cdot\text{mol}^{-1}\cdot\text{s}^{-1}$ for the aqueous-phase reaction with photochemically produced hydroxyl radical of $1 \times 10^{-17} \text{ mol}\cdot\text{L}^{-1}$ (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).

TABLE 16.1.2.3.1
Reported vapor pressures of ethylamine at various temperatures

Stull 1947		Bittrich et al. 1962	
summary of literature data			
t/°C	P/Pa	t/°C	P/Pa
−82.3	133.3	1.95	53329
−66.4	666.6	4.55	59995
−58.3	1333	6.85	66661
−48.6	2666	9.15	73327
−39.8	5333	11.05	79993
−33.4	7999	12.85	86659
−25.1	13332	14.65	93325
−12.3	26664		
2.0	53329		
16.6	101325		
mp/°C	−80.6		

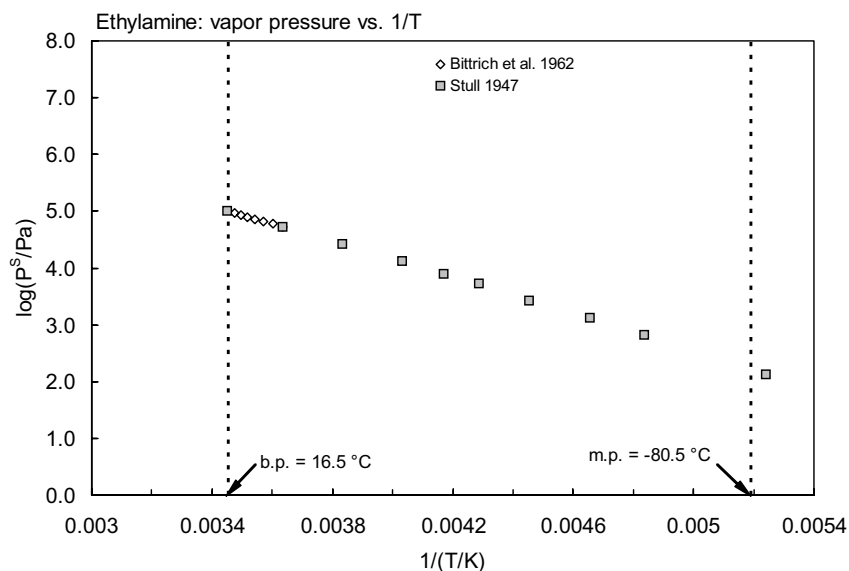
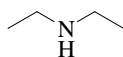


FIGURE 16.1.2.3.1 Logarithm of vapor pressure versus reciprocal temperature for ethylamine.

16.1.2.4 Diethylamine



Common Name: Diethylamine

Synonym: aminoethylethane, *N*-ethylethanamine

Chemical Name: aminoethylethane, diethylamine

CAS Registry No: 109-89-7

Molecular Formula: $C_4H_{11}N$, $CH_3CH_2NHCH_2CH_3$

Molecular Weight: 73.137

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

−49.8 (Lide 2003)

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

55.5 (Lide 2003)

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

0.6993, 0.6926 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach. 1961)

0.7056 (Weast 1982–83)

0.7070, 0.7016 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.4 ($20^{\circ}C$, calculated-density)

109.0 (exptl. at normal bp, Lee et al. 1972)

111.9 (calculated-Le Bas method at normal boiling point.)

Dissociation Constant, pK_a :

10.98 (Perrin 1965; quoted, Howard 1990)

10.80 ($35^{\circ}C$, Perrin 1972)

10.80 (protonated cation + 1, Dean 1985)

11.07 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.38, 29.50 ($25^{\circ}C$, bp, Dreisbach 1961)

31.32, 29.07 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

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

815000 ($14^{\circ}C$, quoted, Verschueren 1983)

miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990)

miscible (Stephenson 1993b)

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

26664* ($21^{\circ}C$, summary of literature data, temp range -33.0 to $55.5^{\circ}C$, Stull 1947)

31130 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.14099 - 1209.9/(229.0 + t/^{\circ}C)$; temp range -15 to $90^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

39997* ($31.45^{\circ}C$, temp range 31.45 – $60.58^{\circ}C$, Bittrich & Kauer 1962)

31471* ($25.17^{\circ}C$, temp range 19.73 – $40.22^{\circ}C$, Kilian & Bittrich 1965)

$\log(P/mmHg) = [-0.2185 \times 7307.5/(T/K)] + 7.701718$; temp range -33.0 to $210^{\circ}C$ (Antoine eq., Weast 1972–73)

26660, 38660 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

30110, 31310 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 4.97981 - 580.448/(143.68 + t/^{\circ}C)$; temp range 31.45 – $60.58^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 5.84728 - 994.478/(203.53 + t/^{\circ}C)$; temp range 19.758 – $40.22^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

31130 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 4.92649 - 583.297/(144.145 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

31490 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.96802 - 1058.538/(-61.331 + T/\text{K})$; temp range 302–328 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.92678 - 1028.405/(-66.2061 + T/\text{K})$; temp range 325–437 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 5.8016 - 583.3/(144.1 + t/^\circ\text{C})$; temp range 31–61°C (Antoine eq., Dean 1992)

$\log(P/\text{mmHg}) = 32.626 - 2.4918 \times 10^3/(T/\text{K}) - 9.3285 \cdot \log(T/\text{K}) + 3.990 \times 10^{-3} \cdot (T/\text{K}) + 1.1732 \times 10^{-12} \cdot (T/\text{K})^2$; temp range 223–497 K (vapor pressure eq., Yaws 1994)

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

2.596 (exptl., Hine & Mookerjee 1975)

2.537, 2.37 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

6.67 (calculated-vapor liquid equilibrium VLE data, Yaws et al. 1991)

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

0.43 (shake flask, Collander 1951)

0.57 (shake flask-titration, Sandell 1962)

0.60, 0.61; 0.70 (calculated-fragment const.; calculated- π const., Rekker 1977)

0.58 (Hansch & Leo 1985)

0.58 (20°C, shake flask-GC, Takayama et al. 1985)

0.81 (HPLC- k' correlation, Eadsforth 1986)

0.58 (recommended, Sangster 1989)

0.58 (recommended, Hansch et al. 1995)

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

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

0.210 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

1.699 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: using Henry's law constant, $t_{1/2} \sim 31.6$ h for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: photooxidation $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 0.21$ d in air, based on an estimated second-order rate constant $k = 77.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5×10^5 radicals/cm³ in air (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 0.21$ d, based on an estimated rate constant $k \sim 77.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5×10^5 radicals/cm³ in air (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.4.1

Reported vapor pressures of diethylamine at various temperatures

Stull 1947		Bittrich & Kauer 1962		Kilian & Bittrich 1965	
summary of literature data					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-33.0	1333	31.45	39997	19.73	24718
-22.6	2666	34.75	46663	25.17	31471
-11.3	5333	38.05	53329	30.31	39343
-4.0	7999	41.1	59995	34.99	47596
6.0	13332	43.85	66661	40.22	58582
21.0	26664	46.5	73327		
38.0	53329	48.85	79993		
55.5	101325	51.10	86659		
		53.20	93325		
mp/°C	-38.9	55.53	101325		
		57.05	106658		
		59.00	113324		
		60.58	119990		

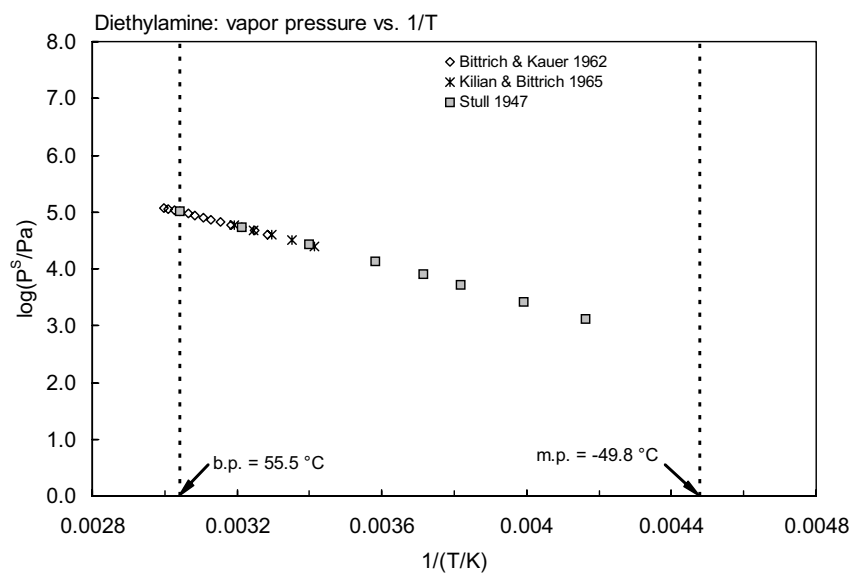
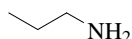


FIGURE 16.1.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for diethylamine.

16.1.2.5 *n*-Propylamine

Common Name: Propylamine

Synonym: 1-aminopropane, 1-propanamine, *n*-propylamine

Chemical Name: aminopropane, *n*-propylamine

CAS Registry No: 107-10-8

Molecular Formula: C₃H₉N, CH₃CH₂CH₂NH₂

Molecular Weight: 59.110

Melting Point (°C):

−84.75 (Lide 2003)

Boiling Point (°C):

47.22 (Lide 2003)

Density (g/cm³ at 20°C):

0.7173 (Dreisbach 1961; Weast 1982–83; Dean 1985; Riddick et al. 1986)

0.7123 (25°C, Dreisbach 1961)

Molar Volume (cm³/mol):

82.4 (liquid molar volume, Kamlet et al. 1986, 1987)

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

Dissociation Constant, pK:

10.74, 10.789 (20°C, Perrin 1972)

10.71 (pK_a, 20°C, Weast 1982–83)

10.57 (pK_{BH}⁺, Dean 1985; Riddick et al. 1986)

10.68 (pK_a, Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.13, 29.73 (25°C, bp, Dreisbach 1961)

31.26, 29.54 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.974 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Dean 1985; Stephenson 1993b)

miscible (Riddick et al. 1986; Howard 1990; Yaws et al. 1990)

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

41800* (interpolated-regression of tabulated data, temp range −64.4 to 48.5°C, Stull 1947)

41050 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 7.2672 − 1218.1/(229.9 + t/°C); temp range −20 to 81°C (Antoine eq. for liquid state, Dreisbach 1961)

42100* (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

log (P/mmHg) = 6.92646 − 1044.028/(t/°C + 210.833); temp range 23–77.6°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)

log [(P/atm) = [1 − 320.379 ± (T/K)] × 10⁴{0.922208 − 10.51259 × 10^{−4}·(T/K) + 11.25530 × 10^{−7}·(T/K)²}, temp range: 34–77.6°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)

log (P/mmHg) = [−0.2185 × 7408.0/(T/K)] + 7.867998; temp range −64.4 to 214.5°C (Antoine eq., Weast 1972–73)

32660 (20°C, 31°C, Verschueren 1983)

38550; 42110 (22.97°C, quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.05146 − 1044.082/(210.84 + t/°C); temp range 22.97–77.6°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1968, Boublik et al. 1984)

42120 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.92651 - 1044.05/(210.84 + t/^{\circ}\text{C})$; temp range: 23–77°C (Antoine eq., Dean 1985, 1992)
 41050 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.05136 - 1044.028/(210.833 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 42120 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.04693 - 1041.725/(-62.596 + T/\text{K})$; temp range 295–351 K (Antoine eq., Stephenson & Malanowski 1987)
 42125 (calculated-Cox eq., Chao et al. 1990)
 $\log (P/\text{mmHg}) = 24.6420 - 2.3152 \times 10^3/(T/\text{K}) - 5.8711 \cdot \log (T/\text{K}) - 4.6258 \times 10^{-11} \cdot (T/\text{K}) + 1.582 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 190–497 (vapor pressure eq., Yaws 1994)

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

1.274 (partial pressure, Butler & Ramchandani 1935)
 0.784; 0.732 (exptl.; calculated-group contribution, Hine & Mookerjee 1975)
 1.330 (calculated-bond contribution, Hine & Mookerjee 1975)
 0.637 (calculated-molecular structure, Russell et al. 1992)
 2.01 (gas stripping-GC, Altschuh et al. 1999)

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

0.28 (shake flask-GC, Korenman et al. 1973)
 0.37, 0.39; 0.31 (calculated-f const.; calculated- π const., Rekker 1977)
 0.48 (shake flask-GC, pH 13, Yakayama et al. 1985)
 0.48 (recommended, Sangster 1989)
 0.48 (recommended, Hansch et al. 1995)

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

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

–0.886 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

< 1.699 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization: using Henry's law constant, $t_{1/2} \sim 2.44$ d was estimated for a model river 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 12$ h in air, based on estimated rate constant $k = 3.21 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 12$ h, based on estimated second-order rate constant of $3.21 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.5.1
Reported vapor pressures of *n*-propylamine at various temperatures

Stull 1947		Osborn & Douslin 1968	
summary of literature data		ebulliometric method	
t/°C	P/Pa	t/°C	P/Pa
-64.4	133.3	22.973	38547
-46.3	666.6	27.750	47359
-37.2	1333	32.564	57803
-27.1	2666	37.414	70109
-16.0	5333	42.304	84525
-9.0	7999	47.229	101325
0.50	13332	52.193	120798
15.0	26664	57.195	143268
31.5	53329	62.235	169052
48.5	101325	67.314	198530
		72.430	232087
mp/°C	-83.0	77.587	270110

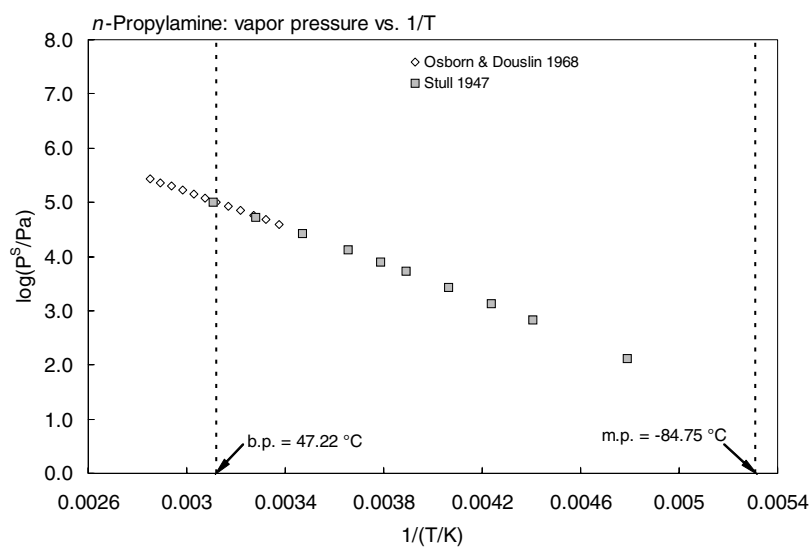
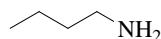


FIGURE 16.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-propylamine.

16.1.2.6 *n*-Butylamine

Common Name: Butylamine

Synonym: 1-aminobutane, *n*-butylamine, 1-butanamine

Chemical Name: 1-aminobutane, *n*-butylamine

CAS Registry No: 109-73-9

Molecular Formula: C₄H₁₁N, CH₃CH₂CH₂CH₂NH₂

Molecular Weight: 73.137

Melting Point (°C):

−49.1 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

77.0 (Lide 2003)

Density (g/cm³ at 20°C):

0.7414 (Dreisbach 1961; Weast 1982–83)

0.7392 (Riddick et al. 1986)

Molar Volume (cm³/mol):

98.8 (20°C, calculated-density)

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

Dissociation Constant, pK:

10.77 (Perrin 1965; pK_a, 20°C, Weast 1982–83; Howard 1990)

10.65 (Perrin 1972)

10.64 (pK_a, protonated + 1, Dean 1985; Sangster 1989)

10.77 (pK_{BH+}, Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.54, 32.11 (25°C, bp, Dreisbach 1961)

35.74, 31.80 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Dean 1985; Howard 1990; Yaws et al. 1990)

miscible (Riddick et al. 1986)

miscible (Stephenson 1993b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

13850 (Hoy 1970; Abraham 1984)

12230 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 7.213 − 1308.4/(224.2 + t/°C); temp range 4–114°C (Antoine eq. for liquid state, Dreisbach 1955)

9600 (20°C, Verschueren 1983)

12230 (quoted lit., Riddick et al. 1986; quoted, Howard 1990)

log (P/kPa) = 6.07009 − 1157.810/(207.80 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

12520 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.2635 − 1258.745/(−54.49 + T/K); temp range 313–350 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 25.0711 − 2.5701 × 10³/(T/K) − 5.8985 · log (T/K) + 7.9399 × 10^{−10} · (T/K) + 1.192 × 10^{−6} · (T/K)²; temp range 124–532 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

1.526 (partial pressure, Butler & Ramchandani 1935)

1.528 (exptl., Hine & Mookerjee 1975)

- 1.676, 1.68 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.880 (calculated-molecular structure, Russell et al. 1992)
 1.785 (gas stripping-GC, Altschuh et al. 1999)

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

- 0.68 (shake flask, Collander 1951)
 0.88 (shake flask-titration, Sandell 1962)
 0.81 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1987)
 0.74 (shake flask-titration, Korenman et al. 1973)
 0.90, 0.92; 0.81 (calculated- f const.; calculated- π const., Rekker 1977)
 0.80 (inter-lab. shake flask average, Eadsforth & Moser 1983)
 0.97 (shake flask-GC, Takayama et al. 1985)
 0.86 (recommended, Sangster 1989)
 0.97 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, $\log BCF$:

- 0.505 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

- 1.903 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
 1.176, 2.021, 2.029 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
 1.880 (soil, quoted exptl., Meylan et al. 1992)
 1.780 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

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

Volatilization: using Henry's law constant, $t_{1/2} = 1.95$ d was predicted for evaporation from a model river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: estimated vapor phase photooxidation $t_{1/2} = 0.479$ d in air, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of 5×10^5 radicals/cm³ (USEPA 1986; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

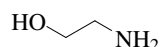
Biotransformation:

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

Half-Lives in the Environment:

Air: estimated vapor phase $t_{1/2} = 0.479$ d, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of 5×10^5 radicals/cm³ (USEPA 1986; quoted, Howard 1990).

16.1.2.7 Ethanolamine



Common Name: Ethanolamine

Synonym: β -aminoethyl alcohol, ethylolamine, 2-hydroxyethylamine, β -hydroxyethylamine, monoethanolamine, MEA

Chemical Name: ethanolamine, 2-aminoethanol

CAS Registry No: 141-43-5

Molecular Formula: $\text{C}_2\text{H}_7\text{NO}$, $\text{HOCH}_2\text{CH}_2\text{NH}_2$

Molecular Weight: 61.098

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

10.5 (Lide 2003)

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

171 (Lide 2003)

Density (g/cm^3 at 20°C):

1.0180 (Weast 1982–83)

1.0147 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

60.4 (Stephenson & Malanowski 1987)

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

Dissociation Constant, pK :

9.48, 9.4994 (Perrin 1972; quoted, Howard 1990)

9.50 (pK_{BH^+} , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_{v} (kJ/mol):

92.09, 49.831 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.50 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} $\text{J}/\text{mol K}$:

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985)

miscible (Riddick et al. 1986; quoted, Howard 1990)

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

893* (65.4°C , Ramsay-Young method, measured range 65.4 – 170.9°C , Matthews et al. 1950)

$\log (P/\text{mmHg}) = 44.008 - 4089/(T/K) - 11.446 \pm \log (T/K)$; temp range 65.4 – 170.9°C (Kirchhoff eq., ebulliometry, Matthews et al. 1950)

8707* (106.1°C , ebulliometry, measured range 106.1 – 170.37°C , McDonald et al. 1959)

$\log (P/\text{mmHg}) = 7.7380 - 1772.11/(186.25 + t/^{\circ}\text{C})$; temp range 106 – 170°C , or pressure range 65.31 – 760 mmHg (ebulliometry, McDonald et al. 1959)

53.32 (20°C , Verschueren 1983)

41.64, 46.67 (extrapolated values-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.54175 - 1554.149/(171.175 + t/^{\circ}\text{C})$; temp range 65.5 – 170.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.86239 - 1725.168/(185.556 + t/^{\circ}\text{C})$; temp range 106.1 – 170.37°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

42.51 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.4568 - 1577.67/(172.37 + t/^{\circ}\text{C})$; temp range 65 – 171°C (Antoine eq., Dean 1985, 1992)

48.0 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.86290 - 1732.11/(186.215 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

47.34 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 6.8629 - 1732.11/(-86.6 + T/K)$; temp range 310 – 444 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

34.66 (from Dow Chemical's Handbook, Howard 1990)

$\log(P/\text{mmHg}) = 72.9125 - 5.8595 \times 10^3/(T/K) - 21.914 \cdot \log(T/K) - 7.1511 \times 10^{-10} \cdot (T/K) + 5.9841 \times 10^{-6} \cdot (T/K)^2$;
temp range 284–638 K (vapor pressure eq., Yaws 1994)

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

0.0041 (calculated-bond method, Hine & Mookerjee 1975)

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

−1.31 (shake flask, Collander 1951)

−1.29; −1.35 (calculated- f const., calculated- π const., Rekker 1977)

−1.31 (recommended, Sangster 1993)

−1.31 (recommended, Hansch et al. 1995)

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

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

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

0.699 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{1/2} = 11$ h in air, based on an estimated rate constant $k \sim 3.5 \times 10^{-11} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air (Atkinson 1987; quoted, Howard 1990).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: half-life of 11 h, based on an estimated rate constant of $3.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.7.1

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

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

Matthews et al. 1950				McDonald et al. 1959	
Ramsay-Young method				ebulliometric method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
65.4	893	137.9	32264	106.1	8707
65.5	947	144.6	42236	108.43	10058
69.5	1160	150.0	54195	112.29	11427
70.0	1253	161.4	73860	114.55	12702
75.4	1760	170.9	100125	116.79	14049
81.1	2320			125.73	20454
86.4	3280	bp/K	444.1	159.79	71862
90.0	3813			169.20	97584
96.4	5440	$\Delta H_v/(\text{kJ mol}^{-1}) = 46.07$ at bp		170.37	101325
101.7	7146	Kirchhoff, Rankine, Dupre			
105.5	8559	eq. 4	P/mmHg	mp/°C	10.31
112.1	11306	A	44.008	eq. 2	P/mmHg
117.3	14012	B	4809	A	7.7380
125.0	19452	C	11.446	B	173211
132.0	25771			C	186.215

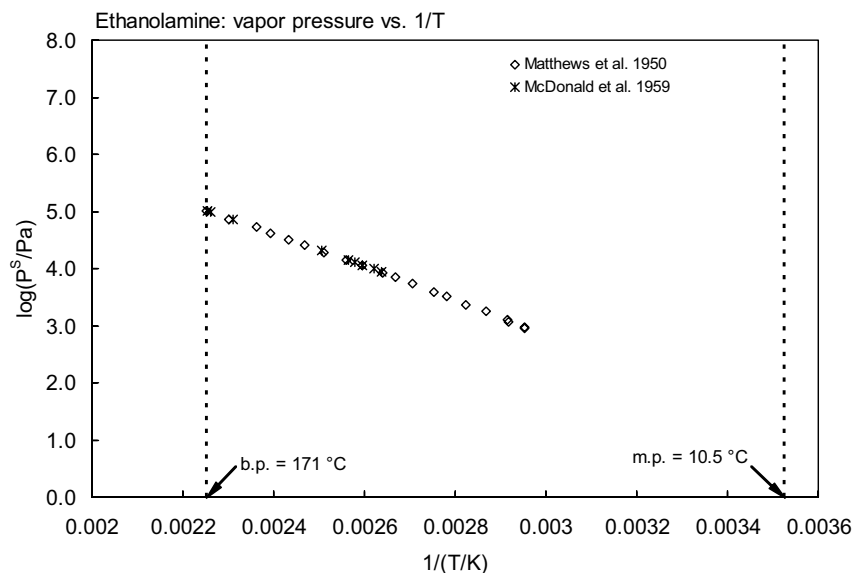
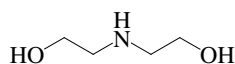


FIGURE 16.1.2.7.1 Logarithm of vapor pressure versus reciprocal temperature for ethanolamine.

16.1.2.8 Diethanolamine



Common Name: Diethanolamine

Synonym: 2,2'-amino-diethanol, 3-aza-1,5-pentanediol, diethylolamine, bis(hydroxyethyl)amine, 2,2'-dihydroxydiethylamine, β,β' -dihydroxydiethylamine, 2,2'-iminobisethanol, 2,2'-iminodiethanol

Chemical Name: diethanolamine

CAS Registry No: 111-42-2

Molecular Formula: $C_4H_{11}NO_2$, $HOCH_2CH_2NHCH_2CH_2OH$

Molecular Weight: 105.136

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

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

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

268.8 (Lide 2003)

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

1.0966 (Weast 1982–83)

1.0936 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

96.5 ($30^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK :

8.88, 8.97 (Perrin 1972)

8.88 (pK_{BH^+} , Dean 1985; Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.3, 65.229 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.104 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.934 (mp at $28^{\circ}C$)

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

954000 (Verschuereen 1983)

964000 (Dean 1985)

954000 ($20^{\circ}C$, Riddick et al. 1986)

miscible (from Dow Chemical's Handbook, Howard 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 1.333 ($20^{\circ}C$, Verschuereen 1983)

0.040 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 8.1388 - 2327.9/(174.4 + t/^{\circ}C)$; temp range 194–241 $^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.030 (quoted lit., Riddick et al. 1986)

$\log(P/kPa) = 7.26458 - 2328.56/(174.399 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 7.26044 - 2326.23/(-98.907 + T/K)$; temp range: 423–542 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

0.0373 (quoted from Dow Chemical's Handbook, Howard 1990)

$\log(P/mmHg) = 122.0877 - 8.8422 \times 10^3/(T/K) - 40.422 \cdot \log(T/K) + 1.4062 \times 10^{-2} \cdot (T/K) + 1.1986 \times 10^{-12} \cdot (T/K)^2$; temp range 301–542 K (vapor pressure eq., Yaws 1994)

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

5.42×10^{-9} (Hine & Mookerjee 1975)

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

- 1.43 (shake flask, Collander 1951)
- 1.51 (calculated-fragment const., Rekker & De Kort 1979)
- 1.43 (recommended, Sangster 1993)
- 1.43 (recommended, Hansch et al 1995)

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

Bioconcentration Factor, $\log BCF$:

- < 0.0 (estimated- K_{OW} , Howard 1990)

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

- 0.602 (soil, estimated- K_{OW} , Howard 1990)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{1/2} = 0.72\text{--}7.2$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 14.4\text{--}168$ h, based on measured half-life in surface water grab sample experiment (Boethling & Alexander 1979; quoted, Howard et al. 1991) and aqueous aerobic screening test data (Gerike & Fischer 1979; Bridie et al. 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 57.6\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.72\text{--}7.2$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991);

atmospheric transformation lifetime by reaction with water was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 14.4\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

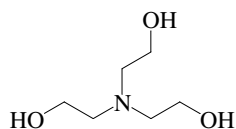
Groundwater: $t_{1/2} = 28.8\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 14.4\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.2.9 Triethanolamine



Common Name: Triethanolamine

Synonym: 2,2',2''-nitrilotriethanol, 2,2',2''-nitrilotrisethanol, triethylolamine, trihydroxytriethylamine, trolamine, tris(hydroxyethyl)-amine, TEA

Chemical Name: triethanolamine

CAS Registry No: 102-71-6

Molecular Formula: $C_6H_{15}NO_3$, $(HOCH_2CH_2)_3N$

Molecular Weight: 149.188

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

20.5 (Lide 2003)

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

335.4 (Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

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

1.1242 (Weast 1982–83; Dean 1985)

1.1196 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

133.3 (Stephenson & Malanowski 1987)

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

Dissociation Constant, pK :

7.92 (Perrin 1972; quoted, Howard 1990)

7.76 (pK_{BH^+} , Dean 1985; Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

67.475 (bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.20 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

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

miscible (Dean 1985; Howard 1990)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 1.33 ($20^{\circ}C$, Verschueren 1983)

0.0131 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 9.19319 - 4543.817/(297.839 + t/^{\circ}C)$, temp range: 252.7 – $305.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.0100 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 10.0675 - 4542.78/(297.76 + t/^{\circ}C)$, temp range: 252 – $305^{\circ}C$ (Antoine eq., Dean 1985, 1992)

< 1.30 ($20^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 7.67989 - 2962.73/(186.75 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 9.53861 - 4951.87/(49.99 + T/K)$, temp range: 523 – $579\ K$, (Antoine eq., Stephenson & Malanowski 1987)

4.79×10^{-4} (quoted from Dow Chemical's Handbook, Howard 1990)

$\log(P/mmHg) = 135.3206 - 1.0312 \times 10^4/(T/K) - 44.637 \cdot \log(T/K) + 1.4368 \times 10^{-2} \cdot (T/K) - 1.7552 \times 10^{-13} \cdot (T/K)^2$; temp range 294 – $787\ K$ (vapor pressure eq., Yaws 1994)

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

3.42×10^{-14} (Hine & Mookerjee 1975)

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

- 1.32, -1.75 (calculated, Verschueren 1983)
- 1.59 (Howard 1990)
- 1.00 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

- < 0.0 (estimated- K_{OW} , Howard 1990)

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

- 0.477 (soil, estimated- K_{OW} , Howard 1990)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{1/2} = 4.0$ h in air, based on an estimated rate constant $k \sim 10.4 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air at 25°C (Atkinson 1987; quoted, Howard 1990).

Biodegradation:

Biotransformation:

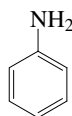
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 4.0$ h, based on an estimated rate constant $k \sim 10.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air at 25°C (Atkinson 1987; quoted, Howard 1990).

16.1.3 AROMATIC AMINES

16.1.3.1 Aniline



Common Name: Aniline

Synonym: phenylamine, aminobenzene, benzeneamine, benzenamine

Chemical Name: aniline

CAS Registry No: 62-53-3

Molecular Formula: $C_6H_5NH_2$

Molecular Weight: 93.127

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

−6.02 (Lide 2003)

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

184.1 (Lide 2003)

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

1.02173, 1.01750 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.02173 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

91.2 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK_a :

4.596 (Perrin 1972; Howard 1989)

4.600 (McLeese et al. 1979; Riddick et al. 1986; Sangster 1989)

4.630 (Weast 1982–83)

4.58, 3.96 (quoted, HPLC, Miyake et al. 1987)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

54.28, 43.17 ($25^{\circ}C$, bp, Dreisbach 1955)

55.843, 44.53 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

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

36650 (Hill & Macy 1924)

36070 (Seidell 1941)

38670 (shake flask-residue volume method, Booth & Everson 1948)

36220 (shake flask-interferometry, Donahue & Bartell 1952)

34100 (Stephen & Stephen 1963)

36600 (Kenaga 1980)

34000 (Verschueren 1983)

56900 (calculated-activity coeff. γ by UNIFAC, Fu & Luthy 1985, 1986)

33800 (selected, Riddick et al. 1986)

34200 (selected, Yaws et al. 1990)

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

133.3 ($43.7^{\circ}C$, static method, measured range 43.7 – $183.9^{\circ}C$, Kahlbaum 1898)

85.71* (extrapolated-regression of tabulated data, temp range 34.8 – $184.4^{\circ}C$ Stull 1947)

$\log(P/mmHg) = 7.57170 - 1941.7/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

10351* ($112.92^{\circ}C$, ebulliometry, measured range 112.92 – $183.93^{\circ}C$, Dreisbach & Shrader 1949)

89.52 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986)

$\log (P/\text{mmHg}) = 7.24179 - 1674.3/(200.0 + t/^{\circ}\text{C})$; temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

6806* (102.59°C, ebulliometry, measured range 102.59–185.15°C, McDonald et al. 1959)

$\log (P/\text{mmHg}) = 7.25375 - 1684.35/(201.175 + t/^{\circ}\text{C})$, temp range 103–185°C (Antoine eq., ebulliometry, McDonald et al. 1959)

133.3* (31.55°C, calculated-thermodynamic properties, temp range 31.55–184.40°C, Hatton et al. 1962)

$\log (P/\text{mmHg}) = [-0.2185 \times 11307.6/(T/\text{K})] + 8.221995$; temp range 34.8–422.4°C (Antoine eq., Weast 1972–73)

88.30 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log (P/\text{mmHg}) = 7.3201 - 1731.515/(205.049 + t/^{\circ}\text{C})$; temp range 102.6–185.2°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1973)

$\log (P/\text{mmHg}) = [-0.2185 \times 11307.6/(T/\text{K})] + 8.221995$; temp range 34.8–422.4°C (Antoine eq., Weast 1972–73)

82.71 (calculated-Cox eq., Chao et al. 1983)

$\log (P/\text{atm}) = [1 - 457.025/(T/\text{K})] \times 10^4 \{0.911551 - 6.64936 \times 10^{-4} \cdot (T/\text{K}) + 5.25455 \times 10^{-7} \cdot (T/\text{K})^2\}$; temp range: 267.3–695.0 K (Cox eq., Chao et al. 1983)

80 ± 6 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)

40.0 (20°C, Verschueren 1983)

88.0, 48.24 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.43196 - 1722.154/(205.002 + t/^{\circ}\text{C})$; temp range 102.6–185.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.68977 - 1234.569/(151.207 + t/^{\circ}\text{C})$; temp range 112.9–183.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

65.18 (Daubert & Danner 1985)

89.30 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.32010 - 1731.515/(206.049 + t/^{\circ}\text{C})$; temp range 102–185°C (Antoine eq., Dean 1985, 1992)

$\log (P/\text{kPa}) = 5.69066 - 1941.7/(230.0 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

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

$\log (P_L/\text{kPa}) = 6.40627 - 1702.817/(-70.155 + T/\text{K})$; temp range 304–458 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 8.1019 - 2728/(T/\text{K})$; temp range 273–338 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.41147 - 1708.239/(-69.454 + T/\text{K})$; temp range 373–458 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.44338 - 1682.348/(-78.065 + T/\text{K})$; temp range: 455–523 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

86.70 (calculated-Cox eq., Chao et al. 1990)

$\log (P/\text{mmHg}) = 124.3764 - 7.1676 \times 10^3/(T/\text{K}) - 42.763 \cdot \log (T/\text{K}) + 1.7336 \times 10^{-2} \cdot (T/\text{K}) + 5.7138 \times 10^{-15} \cdot (T/\text{K})^2$; temp range 267–699 K (vapor pressure eq., Yaws 1994)

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

13778 (Hakuta et al. 1977)

12.16 (measured, Yoshida et al. 1983)

0.193 (gas stripping-GC, Altschuh et al. 1999)

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

0.90 (shake flask-UV, Fujita et al. 1964)

0.90 (shake flask, Iwasa et al. 1965)

0.90 (shake flask-UV, Hansch et al. 1968)

0.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1983, Hansch & Leo 1985)

0.89 (shake flask-UV at pH 5.6, Umeyama et al. 1971)

0.90 (HPLC- k' correlation, Carlson et al. 1975)

0.85 (shake flask, Lu & Metcalf 1975)

0.90 (HPLC-RT correlation, Mirrlees et al. 1976)

0.93 ± 0.05 (shake flask at pH 7, Unger et al. 1978)

0.90, 0.98, 0.85 (shake flask, Hansch & Leo 1979)

0.91 (HPLC- k' correlation, Könnemann et al. 1979)

0.90 (shake flask-UV, Briggs 1981)

- 1.03 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 0.90 (HPLC- k' correlation, Hammers et al. 1982)
 0.90 (inter-laboratory studies. shake flask average, Eadsforth & Moser 1983)
 1.09 (inter-laboratory studies, HPLC-RT correlation, average, Eadsforth & Moser 1983; Brooke et al. 1990)
 1.34, 1.27, 1.08 (HPLC-RT correlation, Harnish et al. 1983)
 1.08 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
 0.79, 0.96 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
 0.89 (shake flask-UV at pH 7.4, El Tayar et al. 1984)
 0.99 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
 0.81, 1.08 (HPLC- k' correlation, Eadsforth 1986)
 0.91 (RP-HPLC-RT correlation, Eadsforth 1986)
 0.98 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
 0.93 (HPLC method average, Ge et al. 1987)
 0.78 (HPLC- k' correlation, Miyake et al. 1987)
 1.18 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.940 ± 0.006 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
 0.90 (recommended, Sangster 1989, 1993)
 0.942 ± 0.010 ; 0.940 ± 0.006 (shake flask/stir-flask method by BRE; RITOX, inter-laboratory studies, Brooke et al. 1990)
 0.90 (shake flask-GC, Alcorn et al. 1993)
 1.21, 0.89, 0.87, 1.09 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
 0.92 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
 0.88 (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

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

Bioconcentration Factor, $\log BCF$:

- 0.78 (fish, Lu & Metcalf 1975)
 0.30 (calculated-S, Kenaga 1980)
 < 1.0 (fish, Freitag et al. 1982)
 < 1.0, 0.602, 3.01 (golden orfe, algae, activated sludge, Freitag et al. 1982)
 0.602 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
 0.845 (alga *Chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)
 < 1.0, < 1.0, 2.70 (golden ide, algae, activated sludge, Freitag et al. 1985)
 2.77 (*Daphnia magna*, based on elimination phase, Dauble et al. 1986)
 1.87 (*Daphnia magna*, based on ^{14}C and exposure water, Dauble et al. 1986)
 0.70 (fish, correlated- K_{OW} , Isnard & Lambert 1988)
 0.78 (quoted, Isnard & Lambert 1988, 1989)
 0.41 (zebrafish, Kalsch et al. 1991)
 0.41 (zebrafish, Zok et al. 1991)
 0.41; 1.04, -0.87, 0.03 (quoted exptl.; calculated values- K_{OW} , Bintein et al. 1993)

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

- 3.11; 2.11 (H-montmorillonite at pH 8.35; pH 6.80, Bailey et al. 1968)
 1.86 (soil average, Moreale & Van Bladel 1976)
 1.41 (average of seven agricultural soils, Briggs 1981)
 3.59 (colloidal organic carbon/ground water, Means et al. 1982)
 2.11; 2.61 (soil; more acidic soil, Pillai et al. 1982)
 2.49; 2.11 (nonsterile Hagerstown soil; sterile Hagerstown soil, Pillai et al. 1982)
 2.96; 2.61 (nonsterile Palouse soil; sterile Palouse soil, Pillai et al. 1982)
 1.17 (soil, quoted as $\log K_{OM}$, Sabljic 1987)
 2.12, 2.05, 2.06 (calculated values: Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
 0.596 (calculated- K_{OW} , Kollig 1993)

- 1.08, 1.25, 0.98 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
 1.41 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.07; 1.65 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 2.70, 1.64, 2.08, 2.04, 2.29 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 2.384, 1.503, 1.279, 1.437, 2.136 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 1.0–1.54 (5 soils, pH 2.8–7.2, batch equilibrium-sorption isotherm, Li et al. 2000)

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

Volatilization: estimated $t_{1/2} = 12$ d from a measured Henry's law constant of 1.2×10^{-4} atm $\text{m}^3 \text{mol}^{-1}$ (Yoshida et al. 1983; quoted, Howard 1989) for a model river of 1-m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);
 volatilization $t_{1/2}(\text{calc}) = 55$ d (Toräng et al. 2002).

Photolysis: first-order rate constants for photosensitized reactions in water with various humic substances as sensitizers: $k = 0.17 \text{ h}^{-1}$ with aquatic humus from Aucilla River, $k = 0.12 \text{ h}^{-1}$ with Aldrich humic acid, $k = 0.091 \text{ h}^{-1}$ with Fluka humic acid and $k = 0.11 \text{ h}^{-1}$ with Contech fulvic acid in sunlight, corresponding to half-lives of 4 to 8 h (Zepp et al. 1981); photolysis $t_{1/2} = > 50$ yr at 15°C and a pH 5–9 (Toräng et al. 2002).

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:

$k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}} = 1.20 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{av.}) = 1.17 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-RF, Rinke & Zetzsch 1984; Witte et al. 1986)

$k_{\text{OH}}^* = 1.10 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range: 239–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{\text{OH}}(\text{calc}) = 1.54 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{\text{OH}}(\text{obs}) \approx 6.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{OH}}(\text{calc.}) = 1.16 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 1.36 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.17 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^*(\text{exptl}) = 1.18 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K, measured range: 265–455 K; and $k_{\text{O}_3} = 1.12 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}}^* = 1.11 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 1.385 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: completely degraded by a soil inoculum in 4 d (Alexander & Lustigman 1966; quoted, Verschuere 1983; Howard 1989);

completely degraded in 20 d by bacteria in river mud (Calamari et al. 1980; quoted, Howard 1989);

$k = 0.23 \text{ d}^{-1}$ and corresponding to a $t_{1/2} = 3$ d in samples of White Lake water at 29°C (Subba-Rao et al. 1982);

average rate of biodegradation $k = 19.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 94.5% removal (Scow 1982);

biodegradation $t_{1/2} = 4.5$ d in unpolluted and $t_{1/2} < 0.5$ d in polluted pond water as model environments (Lyons et al. 1984);

0.46 mM aniline solution degraded by strain Ani1 within 14 d in water (Schnell et al. 1989);

average exptl. $k = 0.044 \text{ h}^{-1}$ compared to the group-contribution method predicted rate constants of 0.050 h^{-1} (nonlinear) and 0.018 h^{-1} (Tabak & Govind 1993);

first-order $k = 1.0 \text{ d}^{-1}$ for batch expt. with Elbe water at 20°C (Börnack et al. 2001);

field first-order degradation $k \sim 1.8 \text{ d}^{-1}$ for 2 different dates with water temperatures of 21.9 and 14.7°C , respectively, in Rhine river and rate constant obtained in laboratory shake flask batch tests with Rhine water averaged 1.5 d^{-1} at 15°C and 2.0 d^{-1} at 20°C (Toräng et al. 2002).

Biotransformation: mean bacteria transformation rate constant for all three sites of $(1.1 \pm 0.8) \times 10^{-11}$ L·organism⁻¹·h⁻¹ (Paris & Wolfe 1987; quoted, Steen 1991).

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

$k_1 = 0.052 \pm 0.0067$ h⁻¹; $k_2 = 7.200 \pm 1.3000$ h⁻¹ (Kalsch et al. 1991)

$k_1 = 11.10 \pm 3.2000$ h⁻¹ (zebrafish, Zok et al. 1991)

Half-Lives in the Environment:

Air: atmospheric lifetimes of 2.3 h in clean troposphere and 1.2 h in moderately polluted atmosphere, based on gas-phase reaction with hydroxyl radical at room temp.; atmospheric lifetimes of 15.0 d in clean troposphere and 5.0 d in moderately polluted atmosphere, based on gas-phase reaction with O₃ at room temp. (Atkinson et al. 1987)

$t_{1/2} \sim 3.3$ h, based on reaction with photochemically produced hydroxyl radical (Howard 1989);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} = 2.3$ d in Rhine river in case of a first order reduction process (Zoeteman et al. 1980; quoted, Howard 1989);

estimated $t_{1/2} = 0.3$ –3.0 d in river waters (Zoeteman et al. 1980);

$t_{1/2} = 4$ to 8 h in May sunlight with both commercial humic acids and aquatic humus as photosensitizers near-surface water and $t_{1/2} \sim 1$ wk in distilled water (Zepp et al. 1981);

$t_{1/2} = 6$ d in eutropic pond and $t_{1/2} = 21$ d in an oligotrophic lake (Subba-Rao et al. 1982; quoted, Howard 1989);

biodegradation $t_{1/2} = 4.5$ d in unpolluted and $t_{1/2} < 0.5$ d in polluted pond water as model environments (Lyons et al. 1984);

$t_{1/2} = 4$ –33 d at 15°C (Ingerslev & Nyholm 2000);

$t_{1/2} \sim 9$ h in the Rhine river at 15 and 22°C (Toräng et al. 2002).

Ground water: estimated $t_{1/2} \sim 30$ –300 d (Zoeteman et al. 1980).

Sediment:

Soil:

Biota:

TABLE 16.1.3.1.1

Reported vapor pressures of aniline 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)					
Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959		Hatton et al. 1962	
summary of literature data		ebulliometry		ebulliometry		calc-thermodynamic properties	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
34.8	133.3	112.92	10351	102.59	6806	31.55	133.3
57.9	666.6	125.16	17039	117.22	12295	41.82	666.6
69.4	1333	153.2	42103	137.5	25439	52.59	1333
82.0	2666	168.21	67701	160.08	51913	68.62	2666
96.7	5333	183.93	101325	182.4	97103	82.11	5333
106.0	7999			184.24	101912	97.02	7999
119.9	13332	bp/°C	183.93	185.15	104589	119.41	13332
140.1	26664					138.90	26664
161.9	53329			mp/°C	–6.02	161.05	53329
184.4	101325					184.40	101325
				eq. 2	P/mmHg		
mp/°C	–6.2			A	7.25375		
				B	1684.35		
				C	201.175		

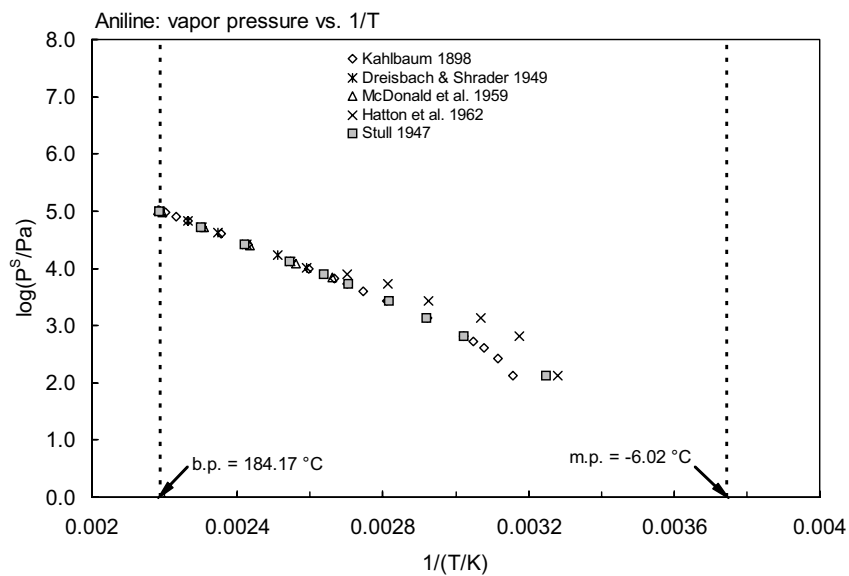
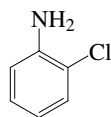


FIGURE 16.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for aniline.

16.1.3.2 2-Chloroaniline



Common Name: 2-Chloroaniline

Synonym: 1-amino-2-chlorobenzene, *o*-aminochlorobenzene, *o*-chloroaniline, 2-chlorophenylamine

Chemical Name: 1-amino-2-chlorobenzene, *o*-chloroaniline, 2-chloroaniline

CAS Registry No: 95-51-2

Molecular Formula: $C_6H_4NH_2Cl$

Molecular Weight: 127.572

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

- −1.94 (β -2-chloroaniline, Dreisbach 1955; Weast 1872–83, Riddick et al. 1986)
- −14.0 (α -2-chloroaniline, Weast 1982–83; Verschueren 1983; Howard 1989)
- −1.9 (Lide 2003)

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

- 208.8 (Kahlbaum 1898; Stull 1947; Dreisbach 1955; Weast 1982–83; Lide 2003)

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

- 1.21266, 1.20787 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)
- 1.21251, 1.20775 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

- 105.2 ($20^{\circ}C$, Stephenson & Malanowski 1987)
- 131.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

- 2.661 (Perrin 1972; quoted, Howard 1989)
- 2.650 (Weast 1982–83)
- 2.640 (protonated cation + 1, Dean 1985)
- 2.640 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

- 57.5 ± 5 ($25^{\circ}C$, Piacente et al. 1985)
- 56.756, 44.35 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

- 11.88 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

- 8760 (Dreisbach 1955)
- 3765 ($20^{\circ}C$, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
- 3763 (calculated- K_{ow} , Müller & Klein 1992)
- 4740 (calculated-group contribution method, Kühne et al. 1995)

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):

- 40.31* (extrapolated-regression of tabulated data, measured range 64.4 – $208.8^{\circ}C$, Kahlbaum 1898)
- 37.77* (extrapolated-regression of tabulated data, temp range 46.3 – $208.8^{\circ}C$, Stull 1947)
- $\log(P/mmHg) = 7.63311 - 2085.5/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)
- 7605* ($124.48^{\circ}C$, ebulliometry, measured range 124.48 – $208.84^{\circ}C$, Dreisbach & Shrader 1949)
- 33.77 (calculated by formula, Dreisbach 1955; selected, Riddick et al. 1986)
- $\log(P/mmHg) = 7.19240 - 1762.74/(200.0 + t/^{\circ}C)$; temp range 110 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)
- $\log(P/mmHg) = [-0.2185 \times 12441.0/(T/K)] + 8.56946$; temp range 46.3 – $208.8^{\circ}C$ (Antoine eq., Weast 1972–73)
- 33.88 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.56265 - 1998.6/(220.0 + t/^{\circ}\text{C})$, temp range 20–108°C (Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.19240 - 1762.74/(200.0 + t/^{\circ}\text{C})$, temp range: 108–300°C (Antoine eq., Dean 1985, 1992)
 35.30* (torsion-weighing effusion, Piacente et al. 1985)
 $\log (P/\text{kPa}) = (8.63 \pm 0.16) - (3006 \pm 56)/(T/\text{K})$; temp range: 287–336 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)
 $\log (P/\text{kPa}) = 6.75801 - 2085.50/(230.0 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 18.97 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.84227 - 1432.2/(-108.81 + T/\text{K})$; temp range 397–482 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 90.6491 - 6.041 \times 10^3/(T/\text{K}) - 31.118 \cdot \log (T/\text{K}) + 1.1564 \times 10^{-2} \cdot (T/\text{K}) + 4.8388 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 271–722 K (vapor pressure eq., Yaws 1994)

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

0.760 (calculated-P/C, Howard 1989)
 0.425 (calculated-P/C, Meylan & Howard 1991)
 0.143 (estimated-bond contribution, Meylan & Howard 1991)

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

1.81 (shake flask, Fujita et al. 1964)
 1.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
 1.92 (exptl., Leo et al. 1971; McCall 1975; Rekker 1977)
 1.92 (HPLC- k' correlation, Carlson et al. 1975)
 1.63 (calculated- π const., Norrington et al. 1975)
 1.61, 1.73 (calculated- π const., calculated- f const., Rekker 1977)
 1.90, 1.92 (shake flask, Hansch & Leo 1979)
 1.74 (HPLC- k' correlation, Könemann et al. 1979)
 1.74 (calculated- f const., Rekker & De Kort 1979)
 1.91 \pm 0.01 (HPLC- k' , Hammers et al. 1982)
 1.99 (HPLC- k' correlated, Hammers et al. 1982)
 1.926 \pm 0.021 (slow-stirring-GC, De Bruijn et al. 1989)
 1.88 (recommended, Sangster 1993)
 1.93 \pm 0.14, 1.55 \pm 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
 1.90 (recommended, Hansch et al. 1995)

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

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

< 2.0 (Kawasaki 1980)
 1.30 (estimated, Canton et al. 1985)
 1.18 (zebrafish, Zok et al. 1991)
 0.301–0.57 (carp, Tsuda et al. 1993)
 1.18; 1.56, 0.73, 0.94 (quoted; calculated values- K_{OW} , Bintein et al. 1993)

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

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

Volatilization: using Henry's law constant, $t_{1/2} \sim 5.6$ d was estimated for a model river of 1-m deep (Lyman et al. 1982; quoted, Howard 1989);
 estimated $t_{1/2} = 64$ d from a representative environmental pond (stagnant) (USEPA 1987; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant of $5.1 \times 10^{-12} \text{ cm}^3/\text{molecule} \cdot \text{s}$ for the reaction with hydroxyl radical in a typical ambient atmosphere at 25°C with $t_{1/2} \sim 2$ d (GEMS 1987; quoted, Howard 1989).

Hydrolysis:

Biodegradation: average biodegradation rate of 25 mg COD $\text{g}^{-1} \text{ h}^{-1}$ for 95.6% removal (Scow 1982).

Biotransformation:

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

$k_1 = 7.10 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.19 \text{ h}^{-1}$ (carp, Tsuda et al. 1993)

Half-Lives in the Environment:

Air: estimated atmospheric $t_{1/2} = 2 \text{ d}$, based on the reaction with sunlight-produced hydroxyl radical (GEMS 1987; quoted, Howard 1989).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 3.6 \text{ h}$ in carp with excretion rate constant $k = 0.19 \text{ h}^{-1}$ (Tsuda et al. 1993).

TABLE 16.1.3.2.1

Reported vapor pressures of 2-chloroaniline 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)					
Kahlbaum 1898		Stull 1947		Piacente et al. 1985		Piacente et al. 1985	
static method		summary of literature data		torsion-weighing effusion		torsion-weighing effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				run 62	average		average
64.4	400	46.3	133.3	14	18	23	36
72.3	666.6	72.3	666.6	20	32	24	41
84.8	1333	84.8	1333	27	45	28	50
92.9	2000	99.2	2666	32	72	30	66
99.2	2666	115.6	5333	34	96	31	62
104.2	3333	125.7	7999	34.5	86	32	83
108.4	4000	139.5	13332	38	117	34	87
112.0	4666	160.0	26664	43	200	35	90
115.2	6333	183.7	53329	34	203	38	112
118.1	6000	208.8	101325	48.5	251	41	167
120.7	6666			52.5	347	43	190
131.4	9999	mp/°C	-	54	362	45	200
139.5	13332			63	505	47	218
160.0	26664					49	269
173.6	39997	Dreisbach & Shrader 1949				51	275
183.7	53329	ebulliometry				51	309
192.0	66661	t/°C	P/Pa			55	343
199.4	79993					56	354
208.8	101325	124.48	7605			57	398
		131.54	10114				
		145.3	16500				
		154.55	42066			overall vapor pressure eq.	
		192.71	67661			eq. 1	P/kPa
		208.84	101325			A	8.63 ± 0.16
						B	3006 ± 56
						ΔH _v /(kJ mol ⁻¹) = 57.5 ± 5	
						at 25°C	

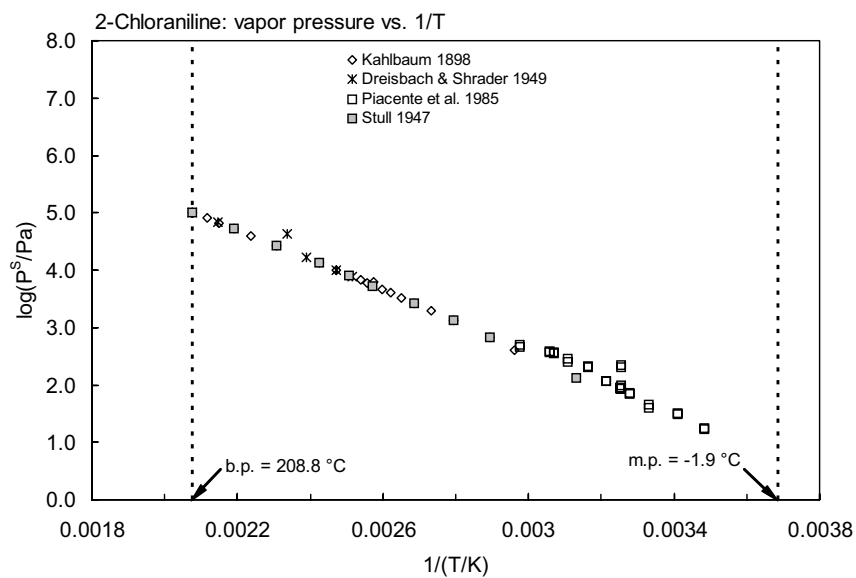
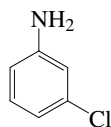


FIGURE 16.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2-chloroaniline.

16.1.3.3 3-Chloroaniline



Common Name: 3-Chloroaniline

Synonym: 1-amino-3-chlorobenzene, *m*-chloroaniline, 3-chlorophenylamine

Chemical Name: 1-amino-3-chlorobenzene, *m*-chloroaniline, 3-chloroaniline

CAS Registry No: 108-42-9

Molecular Formula: $C_6H_4NH_2Cl$

Molecular Weight: 127.572

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

−10.28 (Lide 2003)

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

230.5 (Lide 2003)

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

1.21606 ($20^{\circ}C$, Weast 1982–83)

1.2150 ($22^{\circ}C$, Dean 1985; Budavari 1989)

Molar Volume (cm^3/mol):

105.0 ($22^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

3.52 (Perrin 1972)

3.50 (McLeese et al. 1979)

3.46 (Weast 1982–83)

3.52 (protonated cation + 1, Dean 1985)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

61.04, 46.016 ($25^{\circ}C$, bp, Dreisbach 1955)

60.9 ± 5 ($25^{\circ}C$, Piacente et al. 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.25 (Dreisbach 1955)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

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

5442 ($20^{\circ}C$, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)

5447 (calculated- K_{ow} , Müller & Klein 1992)

4740 (calculated-group contribution method, Kühne et al. 1995)

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

13.14* (extrapolated-regression of tabulated data, measured range 81.7 – $228.5^{\circ}C$, Kahlbaum 1898)

11.94* (extrapolated-regression of tabulated data, temp range 63.5 – $228.5^{\circ}C$, Stull 1947)

11.17 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.23603 - 1857.75/(196.64 + t/^{\circ}C)$; temp range 125 – $350^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 133854.6/(T/K)] + 8.761546$; temp range 63.5 – $228.5^{\circ}C$ (Antoine eq., Weast 1972–73)

11.06 (calculated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.59939 - 2073.75/(215.0 + t/^{\circ}C)$, temp range 15 – $125^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.23603 - 1857.75/(196.64 + t/^{\circ}C)$, temp range 125 – $310^{\circ}C$ (Antoine eq., Dean 1985, 1992)

15.60* (torsion-weighting effusion, Piacente et al. 1985)

$\log (P/\text{kPa}) = (8.86 \pm 0.10) - (3180 \pm 40)/(T/\text{K})$; temp range ~290–345 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)

9.530 (extrapolated from Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.36093 - 1857.75/(-76.51 + T/\text{K})$; temp range 398–573 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 65.6033 - 5.3779 \times 10^3/(T/\text{K}) - 20.518 \cdot \log (T/\text{K}) + 6.7861 \times 10^{-3} \cdot (T/\text{K}) + 2.1167 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 263–751 K (vapor pressure eq., Yaws 1994)

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

0.223 (calculated-P/C)

0.102 (gas stripping-GC, Altschuh et al. 1999)

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

1.88 (shake flask-UV, Fujita et al. 1964)

1.88 (Ichikawa et al. 1969)

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

1.90 (exptl., Leo et al. 1971; Rekker 1977)

1.98 (calculated- π const., Norrington et al. 1975)

1.73, 1.75; 1.61 (calculated-f const., calculated- π const., Rekker 1977)

1.90, 1.88 (shake flask, Hansch & Leo 1979)

1.57 (HPLC- k' correlation, Könemann et al. 1979)

1.89 ± 0.01 (HPLC- k' correlation, Hammers et al. 1982)

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

1.910 ± 0.013 (slow-stirring-GC, De Bruijn et al. 1989)

1.88 (recommended, Sangster 1993)

1.91 ± 0.14 , 1.52 ± 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)

1.88 (recommended, Hansch et al. 1995)

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

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

1.06 (zebrafish, Zok et al. 1991)

-0.097 to 0.342 (average for carp, Tsuda et al. 1993)

1.06; 1.55, 0.70, 0.92 (quoted; calculated values, Bintein et al. 1993)

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

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

Volatilization:

Photolysis: direct aqueous photolysis rate constant $k = 0.393 \pm 0.006 \text{ min}^{-1}$ with a calculated $t_{1/2} = 1.76 \text{ min}$ (Stegeman et al. 1993).

Oxidation:

Hydrolysis: direct photohydrolysis rate constant $k = 0.393 \pm 0.006 \text{ min}^{-1}$ with a calculated $t_{1/2} = 1.76 \text{ min}$ (Stegeman et al. 1993).

Biodegradation: average biodegradation rate of $6.2 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.2% removal (Scow 1982).

Biotransformation: mean bacteria transformation rate constant for all three sites of $(2.2 \pm 1.7) \times 10^{-12} \text{ L} \cdot \text{organism}^{-1} \cdot \text{h}^{-1}$ (Paris & Wolfe 1987; quoted, Steen 1991).

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

$k_1 = 19.1 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.21 \text{ h}^{-1}$ (carp, Tsuda et al. 1993)

Half-Lives in the Environment:

Biota: $t_{1/2} = 3.3 \text{ h}$ in carp with excretion rate $k = 0.21 \text{ h}^{-1}$ (Tsuda et al. 1993).

TABLE 16.1.3.3.1

Reported vapor pressures of 3-chloroaniline 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)					
Kahlbaum 1898		Stull 1947		Piacente et al. 1985			
static method		summary of literature data		torsion-weighing effusion			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				run 63	average	run 64	average
81.7	400	63.5	133.3	19	8	31	19
89.8	666.6	89.8	666.6	29	17	39	41
102	1333	102	1333	36.5	33	42	50
110.4	2000	116.7	2666	43	49	44	52
116.8	2666	133.6	5333	50	89	45	56
122.0	3333	144.1	7999	57.5	145	46	66
126.2	4000	158	13332	65	250	47	70
129.8	4666	179.5	26664	73	376	49	89
133.2	6333	203.5	53329			50	85
136.2	6000	228.5	101325			51	95
138.8	6666					52	105
149.9	9999	mp/°C	–10.4			53	102
158.0	13332					55	126
179.5	26664					57	146
193.2	53329					59	151
203.5	66661					60.5	170
211.9	79993					62	190
228.5	101325					63	204
						65	240
						69	296
				overall vapor pressure eq.			
				eq. 1			
				P/kPa			
				A			
				8.86 ± 0.10			
				B			
				3180 ± 40			
				ΔH _v /(kJ mol ^{–1}) = 60.9 ± 5			
				at 25°C			

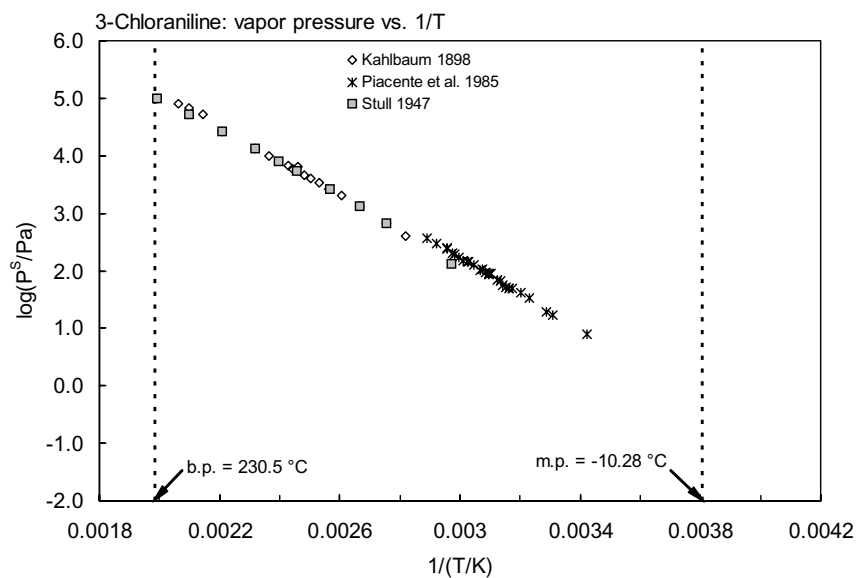
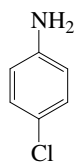


FIGURE 16.1.3.3.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chloroaniline.

16.1.3.4 4-Chloroaniline



Common Name: 4-Chloroaniline

Synonym: 1-amino-4-chlorobenzene, *p*-chloroaniline, 4-chlorophenylamine

Chemical Name: 1-amino-4-chlorobenzene, *p*-chloroaniline, 4-chloroaniline

CAS Registry No: 106-47-8

Molecular Formula: $\text{NH}_2\text{C}_6\text{H}_4\text{Cl}$

Molecular Weight: 127.572

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

70.5 (Lide 2003)

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

232.0 (Weast 1982–83; Verschueren 1983; Howard 1989)

Density (g/cm^3 at 20°C):

1.429 (19°C , Weast 1982–83)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

3.98 (Perrin 1972; Freitag et al. 1984; quoted, Howard 1989)

4.20 (McLeese et al. 1979)

4.15 (Weast 1982–83)

3.99 (protonated + 1, Dean 1985)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

79 ± 5 (25°C , Piacente et al. 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.69 (Tsonopoulos & Prausnitz 1971)

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

57.74 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.358 (mp at 70.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):

3000 (Philpot et al. 1940)

3900 (Kilzer et al. 1979)

2620 (Schmidt-Bleek et al. 1982; Rott et al. 1982)

2487 (calculated-group contribution method, Kühne et al. 1995)

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

1.707* (20°C , Knudsen effusion, measured range 10 – 30°C , Swan & Mack 1925)

15.19* (extrapolated-regression of tabulated data, temp range 59.3 – 230.5°C , Stull 1947)

$\log (P/\text{mmHg}) = [-0.2185 \times 12832.8/(T/\text{K})] + 8.461034$; temp range 59.3 – 230.5°C (Antoine eq., Weast 1972–73)

3.173 (effusion method, DePablo 1976)

3.33 (extrapolated, Verschueren 1977)

2.00, 6.67 (20°C , 30°C , quoted, Verschueren 1983)

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

$\log (P/\text{kPa}) = 3.55438 - 521.556/(47.392 + t/^{\circ}\text{C})$; temp range 90 – 150°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.636* (torsion-weighing effusion, Piacente et al. 1985)

$\log (P/\text{kPa}) = (11.20 \pm 0.20) - (4170 \pm 60)/(T/K)$; temp range ~298–360 K (Antoine eq., combined torsion-weighting effusion, Piacente et al. 1985)

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

$\log (P_s/\text{kPa}) = 13.448 - 4736/(T/K)$, temp range 283–303 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.3489 - 2729/(T/K)$, temp range 363–505 K (Antoine eq.-II, Stephenson & Malanowski 1987)

3.33, 32.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = -15.3259 - 2.8592 \times 10^3/(T/K) + 11.527 \cdot \log (T/K) - 1.8071 \times 10^{-2} \cdot (T/K) + 7.2359 \times 10^{-6} \cdot (T/K)^2$; temp range 343–754 K (vapor pressure eq., Yaws 1994)

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

1.0840 (calculated-P/C, Howard 1989)

0.0395 (calculated-P/C, Meylan & Howard 1991)

0.1430 (estimated-bond contribution, Meylan & Howard 1991)

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

1.84 (Ichikawa et al. 1969)

1.83 (quoted exptl., Leo et al. 1969, 1971; Hansch & Leo 1985)

1.83 (HPLC- k' correlation; Carlson et al. 1975)

1.83 (shake flask, Hansch & Leo 1979)

1.57 (HPLC- k' correlation, Könemann et al. 1979)

1.83, 20.2 (HPLC- k' correlation, Hammers et al. 1982)

1.64 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)

1.88 ± 0.02 (HPLC-RV correlation-ALPM; Garst & Wilson 1984)

2.78 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)

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

1.83 (RP-HPLC- k' correlation, Minick et al. 1988)

1.88 ± 0.014 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)

1.83 (shake flask, Leahy et al. 1989)

1.80, 1.82 (shake flask, HPLC-RT correlation, Wang et al. 1989)

2.01 (centrifugal partition chromatography CPC-RV correlation, El Tayar et al. 1991)

1.83 (recommended, Sangster 1993)

1.83 (pH 7.4, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

< 1.30 (golden orfe for 3-d exposure, Körte et al. 1978)

3.08 (green algae for 24-h exposure of dry wt. basis, Körte et al. 1978)

2.42 (green algae for 24-h exposure of wet wt. basis, Körte et al. 1978)

< 1.0, 2.41, 3.11 (golden orfe, algae, activated sludge, Freitag et al. 1982)

2.42 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)

2.06 (alga *Chlorella fusca*, calculated- K_{ow} , Geyer et al. 1984)

1.11, 2.42, 2.45 (golden ide, algae, activated sludge, Freitag et al. 1985)

0.91 (zebrafish, Zok et al. 1991)

−0.097–0.23 (carp, Tsuda et al. 1993)

0.91; 1.52, 0.63, 0.88 (quoted; calculated values, Bintein et al. 1993)

2.58 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)

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

2.36–2.67 (five Belgium soils, Van Bladel & Moreale 1977)

1.98–3.18 (five German soils, Rott et al. 1982)

3.74 (colloidal org. matter in ground water, Means 1983)

1.86 (calculated-MCI χ , Sabljic 1987)

2.08 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)

1.96, 1.86 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)

- 1.61 (calculated- K_{OW} , Kollig 1993)
 1.96 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.28; 1.86 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.086, 2.21, 2.48, 2.374, 2.973 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 2.801, 2.326, 2.145, 2.420 (second generation Eurosoils ES-1, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

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

Volatilization: estimated $t_{1/2} = 6.4$ h from using Henry's law constant for a model river of 1-m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} = 3$ d in an experimental pond with spiked 4-chloroaniline (Schauerte 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:

$k_{OH} = (8.3 \pm 0.42) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{OH}(\text{obs.}) = 83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH}(\text{calc.}) = 34.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. in air (Atkinson 1985; Atkinson et al. 1985)

$k_{OH}(\text{calc.}) = 54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH}(\text{obs.}) = 83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{OH} = (83 \text{ to } \sim 44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295–296 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

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

$k_1 = 42.9 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.16 \text{ h}^{-1}$ (carp, Tsuda et al. 1993)

$k_1 = 17.74 \text{ h}$, $k_2 = 0.0465 \text{ h}$ (algae *Chlorella fusca*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 4.6$ h, based on estimated reaction rate with photochemically produced hydroxyl radical of 5×10^5 radicals/cm³ in atmosphere (Wahner & Zetzsch 1983; quoted, Howard 1989).

Surface water: estimated $t_{1/2} = 0.3$ –3.0 d in river waters in case of a first order reduction process (Zoeteman et al. 1980);

72.1 mg/L total organic carbon (TOC) degraded to 92% TOC after 5 h illumination with a 250 watt tungsten lamp by photo-Fenton reaction in distilled water (Ruppert et al. 1993).

Groundwater: estimated $t_{1/2} = 30$ –300 d in Rhine River (Zoeteman et al. 1980).

Sediment:

Soil:

Biota: $t_{1/2} = 4.3$ h in carp with excretion rate $k = 0.16 \text{ h}^{-1}$ (Tsuda et al. 1993).

TABLE 16.1.3.4.1

Reported vapor pressures of 4-chloroaniline 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)					
Swan & Mack 1925		Stull 1947		Piacente et al. 1985			
Knudsen effusion		summary of literature data		torsion-weighing effusion			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				Run 58	average	Run 66	average
10	0.513	59.3	133.3	26	3.0	52	56
20	1.707	87.9	666.6	31	6.0	56.5	75
30	6.493	102.1	1333	34	8.0	61	128
		117.8	2666	39	13	63	136
		135.0	5333	40	17	65	152
		145.8	7999	43	20	68	238
eq. 4	P/mmHg	159.9	13332	48	31	71	275
A	415.007	182.3	26664	49.5	35	72	316
B	22322	206.6	53329	53	48		
C	138.475	230.5	101325	59	87		
				60.5	100	overall vapor pressure eq.	
ΔH _v /(kJ mol ⁻¹) = 90.37		mp/°C	70.5	63.5	127	eq. 1	P/kPa
at 20°C				67	170	A	11.20 ± 0.20
				69.5	224	B	4170 ± 60
				82.5	549		
				88.5	832	ΔH _v /(kJ mol ⁻¹) = 70.9 ± 5	
						at 25°C	

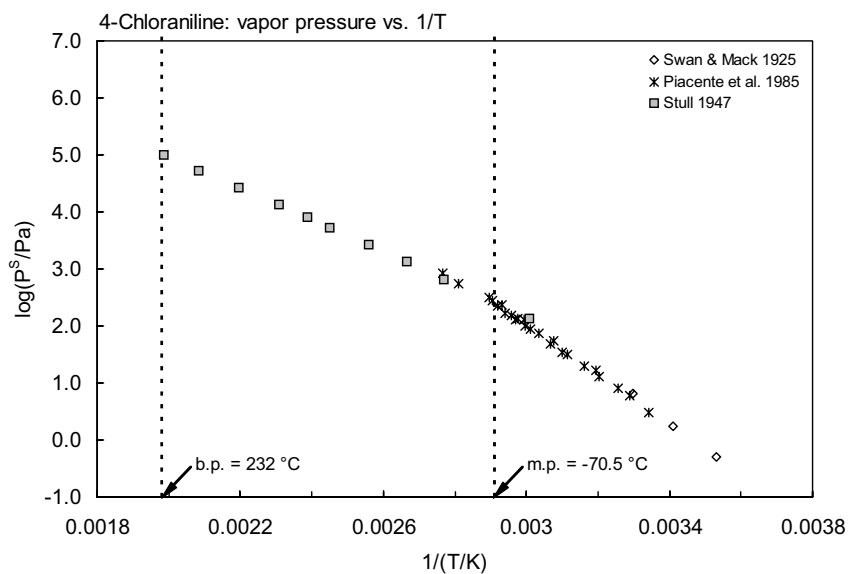
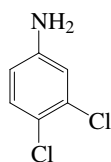


FIGURE 16.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for 4-chloroaniline.

16.1.3.5 3,4-Dichloroaniline



Common Name: 3,4-Dichloroaniline

Synonym:

Chemical Name: 3,4-dichloroaniline

CAS Registry No: 95-76-1

Molecular Formula: $C_6H_5Cl_2N$, $C_6H_3NH_2Cl_2$

Molecular Weight: 162.017

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

72.0 (Weast 1982–83; Lide 2003)

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

272.0 (Weast 1982–83; Lide 2003)

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

Molar Volume (cm^3/mol):

111.7 (calculated-density, Jaworska & Schultz 1993)

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

Dissociation Constant, pK_a :

2.968, 3.0 (Perrin 1972)

2.00 (estimated, Wolff & Crossland 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.346 (mp at $72^{\circ}C$)

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

92.03 ($20^{\circ}C$, Wolff & Crossland 1985)

93.2; 740 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.30 ($20^{\circ}C$, Wolff & Crossland 1985)

2.27 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.6189 - 3060.03/(T/K)$; temp range 420–545 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -15.2685 - 3.3857 \times 10^3/(T/K) + 11.926 \cdot \log(T/K) - 1.9227 \times 10^{-2} \cdot (T/K) + 7.4179 \times 10^{-6} \cdot (T/K)^2$;
temp range 345–800 K (vapor pressure eq., Yaws 1994)

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

2.289 (calculated-P/C)

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

2.69 (unpublished result, Leo et al. 1971, Hansch & Leo 1979)

2.12 (HPLC- k' correlation, Könemann et al. 1979)

2.78 ($20^{\circ}C$, shake flask-UV, Briggs 1981)

2.69, 2.67 (HPLC- k' correlation, Hammers et al. 1982)

2.62 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)

2.30 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)

2.14, 2.63 (HPLC- k' correlation, Eadsforth 1986)

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

2.68 (recommended, Sangster 1993)

2.69 (recommended, Hansch et al. 1995)

2.69 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

1.48 (zebrafish, Zok et al. 1991)

1.48; 2.02, 1.88, 1.75 (fish: quoted; calculated values- K_{OW} , Bintein et al. 1993)

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

2.29 (20°C, sorption isotherm-GC, converted from K_{OM} multiplied by 1.724, Briggs 1981)

1.40 (calculated- K_{OW} , wet sediment, Wolff & Crossland 1985)

2.29 (Sabljic 1987)

2.05 (soil, quoted, Sabljic 1987)

2.29, 2.08 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

2.29 (calculated-MCI $^1\chi$, Sabljic et al. 1995)

2.26, 2.39 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

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

Volatilization: first order rate constant $k(\text{calc}) = 5.0 \times 10^{-3} \text{ d}^{-1}$ (Wolff & Crossland 1985).

Photolysis: phototransformation rate constant $k = 0.12$ to 0.20 d^{-1} (Wolff & Crossland 1985).

Oxidation:

Hydrolysis: not expected to occur (Wolff & Crossland 1985).

Biodegradation:

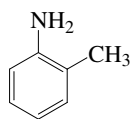
Biotransformation:

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

$k_1 = 78.5 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

Half-Lives in the Environment:

Surface water: overall rate of loss predicted from outdoor ponds was calculated based on direct phototransformation, and indirect phototransformation $k = 0.13$ to 0.22 d^{-1} corresponding to $t_{1/2} = 3.2$ to 5.3 d ; the observed rate of loss varied from 0.11 to 0.17 d^{-1} corresponding to $t_{1/2} = 4.1 - 6.3 \text{ d}$ (Wolff & Crossland 1985).

16.1.3.6 *o*-Toluidine (2-Methylbenzeneamine)

Common Name: *o*-Toluidine

Synonym: 2-aminotoluene, *o*-aminotoluene, 2-methylaniline, 2-methylbenzeneamine

Chemical Name: 2-aminotoluene, *o*-methylaniline, *o*-toluidine

CAS Registry No: 95-53-4

Molecular Formula: C_7H_9N , $C_6H_4(CH_3)NH_2$

Molecular Weight: 107.153

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

−14.41 (Lide 2003)

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

200.3 (Lide 2003)

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

0.9984, 0.99430 (10, $25^{\circ}C$, Dreisbach 1955, Riddick et al. 1986)

0.9984 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

107.3 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.40, 4.447, 4.46 (Perrin 1972)

4.44 (Weast 1982–83)

4.45 (protonated cation + 1, Dean 1985)

4.43 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.739, 44.597 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.535 (Dreisbach 1955)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

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

16330 ($20^{\circ}C$, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)

15000 (quoted, Verschueren 1983)

16300 (calculated- K_{OW} , Müller & Klein 1992)

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

133.3* ($48.2^{\circ}C$, static method, measured range 48.2 – $199.7^{\circ}C$, Kahlbaum 1898)

42.72* (extrapolated-regression of tabulated data, temp range 44 – $199.7^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.60681 - 2033.6/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

7605* ($118.46^{\circ}C$, ebulliometry, measured range 118.46 – $200.30^{\circ}C$, Dreisbach & Shrader 1949)

42.26 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.28896 - 1768.7/(201.0 + t/^{\circ}C)$; temp range 103 – $320^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [-0.2185 \times 12663.4/(T/K)] + 8.440371$; temp range 41 – $203.3^{\circ}C$ (Antoine eq., Weast 1972–73)

42.93 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 473.369/(T/K)] \times 10^{[0.907135 - 6.44774 \times 10^{-4} \cdot (T/K) + 4.94693 \times 10^{-7} \cdot (T/K)^2]}$; temp range: 300.0 – $710.0\ K$ (Cox eq., Chao et al. 1983)

13.33, 40.0 ($20^{\circ}C$, $30^{\circ}C$, quoted, Verschueren 1983)

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

$\log (P/\text{kPa}) = 6.20039 - 1623.158/(186.641 + t/^{\circ}\text{C})$; temp range 118.5–200.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

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

$\log (P/\text{mmHg}) = 6.73171 - 2033.6/(230.0 + t/^{\circ}\text{C})$; temp range: not specified (Antoine eq., Riddick et al. 1986)

34.18 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.08203 - 1627.72/(187.13 + t/^{\circ}\text{C})$; temp range 118–200°C (Antoine eq., Dean 1985, 1992)

36.46 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.26948 - 1672.87/(-81.47 + T/\text{K})$; temp range 391–474 K, (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 96.5685 - 6.2643 \times 10^3/(T/\text{K}) - 32.265 \cdot \log (T/\text{K}) + 1.2361 \times 10^{-2} \cdot (T/\text{K}) + 6.2915 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 249–694 K (vapor pressure eq., Yaws 1994)

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

0.095 (calculated-P/C)

0.201 (gas stripping-GC, Altschuh et al. 1999)

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

1.29 (shake flask-UV, Leo et al. 1971)

1.43 (HPLC- k' correlation, Carlson et al. 1975)

1.63 (RP-HPLC-RT correlation, Veith et al. 1979a)

1.42 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)

1.34 (HPLC-RT correlation, average, Ge et al. 1987)

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

1.32 (recommended, Sangster 1989)

1.44, 1.57 (shake flask, HP:C-RT correlation, Wang et al. 1989)

1.43 (recommended, Sangster 1993)

1.32 (recommended, Hansch et al. 1995)

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

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

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

1.24 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radicals at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 62.4 - 3480 \text{ h}$ in water, based on estimated rate constants for reactions of representative aromatic amines with OH and RO_2 radicals (Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.394 - 3.94 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: decomposition by a soil microflora in $> 64 \text{ d}$ (Alexander & Lustigman 1966; quoted, Verschueren 1983);

aqueous aerobic $t_{1/2} = 24 - 168 \text{ h}$, based on aqueous aerobic screening test data (Baird et al. 1977; Sasaki 1978; quoted, Howard et al. 1991);

average biodegradation $k = 15.1 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.7% removal (Scow 1982);

aqueous anaerobic $t_{1/2} = 96 - 672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.394 - 3.94$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} = 1.0$ d for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

photooxidation $t_{1/2} = 62.4 - 3480$ h, based on estimated rate constants for reactions of representative aromatic amines with OH and RO₂ radicals (Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 48 - 336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24 - 168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.3.6.1

Reported vapor pressures of *o*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949	
static method-manometer*		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
48.2	133.3	44.0	133.3	118.46	7605
55.3	266.6	69.3	666.6	122.22	8851
61.4	400.0	81.4	1333	125.99	10106
65.7	533.3	95.1	2666	139.0	16500
69.3	666.6	110.0	5333	168.06	42066
81.4	1333.2	119.8	7999	184.80	67661
94.9	2666.4	133.0	13332	200.30	101325
103.6	3999.7	153.0	26664		
110.0	5332.9	170.2	53329		
115.1	6666.1	199.7	101325		
125.4	9999.2				
133.0	13332	mp/°C	-16.3		
154.0	26664				
166.2	39997				
176.2	53329				
183.9	66661				
190.5	79993				
196.2	93326				
199.7	101325				

*complete list see [ref.](#)

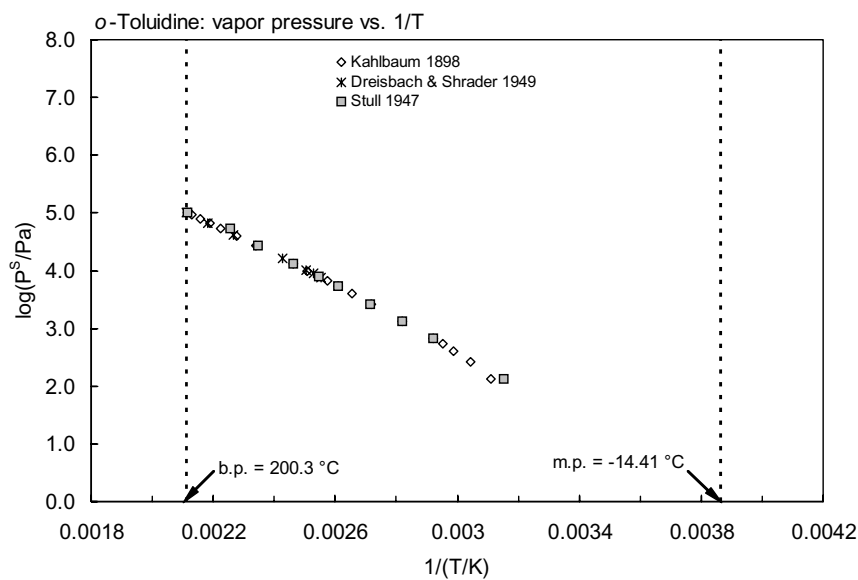
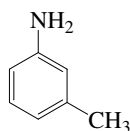


FIGURE 16.1.3.6.1 Logarithm of vapor pressure versus reciprocal temperature for *o*-toluidine.

16.1.3.7 *m*-Toluidine (3-Methylbenzeneamine)

Common Name: *m*-Toluidine

Synonym: 3-aminotoluene, 3-methylbenzeneamine, 3-methylaniline

Chemical Name: 3-aminotoluene, *m*-amino-methylbenzene, *m*-methylaniline, *m*-toluidine

CAS Registry No: 108-44-1

Molecular Formula: $C_6H_4(CH_3)NH_2$

Molecular Weight: 107.153

Melting Point (°C):

−31.3 (Lide 2003)

Boiling Point (°C):

203.3 (Stull 1947; Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):

0.9889 (Dreisbach 1955; Weast 1982–83)

Molar Volume (cm³/mol):

108.4 (20°C, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

4.66, 4.712, 4.72 (Perrin 1972)

4.73 (Weast 1982–83)

4.71 (protonated cation + 1, Dean 1985)

4.70 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

57.283, 44.848 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.08 (Dreisbach 1955)

3.891 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

15031 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)

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

133.3* (49.8°C, static method, measured range 49.8–203.3°C, Kahlbaum 1898)

49.54* (extrapolated-regression of tabulated data, temp range 41–203.3°C, Stull 1947)

$\log(P/\text{mmHg}) = 7.616512 - 2052.0/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

7605* (121.77°C, ebulliometry, measured range 121.77–203.34°C, Dreisbach & Shrader 1949)

36.64 (calculated by formula, Dreisbach 1955)

$\log(P/\text{mmHg}) = 7.27435 - 1772.06/(200.0 + t/^\circ\text{C})$; temp range 105–320°C (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/\text{mmHg}) = [-0.2185 \times 12104.1/(T/K)] + 8.440371$; temp range 41–203°C (Antoine eq., Weast 1972–73)

33.49 (calculated-Cox eq., Chao et al. 1983)

$\log(P/\text{atm}) = [1 - 476.329/(T/K)] \times 10^4 \{0.923479 - 6.91988 \times 10^{-4} \cdot (T/K) + 5.41104 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 280.0–705.0 K (Cox eq., Chao et al. 1983)

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

$\log(P/\text{kPa}) = 6.21454 - 1620.608/(203.346 + t/^\circ\text{C})$; temp range 121.9–203.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

25.66 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.09367 - 1631.43/(183.91 + t/^{\circ}\text{C})$; temp range 122–203°C (Antoine eq., Dean 1985, 1992)
 36.0 (quoted lit., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 17.6292 - 3200.9/(T/\text{K}) - 3.323 \cdot \log (T/\text{K})$, temp range not specified (vapor pressure eq., Riddick et al. 1986)
 26.86 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.27299 - 1669.26/(-85.339 + T/\text{K})$; temp range 394–447 K (Antoine eq., Stephenson & Malanowski 1987)
 25.50 (calculated-Cox eq., Chao et al. 1990)
 $\log (P/\text{mmHg}) = 7.0317 - 3.2034 \times 10^3/(T/\text{K}) + 2.3006 \cdot \log (T/\text{K}) - 9.7791 \times 10^{-3} \cdot (T/\text{K}) + 4.6824 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 243–709 K (vapor pressure eq., Yaws 1994)

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

0.257 (calculated-P/C)
 0.169 (gas stripping-GC, Altschuh et al. 1999)

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

1.40 (shake flask-UV, Fujita et al. 1964)
 1.43 (HPLC- k' correlation, Carlson et al. 1975)
 1.42 (20°C, shake flask-UV, Briggs 1981)
 1.43 (shake flask, Log P Database, Hansch & Leo 1987)
 1.40 (recommended, Sangster 1989)
 1.49, 1.37 (shake flask, HPLC-RT correlation, Wang et al. 1989)
 1.40 (recommended, Hansch et al. 1995)

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

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

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

1.41 (soil, quoted obs. as $\log K_{\text{OM}}$, Sabljic 1987)
 1.65 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982).

Biodegradation: decomposition by a soil microflora in 8 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average biodegradation rate of $30.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.7% removal (Scow 1982).

Biotransformation:

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

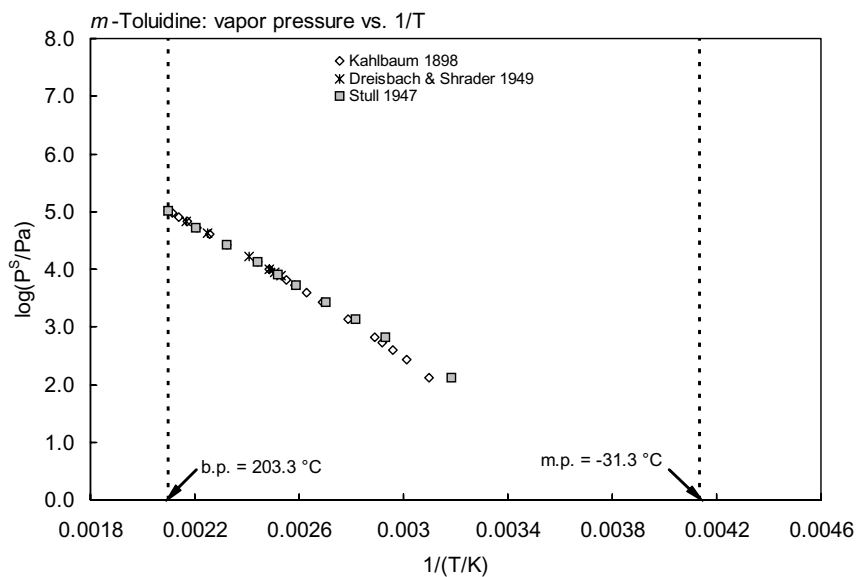
Half-Lives in the Environment:

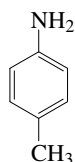
Surface water: estimated $t_{1/2} = 1.0 \text{ d}$ for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.3.7.1

Reported vapor pressures of *m*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949	
static method-manometer*		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
49.8	133.3	41.0	133.3	121.77	7605
58.9	266.6	68.0	666.6	125.57	8851
64.8	400.0	82.0	1333	129.03	10114
69.3	533.3	96.7	2666	142.27	16500
72.8	666.6	113.5	5333	171.18	42066
85.3	1333.2	123.8	7999	187.87	67661
98.5	2666.4	136.7	13332	203.34	101325
107.1	3999.7	157.6	26664		
113.6	5332.9	180.6	53329		
118.7	6666.1	203.3	101325		
129.0	9999.2				
136.6	13332	mp/°C	−31.5		
157.6	26664				
169.8	39997				
179.8	53329				
187.5	66661				
194.0	79993				
199.8	93326				
203.3	101325				

*complete list see [ref.](#)FIGURE 16.1.3.7.1 Logarithm of vapor pressure versus reciprocal temperature for *m*-toluidine.

16.1.3.8 *p*-Toluidine (4-Methylbenzeneamine)

Common Name: *p*-Toluidine

Synonym: 4-aminotoluene, 4-methylaniline, 4-methylbenzenamine

Chemical Name: 4-aminotoluene, *p*-amino-methylbenzene, *p*-methylaniline, *p*-toluidine

CAS Registry No: 106-49-0

Molecular Formula: $C_6H_4(CH_3)NH_2$

Molecular Weight: 107.153

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

43.6 (Lide 2003)

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

200.4 (Lide 2003)

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

0.9619 ($20^{\circ}C$, Weast 1982–83)

1.043 (Verschueren 1983)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

5.02, 5.08, 5.084 (Perrin 1972)

5.08 (Weast 1982–83; Sangster 1989)

5.08 (protonated cation + 1, Dean 1985)

5.17 (shake flask-HPLC/UV, Johnson & Westall 1990)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.195, 44.271 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.32 (Tsonopoulos & Prausnitz 1971)

18.91 (Riddick et al. 1986)

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

54.81 (Tsonopoulos & Prausnitz 1971)

57.61 (observed, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.657 (mp at $43.6^{\circ}C$)

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

65400 (20 – $25^{\circ}C$, shake flask-gravimetric, Dehn 1917)

8965 (Seidell 1941, 1952)

7400 ($21^{\circ}C$, Verschueren 1983)

6643, 5370 ($20^{\circ}C$, shake flask-UV, calculated, Hashimoto et al. 1984)

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

133.3* ($46.9^{\circ}C$, static method, measured range 46.9 – $200.4^{\circ}C$, Kahlbaum 1898)

$\log(P/mmHg) = -2597/(T/K) + 8.366$ (isoteniscope method, temp range not specified, Kobe et al. 1941)

46.27* (extrapolated-regression of tabulated data, temp range 42 – $200.4^{\circ}C$, Stull 1947)

44.70 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.25173 - 1755.0/(201.0 + t/^{\circ}C)$; temp range 103 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [-0.2185 \times 12428.6/(T/K)] + 8.748585$; temp range 42 – $200.4^{\circ}C$ (Antoine eq., Weast 1972–73)

38.13 (calculated-Cox eq., Chao et al. 1983)

- $\log (P/\text{mmHg}) = [1 - 473.445/(T/K)] \times 10^{\{0.915691 - 6.57014 \times 10^{-4} \cdot (T/K) + 5.11261 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 290.0–700.0 K (Cox eq., Chao et al. 1983)
 40.17 (calculated-Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.26022 - 1758.55/(201.0 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Dean 1985, 1992)
 45.0 (quoted lit., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 18.2818 - 3269.3/(T/K) - 3.877 \cdot \log (T/K)$; temp range not specified (vapor pressure eq., Riddick et al. 1986)
 27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.17451 - 1585.0/(-93.44 + T/K)$; temp range 393–474 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = -13.9927 - 2.5795 \times 10^3/(T/K) - 10.823 \cdot \log (T/K) - 1.7705 \times 10^{-2} \cdot (T/K) + 7.6741 \times 10^{-6} \cdot (T/K)^2$; temp range 317–693 K (vapor pressure eq., Yaws 1994)

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

- 0.656 (calculated-P/C)
 0.0768 (gas stripping-GC, Altschuh et al. 1999)

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

- 1.39 (shake flask-UV, Fujita et al. 1964)
 1.41 (HPLC- k' correlation, Carlson et al. 1975)
 1.56 (shake flask-UV, Ezumi & Kubota 1980)
 1.40 (20°C , shake flask-UV, Briggs 1981)
 1.44 ± 0.03 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
 1.42 (HPLC- k' correlation, Haky & Young 1984)
 1.39 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
 1.41 (HPLC-RT correlation, average, Ge et al. 1987)
 1.39 (shake flask, Leahy et al. 1989)
 1.39 (recommended, Sangster 1989, 1993)
 1.38, 1.39 (shake flask, HPLC-RT correlation, Wang et al. 1989)
 1.40 (shake flask-HPLC/UV, Johnson & Westall 1990)
 1.40 (shake flask-UV, Roberts et al. 1991)
 1.40 (32°C , shake flask-UV, pH 7, Takahashi et al. 1993)
 1.39 (recommended, Hansch et al. 1995)

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

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

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

- 2.51, 2.70, 2.71 (Morocco soil, Oakville soil, Milford soil, Graveel et al. 1986)
 1.66 (soil, quoted obs. as $\log K_{OM}$, Sabljic 1987)
 2.74, 2.22, 2.20 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
 1.24 (calculated- K_{OW} , Kollig 1993)
 1.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.21; 1.86 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.28, 2.01, 2.30, 2.084 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 2.138, 2.133, 2.212, 2.041 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask-batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

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

- Volatilization:
 Photolysis:
 Hydrolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982).

Biodegradation: decomposition by a microflora in 4 d (Alexander & Lustigman 1966; quoted, Verschueren 1983); average biodegradation rate of $20 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.7% removal (Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 1.0 \text{ d}$ for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.3.8.1

Reported vapor pressures of *p*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947	
static method-manometer*		summary of literature data	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
46.9	133.3	42.0	133.3
55.9	266.6	68.2	666.6
62.0	400.0	81.8	1333
66.4	533.3	95.8	2666
70.1	666.6	111.5	5333
82.2	1333.2	121.5	7999
95.6	2666.4	133.7	13332
104.3	3999.7	154.0	26664
110.7	5332.9	176.9	53329
115.8	6666.1	200.4	101325
126.1	9999.2		
133.7	13332	mp/ $^\circ\text{C}$	44.5
154.7	26664		
166.9	39997		
176.9	53329		
184.6	66661		
191.1	79993		
196.9	93326		
200.4	101325		

*complete list see [ref.](#)

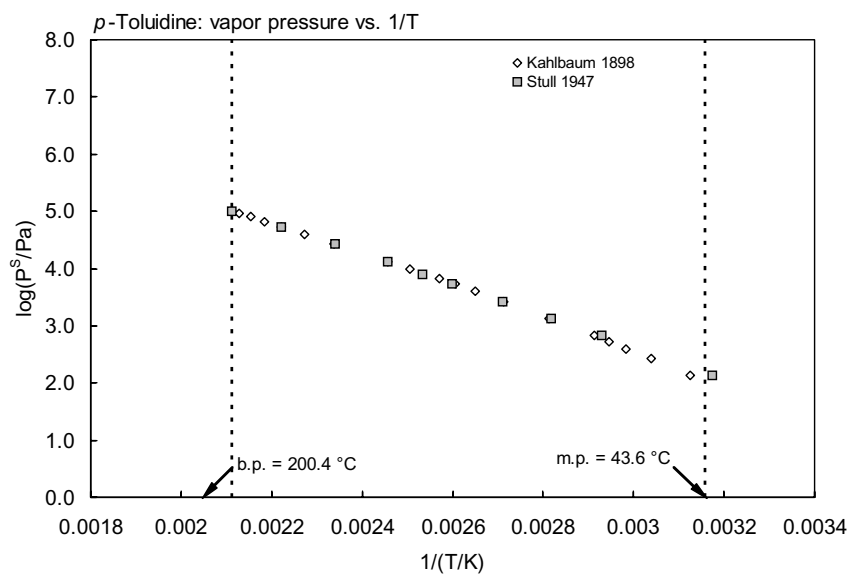
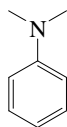


FIGURE 16.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-toluidine.

16.1.3.9 N,N'-Dimethylaniline



Common Name: N,N'-Dimethylaniline

Synonym: N,N'-dimethylbenzenamine

Chemical Name: N,N'-dimethylaniline

CAS Registry No: 121-69-7

Molecular Formula: $C_8H_{11}N$, $C_6H_5N(CH_3)_2$

Molecular Weight: 121.180

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

2.42 (Lide 2003)

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

194.0 (Weast 1982–83)

194.15 (Lide 2003)

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

0.9557 (Weast 1982–83)

Molar Volume (cm^3/mol):

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

Dissociation Constant pK:

5.15 (pK_{BH}^{+} , Riddick et al. 1986)

5.10 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.42 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

41.46 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

1105 (shake flask-GC, Chiou et al. 1982)

1540, 1680 (20, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90^{\circ}C$, Stephenson 1993c)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

106.3 (extrapolated-regression of tabulated data, temp range 20.0 – $193.1^{\circ}C$, Stull 1947)

133.3 ($29.5^{\circ}C$, Stull 1947)

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

$\log(P/atm) = [-0.2185 \times 11320.4/(T/K)] + 8.197379$; temp range: 29.5 – $193^{\circ}C$, (Antoine eq., Weast 1972–73)

68.95 (calculated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 466.445/(T/K)] \times 10^4 \{0.909397 - 7.07673 \times 10^{-4} \pm (T/K) + 5.69581 \times 10^{-7} \pm (T/K)^2\}$; temp range 275.0 – $685.0 K$ (Cox eq., Chao et al. 1983)

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

$\log(P/kPa) = 6.5031 - 1865.084/(211.171 + t/^{\circ}C)$; temp range 71.02 – $196.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

83.91 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.91048 - 946.35/(246.68 + t/^{\circ}C)$; temp range -87 to $7^{\circ}C$ (Antoine eq., Dean 1985, 1992)

670.0 (quoted from Stull 1947, Riddick et al. 1986)

107.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.07329 - 2301.63/(-12.001 + T/K)$; temp range 302 – $467 K$ (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.55663 - 1864.075/(-55.854 + T/K)$; temp range 363 – $418 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 2-.177 - 3.1095 \times 10^3/(T/K) - 4.0127 \cdot \log (T/K) + 5.8538 \times 10^{-10} \cdot (T/K) + 3.5387 \times 10^{-7} \cdot (T/K)^2;$$

temp range 276–687 K (vapor pressure eq., Yaws 1994)

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

11.73 (calculated-P/C)

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

2.31 (shake flask-UV, Fujita et al. 1964)
 2.62 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
 1.66 (shake flask-UV, Leo et al. 1971)
 2.29 (shake flask-UV, Yaguzhinskii et al. 1973)
 2.30 (shake flask at pH 7, Unger et al. 1978)
 2.43 (HPLC-RT correlation, Miyake et al. 1986)
 2.28 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
 2.32 (CPC correlation, El Tayar et al. 1991)
 2.31 (recommended, Sangster 1993)
 2.31 (recommended, Hansch et al. 1995)
 2.05 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

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

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

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

1.99; 2.53; 2.06 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
 2.26, 1.89 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 2.26 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis:

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

$k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}}^*(\text{exptl}) = (1.48 \pm 0.11) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, measured range 278–464 K; $k_{\text{O}_3} = (9.1 \pm 1.0) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}} = 1.5 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere; $k_{\text{O}_3} = 9.1 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of 1.8 d in clean troposphere and 14 h in moderately polluted atmosphere at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 4.66 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs}) = 1.48 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = 1.78 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aqueous screening test data and anaerobic $t_{1/2} = 2880\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp.; atmospheric lifetimes of 1.8 d in clean

troposphere and 14 h in moderately polluted atmosphere, based on the gas-phase reaction with O_3 in air at room temp. (Atkinson et al. 1987);

$t_{1/2} = 2.7\text{--}21$ h, based on photooxidation half-life in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} = 2.3$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 19.3\text{--}1925$ h, based on reaction with singlet oxygen in aqueous solution (Howard et al. 1991)

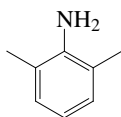
Groundwater: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

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

Biota:

16.1.3.10 2,6-Xylidine (2,6-Dimethylbenzeneamine)



Common Name: 2,6-Xylidine

Synonym: 2,6-dimethylaniline, 2,6-dimethylbenzeneamine

Chemical Name: 2,6-dimethylaniline

CAS Registry No: 87-62-7

Molecular Formula: $C_8H_{11}N$, 2,6- $(CH_3)_2C_6H_3NH_2$

Molecular Weight: 121.180

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

11.20 (Weast 1982–83; Riddick et al. 1986; Lide 2003)

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

214.0 (at 739 mm Hg, Weast 1982–83; Verschueren 1983)

215 (Lide 2003)

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

0.9842 (Weast 1982–83; Riddick et al. 1986)

Molar Volume (cm^3/mol):

123.1 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant pK :

3.95 (pK_{BH}^{+} , Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

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

slightly soluble (Dean 1985; Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

43.03 (extrapolated-regression of tabulated data, temp range 44 – $217.9^{\circ}C$, Stull 1947)

$\log(P/atm) = [1 - 490.795/(T/K)] \times 10^{0.926009 - 6.89676 \times 10^{-4} \cdot (T/K) + 5.31053 \times 10^{-7} \cdot (T/K)^2}$; temp range: 285.0 – 720.0 K (Cox eq., Chao et al. 1983)

17.33 (Howard et al. 1986)

670.0 (quoted from Stull 1947, Riddick et al. 1986)

35.99 (calculated-solvatochromic parameters, Banerjee et al. 1990)

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

17.28 (calculated-P/C from selected value)

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

1.96 (calculated, Verschueren 1983)

1.91 (calculated-CLOGP, Jäckel & Klein 1991)

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982); $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);photooxidation $t_{1/2} = 0.33\text{--}3.3 \text{ h}$ in air, based on estimated reaction rate constant with OH radical (Atkinson 1987; selected, Howard et al. 1991) and photooxidation $t_{1/2} = 62.4\text{--}3480 \text{ h}$ in water, based on reaction rate constants of amine class with $\text{RO}_2\cdot$ and OH radicals in water (Güesten et al. 1981; Mill & Mabey 1985; selected, Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672\text{--}4320 \text{ h}$, based on a biological screening study (Baird et al. 1977; selected Howard et al. 1991) and a soil degradation study (Bollag et al. 1978; selected, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2} = 2688\text{--}17280 \text{ h}$, based on estimated aqueous biodegradation half-lives (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

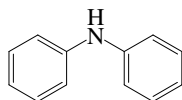
Air: $t_{1/2} = 0.33\text{--}3.3 \text{ h}$, based on estimated photooxidation half-lives in air from estimated reaction rate constant with OH radical in air (Atkinson 1987; selected, Howard et al. 1991).Surface water: estimated $t_{1/2} = 2.0 \text{ d}$ for dimethylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980) $t_{1/2} = 62.4\text{--}3480 \text{ h}$, based on photooxidation half-life in water (Howard et al. 1991).Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 72\text{--}7584 \text{ h}$, based on soil persistence and soil biodegradation studies (Bollag et al. 1978; Medvedev & Davidov 1981; selected, Howard et al. 1991).

Biota:

16.1.3.11 Diphenylamine



Common Name: Diphenylamine

Synonym: N-diphenylamine, N-phenyl aniline, DPA

Chemical Name: N-diphenylamine, diphenylamine

CAS Registry No: 122-39-4

Molecular Formula: $C_{12}H_{11}N$, $C_6H_5NHC_6H_5$

Molecular Weight: 169.222

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

53.2 (Lide 2003)

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

302.0 (Stull 1947; Weast 1982–83; Verschueren 1983; Dean 1985; Lide 2003)

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

1.160 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

145.9 ($20^{\circ}C$ calculated-density)

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

Dissociation Constant, pK_a :

0.89 (Perrin 1972)

0.90 (protonated cation + 1, Dean 1985)

0.78 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.53 (Tsonopoulos & Prausnitz 1971)

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

53.56 (Tsonopoulos & Prausnitz 1971)

54.81; 56.5 (exptl., calculated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.529 (mp at $53.2^{\circ}C$))

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

150 (20 – $25^{\circ}C$, shake flask-gravimetric method, Dehn 1917)

308 (Briggs 1981)

48 ($20^{\circ}C$, shake flask and membrane filter-fluorophotometric, Hashimoto et al. 1982)

52, 54 ($20^{\circ}C$, shake flask and glass fiber filters-fluorophotometric, Hashimoto et al. 1982)

300 (Verschueren 1983)

53 ($20^{\circ}C$, Yalkowsky et al. 1987)

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

0.5682* (extrapolated-regression of tabulated data, temp range 108.3 – $302^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 14920.3/(T/K)] + 8.564067$; temp range 108.3 – $302^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = [1 - 575.114/(T/K)] \times 10^4 \{0.936992 - 6.17195 \times 10^{-4} \cdot (T/K) + 4.32696 \times 10^{-7} \cdot (T/K)^2\}$; temp range 335.0 – $670.0\ K$ (Cox eq., Chao et al. 1983)

0.0612 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 12.704 - 5043.9/(T/K)$; temp range 298 – $323\ K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.15045 - 2778.28/(-35.102 + T/K)$; temp range 381 – $575\ K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.5746 - 2430.7/(-41.15 + T/K)$; temp range 573 – $673\ K$ (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 9.7736 - 3.9008 \times 10^3/(T/K) + 0.91207 \cdot \log(T/K) - 5.898 \times 10^{-3} \cdot (T/K) + 2.3012 \times 10^{-6} \cdot (T/K)^2$; temp range 326 – $817\ K$ (vapor pressure eq., Yaws 1994)

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

- 0.285 (calculated-P/C, Meylan & Howard 1991)
- 0.106 (estimated-bond contribution, Meylan & Howard 1991)
- 0.035 (calculated-P/C from selected values)

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

- 3.23 (shake flask-UV, pH 7.4, Rogers & Cammarata 1969)
- 3.34 (unpublished result, Leo et al. 1971)
- 3.34, 3.50, 3.72 (unpublished results, Rekker 1977)
- 2.37 (RP-HPLC-RT correlation, Veith et al. 1979a)
- 3.45 (Hansch & Leo 1979)
- 3.42 (shake flask-UV, Briggs 1981)
- 3.37 (inter-laboratory shake flask average, Eadsforth & Moser 1983)
- 3.72 ± 0.03 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
- 2.69 (HPLC-RT correlation, average, Ge et al. 1987)
- 3.42 (shake flask, Log P Database, Hansch & Leo 1987)
- 3.50 (recommended, Sangster 1989, 1993)
- 3.70, 3.68 (shake flask, HPLC-RT correlation, Wang et al. 1989)
- 3.50 (recommended, Hansch et al. 1995)
- 2.99, 3.13, 3.04, 3.18 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
- 3.35 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

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

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

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

- 1.48 (fathead minnow, Veith et al. 1979b)
- 1.48, 2.10 (quoted, calculated- K_{OW} , Mackay 1982)

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

- 2.78 (sorption isotherm-GC, converted from K_{OM} organic matter-water in various soils, Briggs 1981)
- 2.78, 3.28 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 3.30 (calculated- K_{OW} , Kollig 1993)
- 2.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 2.80, 2.93 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

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

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 31\text{--}1740 \text{ h}$ in water, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 0.247\text{--}2.47 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis: rate constant $k = 1.2 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ for reactions with hydroxyl radical in aqueous solution, (Buxton et al. 1986; quoted, Armbrust 2000);

measured hydroxy radical rate constant $k = 4.9 \times 10^{13} \text{ M}^{-1} \cdot \text{h}^{-1}$ (Armbrust 2000)

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation screening test data (Malaney 1960; quoted, Howard et al. 1991);

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

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.247\text{--}2.47$ h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 31\text{--}1740$ h in water, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991); $t_{1/2} = 31\text{--}672$ h, based on estimated unacclimated aqueous aerobic degradation half-life and photooxidation half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2} = 336\text{--}1344$ 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 16.1.3.11.1
Reported vapor pressures of diphenylamine at various temperatures

Stull 1947

summary of literature data

$t/^{\circ}\text{C}$	P/Pa
108.3	133.3
141.7	666.6
157.0	1333
175.2	2666
194.3	5333
206.9	7999
222.9	13332
247.5	26664
274.1	53329
302.0	101325
mp/ $^{\circ}\text{C}$	52.9

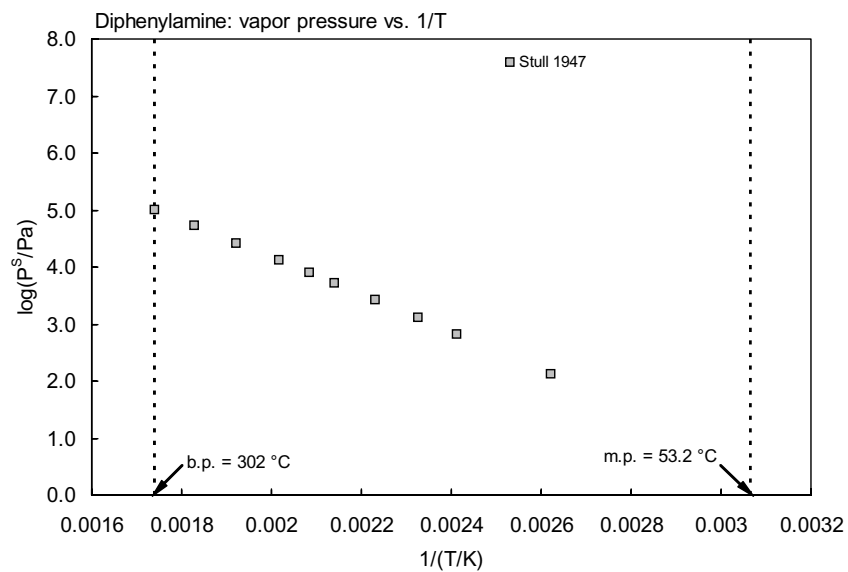
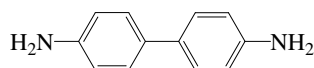


FIGURE 16.1.3.11.1 Logarithm of vapor pressure versus reciprocal temperature for diphenylamine.

16.1.3.12 Benzidine



Common Name: Benzidine

Synonym: *p,p'*-bianiline, 4,4'-diaminobiphenyl, 4,4'-biphenyldiamine, (1,1'-biphenyl)-4,4'-diamine

Chemical Name: *p*-benzidine

CAS Registry No: 92-87-5

Molecular Formula: $C_{12}H_{12}N_2$, $NH_2C_6H_4C_6H_4NH_2$

Molecular Weight: 184.236

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

128 (Weast 1982–83)

120 (Lide 2003)

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

400 (Weast 1982–83)

401 (Lide 2003)

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

1.250 (Verschuereen 1983)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

4.66 (pK_1), 3.57 (pK_2) ($30^{\circ}C$, Perrin 1965; quoted, Mabey et al. 1982; Howard 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.117 (mp at $120^{\circ}C$)

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

400 ($12^{\circ}C$, Verschuereen 1977, 1983)

520 (Shriner et al. 1978)

360 ($24^{\circ}C$ at pH 5.9, shake flask-LSC, Means et al. 1980)

276 ($20^{\circ}C$, Schmidt-Bleek et al. 1982)

359 (Gerstl & Helling 1987)

Vapor Pressure (Pa at $25^{\circ}C$):

0.724 (calculated-Trouton's rule, Mabey et al. 1982)

1.0×10^{-6} ($20^{\circ}C$, Schmidt-Bleek et al. 1982)

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

3.93×10^{-6} (estimated, Hine & Mookerjee 1975)

0.0394 (calculated-P/C at $12^{\circ}C$, Mabey et al. 1982)

4.60×10^{-7} (calculated-P/C, this work)

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

1.34 (shake flask, Korenman 1971)

1.34 (recommended, Sangster 1993)

1.34 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

1.74, 2.66, 2.81, 3.4 (fish, mosquitoes, snail, algae; Lu et al. 1977)

1.60 (bluegills, USEPA 1980; quoted, Howard 1989)

1.00 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

1.90, 2.93, 3.08 (golden ide, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC} :

- 1.66 (soil/sediment, equilibrium sorption isotherm by shake flask-LSC at pH 5.9, Means et al. 1980)
- 1.02 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
- 5.95; 5.68; 5.35; 5.91 (Russell soil; Chalmers soil; Kokomo soil; Milford soil, Graveel et al. 1986)
- 3.00 (calculated-MCI χ , Gerstl & Helling 1987)
- 3.46, 3.44 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.26 (calculated- K_{OW} , Kollig 1993)
- 3.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical of $1.1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 0.312\text{--}3.12 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 48\text{--}192 \text{ h}$, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

overall biodegradation $t_{1/2} = 76 \text{ d}$, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989);

aqueous aerobic $t_{1/2} = 192\text{--}768 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.312\text{--}3.12 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated $t_{1/2} \sim 1 \text{ d}$ for the reaction with hydroxyl radical and ozone (Howard 1989);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

Surface water: estimated $t_{1/2} \sim 1 \text{ d}$ for the reaction with radicals and redox reactions with naturally occurring cations, etc. and perhaps with photodegradation (Howard 1989);

$t_{1/2} = 31.2\text{--}192 \text{ h}$, based on estimated photooxidation half-life in water and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 96\text{--}484 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

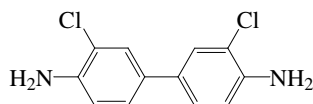
Soil: $t_{1/2} < 10 \text{ d}$ in soil (USEPA 1979; quoted, Ryan et al. 1988);

$t_{1/2} = 48\text{--}192 \text{ h}$, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

overall biodegradation $t_{1/2} = 76 \text{ d}$, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989).

Biota: depuration $t_{1/2} \sim 7 \text{ d}$ from bluegills (Lu et al. 1977; quoted, Howard 1989).

16.1.3.13 3,3'-Dichlorobenzidine



Common Name: 3,3'-Dichlorobenzidine

Synonym: 3,3'-dichloro-4,4'-diamino(1,1'-biphenyl), DCB

Chemical Name: 3,3'-dichlorobenzidine

CAS Registry No: 91-94-1

Molecular Formula: $C_{12}H_{10}Cl_2N_2$, $NH_2C_6H_3(Cl)C_6H_3(Cl)NH_2$

Molecular Weight: 253.126

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

132.5 (Lide 2003)

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

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

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_b :

11.7 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0882 (mp at $132.5^{\circ}C$)

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

4.00 ($22^{\circ}C$, as dihydrochloride, Banerjee et al. 1978)

3.99 ($22^{\circ}C$, at pH 6.9 as DCB.2HCl, quoted, Verschueren 1983)

3.11 (shake flask-UV/LSC, Banerjee et al. 1980)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00133 (estimated, Mabey et al. 1982)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

0.0811 (calculated-P/C, Mabey et al. 1982)

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

3.02 (calculated as per Leo et al.1971)

3.51 ($23^{\circ}C$, shake flask, Banerjee et al. 1980)

3.35 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

3.51 (recommended, Sangster 1993)

3.51 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

2.70 (bluegill sunfish, Appleton & Sikka 1980)

2.97 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

2.79, 2.97, 3.49 (fish, algae, activated sludge, Freitag et al. 1985)

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

3.19 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

4.35, 3.87 (soil: quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

3.30 (calculated- K_{OW} , Kollig 1993)

4.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis:

direct aqueous photolysis rate constant $k = 2.1 \times 10^{-6} \text{ h}^{-1}$ in summer at 40°N latitude (Mabey et al. 1982); both aqueous and atmospheric photolysis $t_{1/2} = 0.025\text{--}0.075 \text{ h}$, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Callahan et al. 1979; Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 31.2\text{--}1740 \text{ h}$ in water, based on estimated rate constants for reactions with OH and RO_2 radicals in water (Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.905\text{--}9.05 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on lake die-away study test data (Appleton et al. 1978; quoted, Howard et al. 1991) and a soil die-away test (Boyd et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^{-12} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.905\text{--}9.05 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated $t_{1/2} \sim 1 \text{ d}$ for the reaction with hydroxyl radical and ozone (Howard 1989);

atmospheric transformation lifetime by photolysis was estimated to be $< 1 \text{ d}$ (Kelly et al 1994).

Surface water: $t_{1/2} = 0.025\text{--}0.075 \text{ h}$, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, Howard et al. 1991).

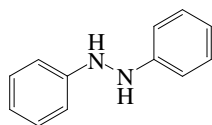
Ground water: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} = 30 \text{ min}$ by suspended microcrystalline clays may be considered the most important fate process in the aquatic environment (Callahan et al. 1979).

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

Biota:

16.1.3.14 N,N'-Bianiline



Common Name: N,N'-Bianiline

Synonym: 1,2-diphenylhydrazine, hydrazobenzene

Chemical Name: 1,2-diphenylhydrazine, hydrazobenzene

CAS Registry No: 122-66-7

Molecular Formula: $C_{12}H_{12}N_2$, $C_6H_5NHNHC_6H_5$

Molecular Weight: 184.236

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

131 (Weast 1982–83; Lide 2003)

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

293 (as azobenzene, IARC 1975)

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

1.158 ($16^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

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

Dissociation constant pK_b :

13.2 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.0912 (mp at $131^{\circ}C$))

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

0.252 ($20^{\circ}C$, as azobenzene, Takagishi et al. 1968)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00347 (quoted, Mabey et al. 1982)

$\log(P/mmHg) = 16.8982 - 5.0039 \times 10^3/(T/K) - 0.35846 \cdot \log(T/K) - 9.9629 \times 10^{-3} \cdot (T/K) + 4.2938 \times 10^{-6} \cdot (T/K)^2$;
temp range 404–573 K (vapor pressure eq., Yaws 1994)

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

3.45×10^{-4} (calculated-P/C, Mabey et al. 1982)

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

3.82 (shake flask-UV as for azobenzene, Fujita et al. 1964)

3.03 (calculated as per Leo et al. 1971, Callahan et al. 1979)

2.94 (shake flask, Hansch & Leo 1979; 1987)

2.94 (recommended, Sangster 1993)

2.94 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

2.46 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

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

2.62 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.40 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical, $k < 1 \times 10^9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 31 - 1740 \text{ h}$, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.3 - 3.0 \text{ h}$ in air, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 672 - 4320 \text{ h}$, based on acclimated aerobic aqueous screening test data (Malaney 1960; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2880 - 17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: bacterial transformation $k = 1 \times 10^{-10} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.3 - 3.0 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

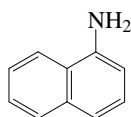
Surface water: photooxidation $t_{1/2} = 31 - 1740 \text{ h}$, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991).

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

Sediment:

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

Biota:

16.1.3.15 α -Naphthylamine (1-Aminonaphthalene)

Common Name: 1-Naphthylamine

Synonym: 1-naphthalenamine, α -naphthylamine, 1-NA, 1-aminonaphthalene, naphthalidine

Chemical Name: 1-naphthalenamine

CAS Registry No: 134-32-7

Molecular Formula: $C_{10}H_7NH_2$

Molecular Weight: 143.185

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

49.2 (Lide 2003)

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

300.7 (Lide 2003)

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

1.1229 ($25^{\circ}C$, Weast 1982–8)

1.123 (Dean 1985)

Molar Volume (cm^3/mol):

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

Dissociation Constant pK_a :

3.92 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.23 ± 0.105 (Tsonopoulos & Prausnitz 1971)

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

44.35 ± 3.35 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.579 (mp at $49.2^{\circ}C$)

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

1700 (Verschueren 1983)

590 parts in water (Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.803 (extrapolated-regression of tabulated data, temp range 104.3 – $300.8^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 14529.5/(T/K)] + 8.29900$; temp range 104.3 – $300.8^{\circ}C$ (Antoine eq., Weast 1972–73)

0.557 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 574.066/(T/K)] \times 10^4 \{0.822931 - 2.94554 \times 10^{-4} \cdot (T/K) + 2.19845 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 325.0 – $645.0\ K$ (Cox eq., Chao et al. 1983)

0.446 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.88407 - 2570.55/(-46.989 + T/K)$; temp range 377 – $574\ K$ (Antoine eq., Stephenson & Malanowski 1987)

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

6.197 (gas stripping-GC, Altschuh et al. 1999)

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

2.23 (Leo et al. 1969)

2.25 (shake flask, Hansch & Leo 1979)

2.27 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)

2.33 (HPLC- k' correlation, Minick et al. 1988)

2.25 (recommended, Sangster 1993)

2.25 (recommended, Hansch et al. 1995)

2.34 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

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

Bioconcentration Factor, $\log BCF$:

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

3.58, 3.43, 3.50	(Milford soil, Morocco soil, Oakville soil, Graveel et al. 1986)
2.63, 2.68, 3.15	(sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
3.51, 3.48	(soil, quoted exptl., calculated-MCI χ , Meylan et al. 1992)
3.51	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.0–2.65	(5 soils, pH 2.8–7.4, batch equilibrium-sorption isotherm, Li et al. 2000)

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

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

atmospheric $t_{1/2} = 0.292\text{--}2.92 \text{ h}$, based on estimated rate constants for the reaction with OH radical in air and aqueous photooxidation $t_{1/2} = 62.4\text{--}3480 \text{ h}$, based on estimated rate constants for reaction of representative aromatic amines with OH and RO_2 radicals in aqueous solution (Howard et al. 1991);

photooxidation $t_{1/2} = 0.08\text{--}0.13 \text{ h}$ under sunlight and $t_{1/2} = 0.25\text{--}9.1 \text{ h}$ under UV light when adsorbed on silica; $t_{1/2} = 0.10\text{--}0.15 \text{ h}$ under sunlight and $t_{1/2} = 0.15\text{--}10.5 \text{ h}$ under UV light when adsorbed on alumina on the TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672\text{--}4320 \text{ h}$ and aqueous anaerobic biodegradation $t_{1/2} = 2688\text{--}17280 \text{ h}$, based on slow biodegradation observed in aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.292\text{--}2.92 \text{ h}$, based on estimated photooxidation half-life in air (Howard et al. 1991).

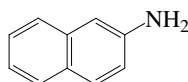
Surface water: $t_{1/2} = 0.62\text{--}3840 \text{ h}$, based on estimated rate constants for reactions of aromatic amines with OH and RO_2 radicals in aqueous solutions (Howard et al. 1991).

Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Biota:

16.1.3.16 β -Naphthylamine (2-Aminonaphthalene)

Common Name: 2-Naphthylamine

Synonym: 2-naphthalenamine, β -naphthylamine, 2-NA, 2-aminonaphthalene, naphthalidine

Chemical Name: 2-naphthalenamine

CAS Registry No: 91-59-8

Molecular Formula: $C_{10}H_7NH_2$

Molecular Weight: 143.185

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

113 (Weast 1982–83; Lide 2003)

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

306.2 (Lide 2003)

Density (g/cm^3):

1.0614 (at $98^{\circ}C$, Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

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

Dissociation Constant pK_a :

4.15 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.97 (Tsonopoulos & Prausnitz 1971)

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

57.32 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.137 (mp at $113^{\circ}C$)

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

6.40 ($18^{\circ}C$, Ciusa 1922; quoted, Tsonopoulos & Prausnitz 1971)

0.19 (18 – $20^{\circ}C$, Neish 1948; quoted, Tsonopoulos & Prausnitz 1971)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.634 (extrapolated-regression of tabulated data, temp range 108 – $306.1^{\circ}C$, Stull 1947)

$\log (P/atm) = [-0.2185 \times 14679.6/(T/K)] + 8.435133$; temp range 108 – $306.1^{\circ}C$ (Antoine eq., Weast 1972–73)

0.369 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/atm) = [1 - 579.422/(T/K)] \times 10^{\{0.860256 - 4.44286 \times 10^{-4} \cdot (T/K) + 3.71453 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 385.0 – $645.0\ K$ (Cox eq., Chao et al. 1983)

0.035 (Howard et al. 1986)

0.035 (interpolated, solid, Antoine eq., Stephenson & Malanowski 1987)

0.362 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 8.4859 - 3859/(T/K)$, temp range: 283 – $323\ K$, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.88978 - 2604.31/(-46.068 + T/K)$, temp range 388 – $579\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

0.340 (calculated-solvatochromic parameters, Banerjee et al. 1990)

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

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

2.28 (shake flask, Hansch & Leo 1979)

2.26 ($20^{\circ}C$, shake flask, Korenman & Polumestnaya, 1982)

2.40 (calculated-UNIFAC activity coeff., Campbell & Luthy 1985)

2.40 (shake flask-AS, pH 7.5, Martin-Villodre et al. 1986)

2.34 (recommended, Sangster 1993)

2.28 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

1.77 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radicals at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 0.30\text{--}2.90 \text{ h}$ in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 62\text{--}3480 \text{ h}$, based on estimated rate constants for reaction of representative aromatic amines with OH and RO_2 radicals in aqueous solution (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.05\text{--}0.14 \text{ h}$ under sunlight and $0.20\text{--}10.0 \text{ h}$ under UV light when adsorbed on silica and $t_{1/2} = 0.16\text{--}0.19 \text{ h}$ under sunlight and $t_{1/2} = 0.22\text{--}10.8 \text{ h}$ under UV light when adsorbed on alumina TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1979) and unacclimated soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2} = 2880\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.30\text{--}2.90 \text{ h}$, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 62.0\text{--}3840 \text{ h}$, based on estimated rate constants for reactions of aromatic amines with OH and RO_2 radicals in aqueous solutions (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991).

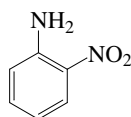
Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1991) and unacclimated aerobic soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1981).

Biota:

16.1.3.17 2-Nitroaniline



Common Name: 2-Nitroaniline

Synonym: 1-amino-2-nitrobenzene, *o*-aminonitrobenzene, *o*-nitroaniline, 2-nitrophenylamine, 2-nitrobenzeneamine

Chemical Name: 1-amino-2-nitrobenzene, *o*-nitroaniline, 2-nitroaniline

CAS Registry No: 88-74-4

Molecular Formula: $C_6H_6N_2O_2$, $C_6H_4NH_2NO_2$

Molecular Weight: 138.124

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

71.0 (Lide 2003)

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

284 (Lide 2003)

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

1.442 ($15^{\circ}C$, Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

16.11 (Tsonopoulos & Prausnitz 1971)

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

46.86 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.354 (mp at $71.0^{\circ}C$)

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

1212, 2423 ($25, 40^{\circ}C$, synthetic method-shake flask-titration, Collet & Johnson 1926)

1740 (calculated- K_{ow} , Yalkowsky & Morozowich 1980)

1260 (Verschueren 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 8.81842 - 3336.52/(T/K)$; measured range $150\text{--}215^{\circ}C$ (isoteniscope, Berliner & May 1925)

$\log (P/mmHg) = 9.55950 - 4037.7/(T/K)$; measured range $190\text{--}250^{\circ}C$ (isoteniscope, Berliner & May 1925)

0.620 (extrapolated-regression of tabulated data, temp range $104\text{--}284.5^{\circ}C$, Stull 1947)

0.072 (Knudsen method, calculated-Antoine eq., Hoyer & Peperle 1958)

$\log (P/mmHg) = 12.50 - 4701/(T/K)$, temp range $0\text{--}50^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

$\log (P/mmHg) = [-0.2185 \times 15284.0/(T/K)] + 8.868383$; temp range $104\text{--}284.5^{\circ}C$ (Antoine eq., Weast 1972–73)

< 13.3 ($30^{\circ}C$, Verschueren 1983)

0.650 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 8.8684 - 3336.5/(T/K)$; temp range $150\text{--}260^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log (P_s/kPa) = 11.625 - 4701/(T/K)$; temp range $273\text{--}323\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 11.3629 - 7444.3/(240.83 + T/K)$; temp range $423\text{--}553\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/mmHg) = -112.5774 - 1.5945 \times 10^3/(T/K) + 54.577 \cdot \log (T/K) - 7.6775 \times 10^{-2} \cdot (T/K) + 3.6152 \times 10^{-5} \cdot (T/K)^2$; temp range $345\text{--}558\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

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

1.44 (shake flask-UV, Fujita et al. 1964)

1.83 (shake flask-UV, Hansch & Anderson 1967)

1.62 (HPLC-RT correlation, Carlson et al. 1975)

1.81 (Hansch & Leo 1979)

- 1.72 (shake flask, Eadsforth & Moser 1983)
- 1.67 (calculated-HPLC- k' correlation, Deneer et al. 1987)
- 1.50 (calculated-linear extrapolation exptl. log k at various solvent compositions, Deneer et al. 1987)
- 1.93, 1.73 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
- 1.85 (recommended, Sangster 1993)
- 1.80 \pm 0.14, 1.35 \pm 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
- 1.85 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

0.91; 1.49, 0.55, 0.83 (quoted exptl.; calculated values- K_{OW} , Bintein et al. 1993)

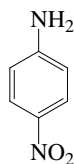
Sorption Partition Coefficient, log K_{OC} :

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

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 1.4$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

16.1.3.18 4-Nitroaniline



Common Name: 4-Nitroaniline

Synonym: 1-amino-4-nitrobenzene, *p*-aminonitrobenzene, *p*-nitroaniline, 4-nitrobenzenamine, 4-nitrophenylamine

Chemical Name: 1-amino-4-nitrobenzene, *p*-nitroaniline, 4-nitroaniline

CAS Registry No: 100-01-6

Molecular Formula: $C_6H_6N_2O_2$, $C_6H_4NH_2NO_2$

Molecular Weight: 138.124

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

147.5 (Lide 2003)

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

332 (Lide 2003)

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

1.424 (Weast 1982–83; Verschueren 1983)

1.4370 ($14^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.09 (Tsonopoulos & Prausnitz 1971)

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

50.21 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.0628 (mp at $147.5^{\circ}C$)

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

568, 1157 ($25, 40^{\circ}C$, synthetic method-shake flask-titration, Collet & Johnson 1926)

728 ($30^{\circ}C$, shake flask-interferometry, Gross et al. 1931)

603 (calculated- K_{ow} , Yalkowsky & Morozowich 1980)

380 ($20^{\circ}C$, shake flask-membrane filter-fluorophotometry, Hashimoto et al. 1982)

390, 400 ($20^{\circ}C$, shake flask-glass fiber filters-fluorophotometry, Hashimoto et al. 1982)

800; 22000 ($19^{\circ}C, 100^{\circ}C$, Verschueren 1983)

800 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 9.55950 - 4037.7/(T/K)$; measured range 190 – $250^{\circ}C$ (isoteniscope, Berliner & May 1925)

0.035 (extrapolated-regression of tabulated data, temp range 142.4 – $336^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 13.69 - 5707/(T/K)$, temp range 30 – $90^{\circ}C$, (Knudsen effusion method, Hoyer & Peperle 1958)

$\log(P/mmHg) = [-0.2185 \times 17220.2/(T/K)] + 9.041879$; temp range 142.4 – $336^{\circ}C$ (Antoine eq., Weast 1972–73)

0.200, 0.933 ($20^{\circ}C, 30^{\circ}C$, Verschueren 1983)

0.014 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 9.5595 - 4039.73/(T/K)$; temp range 190 – $260^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_s/kPa) = 11.1109 - 5093/(T/K)$; temp range 346 – $366\ K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.7988 - 4071.3/(T/K)$; temp range 473 – $538\ K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 56.1642 - 5.3655 \times 10^3/(T/K) - 17.958 \cdot \log(T/K) + 9.092 \times 10^{-3} \cdot (T/K) + 7.0305 \times 10^{-10} \cdot (T/K)^2$; temp range 421 – $609\ K$ (vapor pressure eq., Yaws 1994)

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

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

- 1.39 (shake flask-UV, Fujita et al. 1964; Hansch & Leo 1979)
- 0.59 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
- 1.16 (HPLC- k' correlation, Deneer et al. 1987)
- 1.10 (calculated-linear extrapolation exptl. values of $\log k$ at various solvent compositions, Deneer et al. 1987)
- 1.15 (HPLC-RT correlation, Wang et al. 1989)
- 1.51, 1.36 (25°C , 60°C , shake flask-UV, Kramer & Henze 1990)
- 1.30 (CPC-RV correlation, Tsai et al. 1991)
- 1.30 (CPC-RV correlation, El Tayar et al. 1991)
- 1.35 (recommended, Sangster 1993)
- 1.39 ± 0.14 , 0.75 ± 0.48 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
- 1.37 (recommended, Hansch et al. 1995)

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

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

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

- 2.26; 2.66; 2.12 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
- 0.64; 1.25, -0.18 , 0.41 (quoted exptl.; calculated values- K_{OW} , Bintein et al. 1993)
- 2.16, 2.22, 2.19 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
- 1.86, 1.84 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

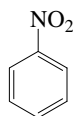
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Surface water: estimated $t_{1/2} = 2.3$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

16.1.4 NITROAROMATIC COMPOUNDS

16.1.4.1 Nitrobenzene



Common Name: Nitrobenzene

Synonym: nitrobenzol, oil of mirbane

Chemical Name: nitrobenzene

CAS Registry No: 98-95-3

Molecular Formula: $C_6H_5NO_2$

Molecular Weight: 123.110

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

5.7 (Stull 1947; Dreisbach 1955; Weast 1982–83; Howard 1989; Lide 2003)

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

210.8 (Weast 1982–83; Lide 2003)

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

1.2032, 1.1982 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.2036 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

102.0 (calculated from density, Rohrschneider 1973; Chiou 1985)

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

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

55.186, 43.421 ($25^{\circ}C$, bp, Dreisbach 1961)

55.013, 40.769 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.59 (Dreisbach 1955)

12.13 (Tsonopoulos & Prausnitz 1971)

11.63 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

43.51 (Tsonopoulos & Prausnitz 1971)

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

1780, 2050 (15, $30^{\circ}C$, shake flask-interferometry, Gross et al. 1931)

2060* ($30^{\circ}C$, shake flask-interferometry and titration, measured range 0 – $60^{\circ}C$, Vermillion et al. 1941)

1204 (shake flask-centrifuge, Booth & Everson 1948)

1930 (Seidell 1941)

2018 (shake flask-interferometry, Donahue & Bartell 1952)

1950 (Deno & Berkheimer 1960)

2259 ($35^{\circ}C$, shake flask-UV spectrophotometry, Hine et al. 1963)

2060 (Hansch et al. 1968)

1900 ($20^{\circ}C$, Verschueren 1977, 1983)

2093 (shake flask-LSC, Banerjee et al. 1980)

2090 (shake flask-radioactive analysis, Veith et al. 1980)

2043 (20 – $27^{\circ}C$, shake flask-GC, Chiou 1985)

1900 ($20^{\circ}C$, Riddick et al. 1986; quoted, Howard 1989)

1930* ($20^{\circ}C$, shake flask-UV spectrophotometry, measured range 10 – $40^{\circ}C$, Beneš & Dohnal 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):

- 133.3* (53.1°C, static-manometer, measured range 53.1–208.3°C, Kahlbaum 1898)
 38.80 (saturated vapor density-gas saturation, Puck & Wise 1946)
 42.06* (extrapolated-regression of tabulated data, temp range 44.4–210.6°C, Stull 1947)
 10063* (134.1°C, ebulliometry, measured range 134.1–210.629°C, Brown 1952)
 37.86 (calculated by formula, Dreisbach 1955; quoted, Hine & Mookerjee 1975)
 $\log(P/\text{mmHg}) = 7.08283 - 1722.2/(199.0 + t/^\circ\text{C})$; temp range 108–300°C (Antoine eq. for liquid state, Dreisbach 1955)
 32.3* (23.14°C, gas saturation, measured range 6.09–23.14°C, Lynch & Wilke 1960)
 $\log(P/\text{mmHg}) = 7.545 - 2064/(t/^\circ\text{C} + 230)$; temp range 6.09–23.14°C (gas saturation, Lynch & Wilke 1960)
 80.0 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)
 $\log(P/\text{mmHg}) = [-0.2185 \times 12168.2/(T/\text{K})] + 8.416268$; temp range 44.4–210.6°C (Antoine eq., Weast 1972–73)
 34.60 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 7.11562 - 1746.585/(201.783 + t/^\circ\text{C})$, temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 20.00 (20°C, Verschueren 1977, 1983)
 28.37 (calculated-bp, Mackay et al. 1982)
 34.36 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.23424 - 1741.779/(201.257 + t/^\circ\text{C})$; temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 4.06596 - 323.457/(-58.276 + t/^\circ\text{C})$; temp range 239–291°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 34.63 (extrapolated-Antoine eq., Dean 1985; 1992)
 $\log(P/\text{mmHg}) = 6.91048 - 946.35/(246.68 + t/^\circ\text{C})$; temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
 37.0 (quoted lit., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.670 - 2064.0/(230.0 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 37.65 (extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.22069 - 1732.222/(-72.886 + T/\text{K})$; temp range 407–484 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.6699 - 2064/(-43.15 + T/\text{K})$; temp range 279–296 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 33.33 (Howard et al. 1986)
 $\log(P/\text{mmHg}) = -54.4937 - 2.1123 \times 10^3/(T/\text{K}) + 29.321 \cdot \log(T/\text{K}) - 4.4839 \times 10^{-2} \cdot (T/\text{K}) + 2.0162 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 279–719 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

- 2.367, 4.51, 4.723 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.327 (calculated-P/C, Mabey et al. 1982)
 2.472 (estimated, Lyman et al. 1982)
 5.06 (calculated-molecular structure, Russell et al. 1992)
 0.868 (gas stripping-GC, Altschuh et al. 1999)

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

- 1.85 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1969, 1971; Hansch & Leo 1979, 1985;)
 1.74 (Neely et al. 1974)
 1.85, 1.84 (Hansch & Leo 1979)
 1.82 (HPLC-RT correlation, Veith et al. 1979a)
 1.83 (shake flask-LSC, Banerjee et al. 1980)
 1.98, 1.78 (HPLC-k' correlation, McDuffie 1981)
 1.85 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982;)
 1.88 (shake flask-UV, Unger & Chiang 1981)
 1.99 (RP-HPLC-k' correlation, Miyake & Terada 1982)
 1.83, 1.84 (calculated-activity coeff. γ from UNIFAC, octanol and water solubility considered; calculated-activity coeff. γ from UNIFAC, octanol and water solubility not considered, Arbuckle 1983)
 1.85, 1.88 (lit. values, Verschueren 1983)

- 1.83 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
- 1.84 (calculated-activity coefficient γ from UNIFAC, Campbell & Luthy 1985)
- 1.87 (Lu et al. 1986)
- 1.85 (RP-HPLC- k' correlation, Minick et al. 1988)
- 1.89 (HPLC- k' correlation, Deneer et al. 1987)
- 1.84 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
- 1.70 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 1.828 ± 0.001 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
- 1.85 (recommended, Sangster 1989, 1993)
- 1.836 ± 0.051; 1.828 ± 0.001 (average values, stir-flask method by BRE; by RITOX, Brooke et al. 1990)
- 1.83, 1.85, 1.88 (CPC-retention volume correlation; Gluck & Martin 1990)
- 1.94, 2.25 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
- 1.57 (shake flask-UV, Nakagawa et al. 1992)
- 1.85 (shake flask-GC, Alcron et al. 1993)
- 1.85 (recommended, Hansch et al. 1995)
- 2.25, 2.12, 2.20, 2.23 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
- 1.88 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
- 1.93 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

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

Bioconcentration Factor, log BCF:

- 1.18 (fathead minnows, Veith et al. 1979b)
- 0.06 (calculated- K_{OW} , Veith et al. 1980)
- < 1.0; 1.36 (golden orfe; green algae, Freitag et al. 1982)
- 1.38; 1.42 (alga *Chlorella fusca*, wet wt. basis; calculated- K_{OW} , Geyer et al. 1984)
- 0.78 (*P. reticulata*, Canton et al. 1985; quoted, Howard 1989)
- < 1.0, 1.38, 1.60 (golden orfe, algae, activated sludge, Freitag et al. 1982)
- < 1.0, 1.30, 1.60 (golden ide, algae, activated sludge, Freitag et al. 1985)
- 1.47 ± 0.12 (guppy-fat wt. basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K_{OC} :

- 1.94 (20°C, sorption isotherm-GC, converted from K_{OM} multiplied by 1.724, Briggs 1981)
- 2.30 (Lincoln fine sand, calculated exptl. value, Wilson et al. 1981)
- 2.23, 2.57 (Danish subsoils, Loekke 1985)
- 1.63, 1.84 (two Norwegian organic soils, Seip et al. 1986)
- 1.70 (soil, quoted, Sabljic 1987)
- 1.95 ± 0.84, 2.02 ± 1.18; 1.99 (Captina slit loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 1.43 (predicted- K_{OW} , Walton et al. 1992)
- 1.51 (calculated- K_{OW} , Kolliq 1993)
- 2.20 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 2.05, 2.16, 2.15 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
- 1.99, 1.84 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 2.20; 2.28 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.51, 2.03, 2.26, 2.09, 1.90 (soil: calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

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

- Volatilization: $t_{1/2}(\text{calc}) \approx 200$ h from water bodies (Mackay & Leinonen 1975; quoted, Callahan et al. 1979)
- $t_{1/2} = 45$ d was estimated in a model river 1 m deep with a 1.0 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: aqueous photolysis $t_{1/2} = 67\text{--}200$ d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; Howard 1989; Howard et al. 1991); atmospheric photolysis $t_{1/2} = 67\text{--}200$ d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; quoted, Howard 1989; Howard et al. 1991); rate constant $k = 2.37 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Hydrolysis:

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 $t_{1/2} = 125$ d to 22 yr in water, based on measured rate constant for reaction with hydroxyl radical in water (Dorfman & Adams 1973; Anbar & Neta 1967; quoted, Howard et al. 1991)

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

$k = (0.09 \pm 0.02) \text{ M}^{-1} \text{ s}^{-1}$ for 5–10 mM to react with ozone in water using 50–1000 mM of *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}}(\text{obs.}) = 0.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Becker et al. 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = 0.21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Zetzsch 1982)

$k_{\text{OH}}(\text{calc}) = 0.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $0.27 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985; Atkinson et al. 1985)

$k_{\text{OH}}^* = 0.137 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K, measured range 259–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{\text{OH}}(\text{calc}) = 1.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (addition of OH for different positions of the electrophilic attack, Witte et al. 1986)

$k_{\text{O}_3} < 7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}} = 1.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes $\tau = 180$ d in clean troposphere and 90 d in moderately polluted atmosphere; $k_{\text{O}_3} < 7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes $\tau > 6$ yr in clean troposphere and $\tau > 2$ yr in moderately polluted atmosphere at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 2.5 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.4 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (0.16 - < 0.90) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (review, Atkinson 1989)

phototransformation decay rate constant of 0.17 min^{-1} on 0.20 g/L of TiO_2 , 8.8 min^{-1} on 0.20 g/L of ZnO and 3.1 min^{-1} on 1.0 g/L of Al_2O_3 (Minero et al. 1994)

Abiotic Transformation: Degradation in reductive environment:

$k = 0.187 \text{ min}^{-1}$ with solute concn of 50 μM in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

$k = (7.39 \pm 1.28) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ in H_2S with (mercapto)juglone (an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Biodegradation:

decomposition by a soil microflora in more than 64 d (Alexander & Lustigman 1966; quoted, Verschuere 1983)

$t_{1/2}(\text{aq. anaerobic}) = 48\text{--}300$ h, based on anaerobic natural die-away test data for 2,4-dinitrotoluene (Spanggard et al. 1980; quoted, Howard et al. 1991)

$k = 14 \text{ mg COD g}^{-1} \text{ h}^{-1}$ average biodegradation rate for 98% removal (Scow 1982)

$t_{1/2}(\text{aq. aerobic}) = 322\text{--}4728$ h, based on aerobic soil column biodegradation study data (Kincannon & Lin 1985; quoted, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 13$ d, $t_{1/2}(\text{anaerobic}) = 2$ d in natural waters (Capel & Larson 1995)

Biotransformation: first-order rate constant of 0.7 d^{-1} corresponding to a half-life of 1 d in adopted activated sludge under aerobic conditions (Mills et al. 1982); rate constant for bacterial transformation of $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: atmospheric lifetimes: $\tau = 180$ d in clean troposphere and $\tau = 90$ d in moderately polluted atmosphere, based on gas-phase reaction with OH radical in atmosphere at room temp. and atmospheric lifetimes $\tau > 6$ yr in clean troposphere and $\tau > 2$ yr in moderately polluted atmosphere, based on gas-phase reaction with O_3 (estimated rate constant) in atmosphere at room temp. (Atkinson et al. 1987);

photooxidation $t_{1/2} = 0.544 - 5.44$ h, based on measured rate constant for reaction with hydroxyl radical in air (Atkinson et al. 1987; quoted, Howard 1989; Howard et al. 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2} = 125$ d to 22 yr, based on measured rate constant for reaction with hydroxyl radical in water (Dorfman & Adams 1973; Anbar & Neta 1967; quoted, Howard et al. 1991);

estimated $t_{1/2} = 0.3 - 3.0$ d in rivers (Zoeteman et al. 1980);

$t_{1/2} = 322 - 4728$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 13$ d, $t_{1/2}(\text{anaerobic}) = 2$ d in natural waters (Capel & Larson 1995).

Groundwater: estimated $t_{1/2} = 1.0$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 48 - 9456$ h, based on estimated unacclimated aqueous anaerobic biodegradation half-life for 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated degradation $t_{1/2} = 625$ d in activated sludge (Freitag et al. 1985; quoted, Anderson et al. 1991)

$t_{1/2} = 322 - 4728$ h, based on aerobic soil column biodegradation study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

calculated $t_{1/2} = 9.1$ d from first-order kinetic of degradation rate in sterilized soils (Anderson et al. 1991).

Biota:

TABLE 16.1.4.1.1

Reported aqueous solubilities of nitrobenzene at various temperatures

Gross et al. 1931		Vermillion et al. 1941		Beneš & Dohnal 1999	
shake flask-interferometry		interferometry		shake flask-UV	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
15	1780	0	1660	10	1770
30	2050	6	1700	20	1930
		30	2060	30	2060
		60	3120	40	2200
		titration		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 5.4 \pm 0.2$	
		30	2060	at 25°C .	
		50	2640		

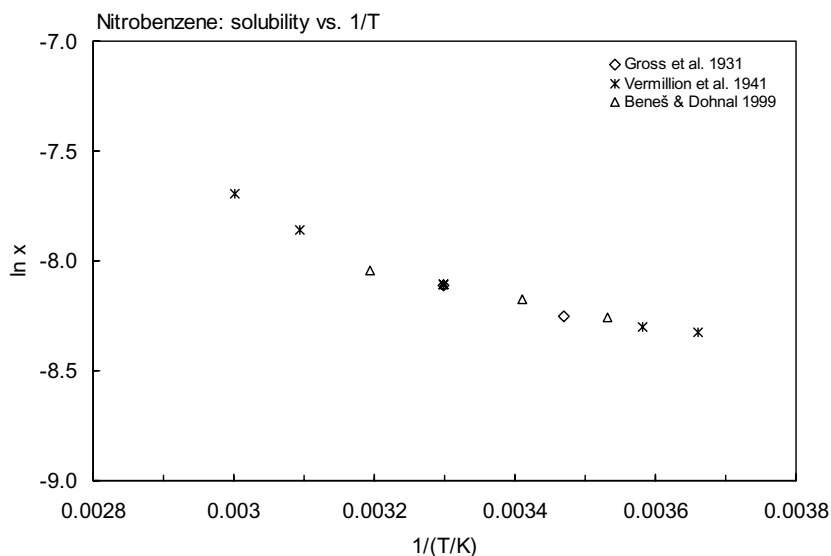


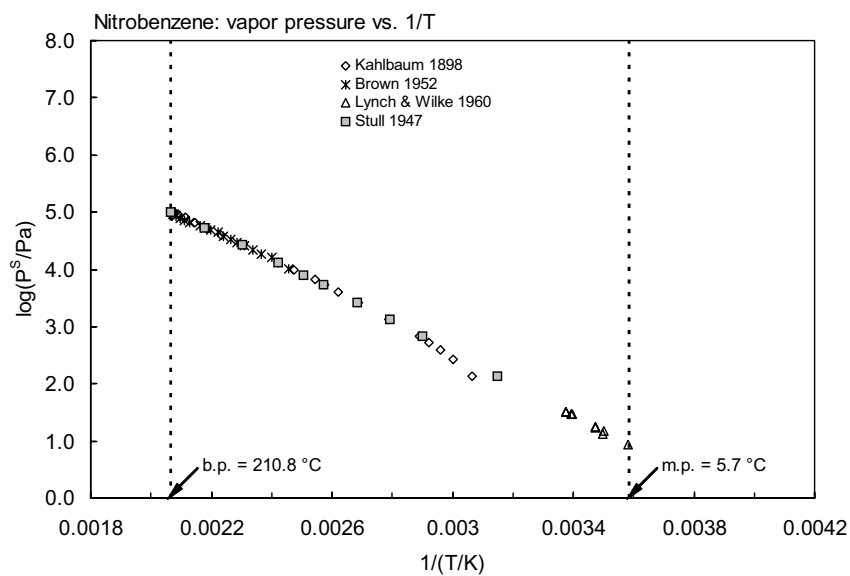
FIGURE 16.1.4.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for nitrobenzene.

TABLE 16.1.4.1.2

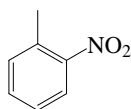
Reported vapor pressures of nitrobenzene at various temperatures and the coefficients for the vapor pressure equations

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)					
Kahlbaum 1898*		Stull 1947		Lynch & Wilke 1960		Brown 1952	
static-manometer		summary of literature data		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
53.1	133.3	44.4	133.3	6.09	8.799	134.1	10063
59.8	266.6	71.6	666.6	12.57	14.80	139.75	13372
64.9	400.0	84.9	1333	12.67	13.33	143.17	16084
69.2	533.3	99.3	2666	14.67	16.93	149.73	18692
72.9	666.6	115.4	5333	14.72	17.73	154.61	21866
85.4	1333.2	125.8	7999	21.37	29.06	159.77	25704
99.1	2666.4	139.9	13332	21.54	29.33	164.45	29641
108.2	3999.7	161.2	26664	23.12	32.26	168.72	33649
114.9	5332.9	185.8	53329	23.14	32.26	172.96	38002
120.0	6666.1	210.6	101325			176.48	44455
131.1	9999.2			bp/°C	210.8	182.07	49014
139.9	13332	mp/°C	5.7			185.70	54019
160.5	26664			eq. 2	P/mmHg	188.90	58839
174.5	39997			A	7.545	196.63	65426
184.5	53329			B	2064	200.41	71843
192.5	66661			C	230	203.88	78997
199.5	79993					206.62	86075
205.0	93326					209.49	92023
208.3	101325					210.626	101322
						210.629	101330

*complete list see [ref.](#)



16.1.4.2 2-Nitrotoluene



Common Name: 2-Nitrotoluene

Synonym: 1-methyl-2-nitrobenzene, *o*-nitrotoluene, 2-methylnitrobenzene

Chemical Name: 2-nitrotoluene, *o*-nitrotoluene

CAS Registry No: 88-72-2

Molecular Formula: $C_7H_7NO_2$, $CH_3C_6H_4NO_2$

Molecular Weight: 137.137

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

−10.4 (Lide 2003)

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

222 (Lide 2003)

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

1.15693, 1.15232 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

1.1629 (Weast 1982–83)

Molar Volume (cm^3/mol):

117.9 ($20^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

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

652 ($30^{\circ}C$, shake flask-interferometer, Gross et al. 1933)

656 (quoted, Deno & Berkheimer 1960)

< 233 (shake flask-centrifuge, Booth & Everson 1948)

324 (Hansch et al. 1968)

656, 2076 (quoted, predicted- K_{ow} , Valvani et al. 1981)

652 ($30^{\circ}C$, Verschueren 1983)

656, 771 (quoted, calculated-fragment const., Wakita et al. 1986)

641; 444 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

609* ($20^{\circ}C$, shake flask-UV spectrophotometry, measured range 10 – $40^{\circ}C$, Beneš & Dohnal 1999)

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

23.97* (extrapolated-regression of tabulated data, Kahlbaum 1898)

27.69* (extrapolated-regression of tabulated data, temp range 50 – $222.3^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.49454 - 2086.1/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

3640* ($115.842^{\circ}C$, ebulliometry, measured range 115.842 – $174.744^{\circ}C$, Dreisbach & Shrader 1949)

$\log(P/mmHg) = [-0.2185 \times 12239.7/(T/K)] + 8.286642$; temp range 50 – $222.3^{\circ}C$ (Antoine eq., Weast 1972–73)

13.33 ($20^{\circ}C$, Verschueren 1983)

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

$\log(P/kPa) = 5.01415 - 967.744/(99.208 + t/^{\circ}C)$; temp range 129.31 – $222.2^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.440 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 5.851 - 946/(96 + t/^{\circ}C)$, temp range 129 – $222^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.32043 - 1827.66/(-71.63 + T/K)$; temp range 402 – 496 K (Antoine eq., Stephenson & Malanowski 1987)

24.80* (ebulliometry, average from extrapolated-Antoine eq., Aim 1994)

$\log(P/\text{mmHg}) = 7.8266 - 2.9906 \times 10^3/(T/K) + 1.1064 \cdot \log(T/K) - 4.9168 \times 10^{-3} \cdot (T/K) + 2.2375 \times 10^{-6} \cdot (T/K)^2$;
temp range 270–720 K (vapor pressure eq., Yaws 1994)

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

5.811 (exptl., Hine & Mookerjee 1975)

4.723, 4.616 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

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

2.30 (Leo et al. 1971; Hansch & Leo 1985)

2.30 (HPLC- k' correlation, Deneer et al. 1987)

2.30 (unpublished data quoted from CLOGP Database and recommended, Sangster 1989)

2.39, 2.43, 2.58 (CPC-RV correlation, Gluck & Martin 1990)

2.46, 2.60; 2.30 (25°C, 60°C, shake flask-UV; quoted lit. value, Kramer & Henze 1990)

2.13 (shake flask-UV, Nakagawa et al. 1992)

2.30 (recommended, Sangster 1993)

2.40 ± 0.15 , 2.21 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)

2.30 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

< 2.0 (*carpinus carpio*, Sasaki 1978; Kawasaki 1980)

1.52, 1.20 (calculated- K_{OW} , S, Lyman et al. 1982; quoted, Howard 1989)

2.28 ± 0.06 (guppy-fat basis, Deneer et al. 1987)

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

2.63, 2.09 (soil, calculated- K_{OW} , S, Lyman et al. 1982; quoted, Howard 1989)

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

Volatilization: estimated $t_{1/2} = 21$ h using Henry's law constant for a model river 1-m deep flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant $k = 3.0 \times 10^{-11} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ for the reaction with $8 \times 10^{-5} \text{ molecules/cm}^3$ photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); rate constant $k = 7.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at 298 K (Atkinson 1989).

Hydrolysis:

Abiotic Transformation: Degradation in reductive environment:

$k = 0.141 \text{ min}^{-1}$ with solute concn of 50 μM in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

Biodegradation: average biodegradation rate of 32.5 mg COD $\text{g}^{-1} \text{ h}^{-1}$ for 98% removal (Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 8$ h, based on a rate constant $k = 3.0 \times 10^{-11} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ for the reaction with $8 \times 10^{-5} \text{ molecules/cm}^3$ photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989).

Surface water: estimated $t_{1/2} = 3.2$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
midday $t_{1/2}(\text{calc}) = 45$ min in Aucilla River water due to indirect photolysis using an experimentally determined reaction rate constant $k = 0.92 \text{ h}^{-1}$ (Zepp et al. 1984; quoted, Howard 1989);

estimated $t_{1/2} = 3.2$ d for a river 4 to 5 m deep, based on monitoring data (Zoeteman et al. 1980; quoted, Howard 1989).

Ground water:

Sediment:

Soil:

Biota:

TABLE 16.1.4.2.1
Reported aqueous solubilities of 2-nitrotoluene at various temperatures

Gross et al. 1931		Beneš & Dohnal 1999	
shake flask-interferometry		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	-	10	531
30	652	20	609
		30	688
		40	773
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 9.4 \pm 0.1$			
25°C			

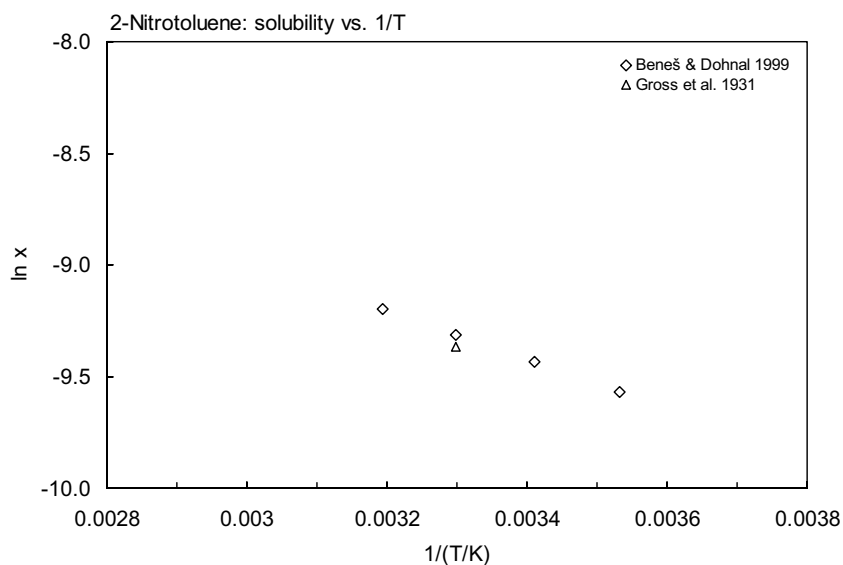


FIGURE 16.1.4.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-nitrotoluene.

TABLE 16.1.4.2.2
Reported vapor pressures of 2-nitrotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Kahlbaum 1898	Stull 1947	Dreisbach & Shrader 1949	Aim 1994				
static method	summary of literature data	ebulliometry	comparative ebulliometry				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
81.8	666.6	50.0	133.3	129.31	6287	115.842	3640
94.8	1333.2	79.1	666.6	134.51	7605	115.847	3639
109.6	2666.4	93.8	1333	138.75	8851	127.245	5773
114.8	3333.1	109.6	2666	142.43	10114	127.268	5778

TABLE 16.1.4.2.2 (Continued)

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Aim 1994	
static method		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
119.2	3999.7	126.3	5333	156.61	16500	137.028	8376
122.8	4666.3	137.6	7999	185.48	42077	137.052	8375
126.1	5333	151.5	13332	205.48	67661	144.838	11104
131.7	6666	173.7	26664	222.15	101325	151.379	13955
150.6	13332	197.7	53329			151.415	13946
172.4	26664	222.3	101325	bp/°C	222.15	157.004	16843
186.1	39997					157.028	16827
196.0	53329	mp/°C	-4.1			162.792	20322
204.2	66661					162.840	20311
211.3	79993					168.856	24597
217.5	93326					168.917	24587
220.4	101325					174.744	29405
						mp/°C	-2.90
						bp/°C	222.946
						eq. 3	P/kPa
						A	6.45342
						B	1906.532
						C	65.441
						for temp range: 115–175°C	

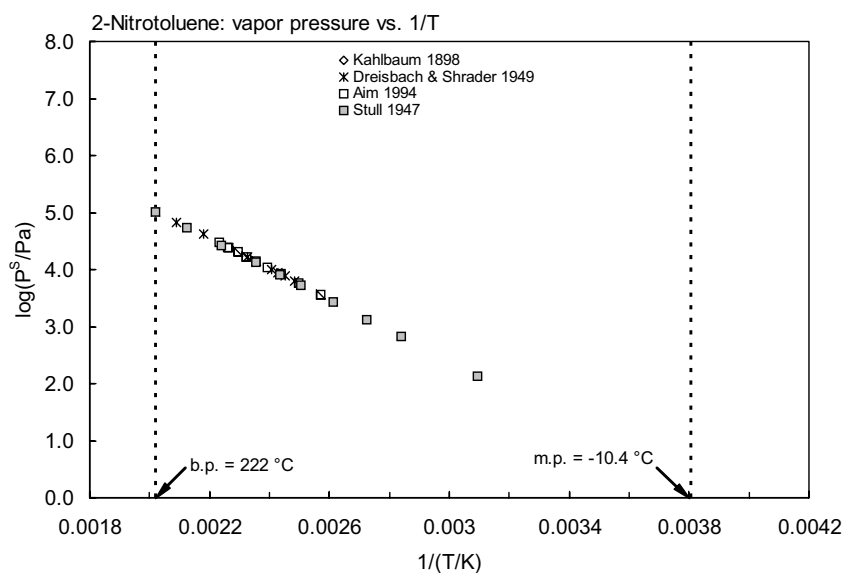
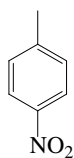


FIGURE 16.1.4.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-nitrotoluene.

16.1.4.3 4-Nitrotoluene



Common Name: 4-Nitrotoluene

Synonym: 1-methyl-4-nitrobenzene, *p*-nitrotoluene, 4-methylnitrobenzene

Chemical Name: 4-nitrotoluene, *p*-nitrotoluene

CAS Registry No: 99-99-0

Molecular Formula: $\text{CH}_3\text{C}_6\text{H}_4\text{NO}_2$

Molecular Weight: 137.137

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

51.63 (Lide 2003)

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

238.3 (Stull 1947; Weast 1982–83; Dean 1985; Howard 1989)

Density (g/cm^3 at 20°C):

1.16278, 1.15799 (20°C , 25°C , Dreisbach & Martin 1949)

1.392 (Dean 1985)

Molar Volume (cm^3/mol):

124.2 (75°C , Stephenson & Malanowski 1987)

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

Dissociation Constant, pK :

–11.27 (Perrin 1972)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.15 (Tsonopoulos & Prausnitz 1971)

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

50.21 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.548 (mp at 51.63°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

442 (30°C , shake flask-interferometer, Gross et al. 1933)

< 278 (shake flask-centrifuge, Booth & Everson 1948)

302 (Tsonopoulos & Prausnitz 1971)

442 (30°C , Verschueren 1983)

288 (20°C , shake flask-UV spectrophotometry, Hashimoto et al. 1984)

307 (calculated-group contribution method, Kühne et al. 1995)

242* (20°C , shake flask-UV spectrophotometry, measured range 10 – 40°C , Beneš & Dohnal 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):

13.98* (extrapolated-regression of tabulated data, measured range 92 – 237°C , Kahlbaum 1898)

$\log (P/\text{mmHg}) = -2630/(T/\text{K}) + 8.025$ (isoteniscopes method, temp range not specified, Kobe et al. 1941)

22.81* (extrapolated-regression of tabulated data, temp range 53.7 – 238.2°C , Stull 1947)

$\log (P/\text{mmHg}) = 7.52323 - 2150.6/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

8851* (147.71°C , ebulliometry, measured range 147.71 – 233.25°C , Dreisbach & Shrader 1949)

0.622* (23.886°C , Knudsen effusion, measured range 297.036 – 309.518 K , Lenchitz & Velicky 1970)

$\log (P/\text{mmHg}) = 11.5424 - 4130.0708/(T/\text{K})$; temp range 297 – 310 K (Knudsen effusion, Lenchitz & Velicky 1970)

$\log (P/\text{mmHg}) = [-0.2185 \times 11915.0/(T/\text{K})] + 7.965025$; temp range 53.7 – 238.3°C (Antoine eq., Weast 1972–73)

5.50* (ebulliometry, fitted to Antoine eq., measured range 144 – 239°C , Ambrose & Gundry 1980)

9.50 (extrapolated-supercooled liq., Ambrose & Gundry 1980)

- 13.33 (20°C, Verschueren 1983; quoted, Howard 1989)
 8.347 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.11507 - 1716.897/(184.543 + t/^\circ\text{C})$; temp range 147.7–233.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 8.38 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.9948 - 1720.39/(184.9 + t/^\circ\text{C})$; temp range 148–233°C (Antoine eq., Dean 1985, 1992)
 0.653 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_g/\text{kPa}) = 10.6673 - 4130.07/(T/\text{K})$; temp range 296–310 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.40605 - 2889.12/(23.37 + T/\text{K})$; temp range 423–512 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 15.18* (ebulliometry, average of extrapolated-Antoine eq., Aim 1994)
 $\log(P/\text{mmHg}) = 9.9641 - 2.6549 \times 10^3/(T/\text{K}) - 0.80182 \cdot \log(T/\text{K}) + 5.3926 \times 10^{-4} \cdot (T/\text{K}) - 4.109 \times 10^{-14} \cdot (T/\text{K})^2$;
 temp range 325–736 K (vapor pressure eq., Yaws 1994)

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

- 5.065 (calculated, Hine & Mookerjee 1975)

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

- 2.37 (shake flask-UV, Fujita et al. 1964)
 2.40 (unpublished result, Leo et al. 1971)
 2.34 (HPLC- k' correlation, Deneer et al. 1987)
 2.42 (recommended, Sangster 1989)
 2.10, 2.05 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
 2.61 (shake flask-UV, Nakagawa et al. 1992)
 2.37 (recommended, Sangster 1993)
 2.37 ± 0.15 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)
 2.42 (recommended, Hansch et al. 1995)
 2.18 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

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

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

- < 2.0 (*Carprinus carpio*, Sasaki 1978; Kawasaki 1980)
 1.57, 1.30 (calculated- K_{ow} , S, Lyman et al. 1982; quoted, Howard 1989)
 2.37 ± 0.05 (guppy-fat basis, Deneer et al. 1987)

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

- 2.67, 2.18 (soil, calculated- K_{ow} , S, Lyman et al. 1982; quoted, Howard 1989)

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

Volatilization: based on Henry's law constant an estimated $t_{1/2} = 25$ h was obtained for a model river of 1- m deep with a current of 1 m/s and wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 8.0$ h in air, based on measured rate constant $k = 3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the reaction with photochemically produced $8 \times 10^5 \text{ molecules/cm}^3$ hydroxyl radical (GEMS 1986; quoted, Howard 1989).

Hydrolysis:

Abiotic Transformation: Degradation in reductive environment:

$k = 0.101 \text{ min}^{-1}$ with solute concn of 50 μM in a 19 d-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

Biodegradation: average biodegradation rate of 32.5 mg COD $\text{g}^{-1} \text{ h}^{-1}$ for 98% removal (Scow 1982).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 8.0$ h, based on measured rate constant of 3×10^{-11} cm³ molecule⁻¹ s⁻¹ at 25°C for the reaction with photochemically produced 8×10^5 molecules/cm³ hydroxyl radical (GEMS 1986; quoted, Howard 1989).

Surface water: estimated $t_{1/2} = 2.7$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980) estimated $t_{1/2} = 2.7$ d, based on monitoring data for a river of 4 to 5-m deep (Zoeteman et al. 1980; quoted, Howard 1989).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 16.1.4.3.1
Reported aqueous solubilities of 4-nitrotoluene at various temperatures

Gross et al. 1931		Beneš & Dohnal 1999	
shake flask-interferometry		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	-	10	179
30	442	20	242
		30	322
		40	418
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 21.1 \pm 0.1$			
25°C			

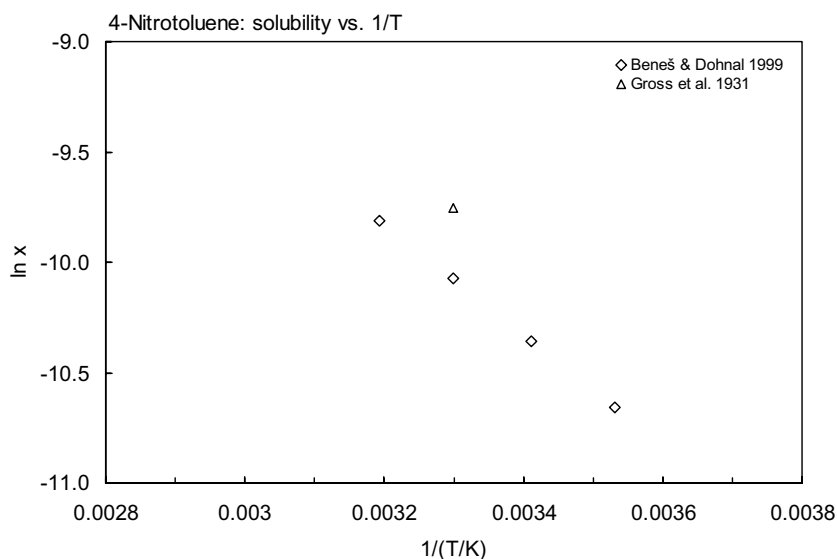


FIGURE 16.1.4.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-nitrotoluene.

TABLE 16.1.4.3.2

Reported vapor pressures of 4-nitrotoluene at various temperatures and the coefficients for the vapor pressure equations

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

1.

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Lenchitz & Velicky 1970	
static method-manometer		summary of literature data		ebulliometry		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
92.3	666.6	53.7	133.3	147.71	8851	23.886	0.6218
105.6	1333.2	85.0	666.6	151.43	10114	23.888	0.6283
120.3	2666.4	100.5	1333	165.98	16500	26.042	0.7311
125.7	3333	117.7	2666	197.75	42077	26.06	0.7330
130.4	3999.7	136.0	5333	216.17	67661	28.029	0.9426
134.4	4666	147.9	7999	233.25	101325	28.065	0.8994
137.9	5333	163.0	13332			30.205	1.0348
143.8	6666	186.7	26664	bp/°C	233.25	30.207	1.0423
164.0	13332	212.5	53329			32.012	1.3291
186.5	26664	238.3	101325			32.033	1.2987
201.2	39997					34.16	1.6681
212.2	53329	mp/°C	51.9			34.165	1.6551
220.8	66661					35.348	2.3313
228.4	79993					35.358	2.2839
234.8	93326					36.368	2.3087
237.7	101325						
						mp/°C	51.5
						enthalpy of sublimation:	
						$\Delta H_{\text{sub}} = 43.095 \text{ kJ mol}^{-1}$	
						at 25°C	
						eq. 1	P/mmHg
						A	11.5424
						B	4130.0828

2.

Ambrose & Gundry 1980		Aim 1994	
bubble-cap ebulliometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
143.498	5649	128.161	3639
148.11	7742	128.167	3639
153.159	9254	140.078	5776
158.081	10956	140.132	5787
163.205	12999	150.293	8378
168.438	15403	150.369	8400
173.494	18066	158.455	11107
180.103	22110	158.487	11118
185.757	26135	165.32	13946

(Continued)

TABLE 16.1.4.3.2 (Continued)

Ambrose & Gundry 1980		Aim 1994	
bubble-cap ebulliometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
192.227	31460	165.32	13967
198.564	37505	171.181	16823
205.643	44864	171.225	16845
212.568	54256	171.236	16848
218.948	63659	177.246	20306
225.722	75033	177.30	20332
233.058	89121	183.698	24639
238.685	101268		
239.269	102565	mp/°C	51.5
		bp/°C	238.343
tp/°C	51.64		
bp/°C	238.675	eq. 2	P/kPa
$\Delta H_{\text{fus}} = 16.81 \text{ kJ mol}^{-1}$		A	6.36793
$\Delta H_{\text{v}} = 46.60 \text{ kJ mol}^{-1}$, at bp		B	1931.718
		C	68.661
eq. 3	P/kPa	for temp range: 128–184°C	
A	6.27217		
B	1682.295		
C	−75.321		
for temp range: 416 to 513 K			
vapor pressure eq. for solid:			
eq. 1	P/kPa		
A	32.2514		
B	9018.0		
at triple pt	P = 67.72 Pa		
at 298.15 K	P = 5.5Pa		

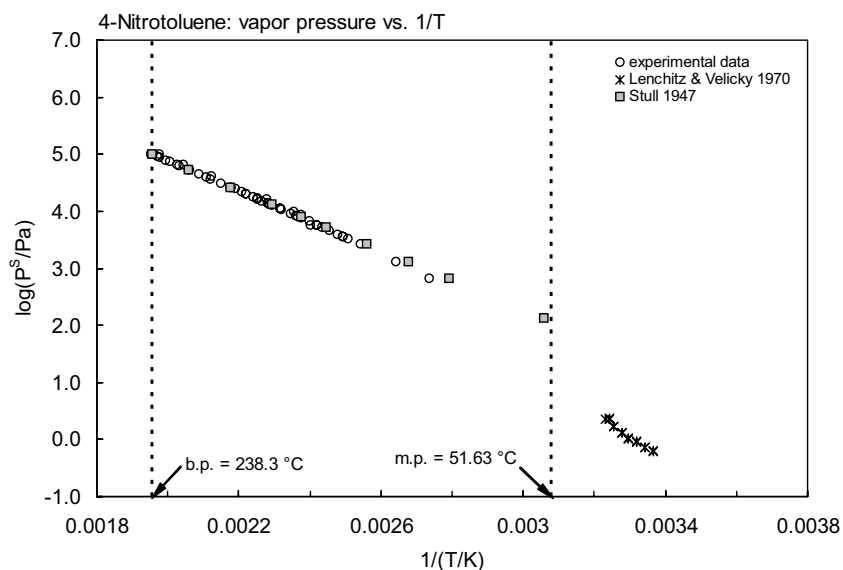
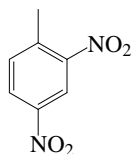


FIGURE 16.1.4.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-nitrotoluene.

16.1.4.4 2,4-Dinitrotoluene (DNT)



Common Name: 2,4-Dinitrotoluene

Synonym: dinitrotoluol, 1-methyl-2,4-dinitrobenzene, DNT

Chemical Name: 2,4-dinitrotoluene, 1-methyl-2,4-dinitrobenzene

CAS Registry No: 121-14-2

Molecular Formula: $C_7H_6N_2O_4$, $CH_3C_6H_3(NO_2)_2$

Molecular Weight: 182.134

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

70.5 (Lide 2003)

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

300 dec. (Weast 1982–83; Lide 2003)

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

1.521 ($15^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK:

–13.53 (Perrin 1972)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

58.99 (Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.358 (mp at $70.5^{\circ}C$)

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

270 ($22^{\circ}C$, Verschueren 1977, 1983)

300 ($22^{\circ}C$, Dunlap 1981)

276; 145 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

199 ($25.2^{\circ}C$, shake flask-HPLC/UV, Phelan & Barnett 2001)

188* ($22^{\circ}C$, shake flask-HPLC/UV, measured range 12.4 – $61.8^{\circ}C$, Phelan & Barnett 2001)

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

0.133* ($59^{\circ}C$, Knudsen effusion, measured range 59 – $69^{\circ}C$, Lenchitz & Velicky 1970)

0.00321 (extrapolated-Antoine eq., Lenchitz & Velicky 1970)

$\log (P/mmHg) = 12.6177 - 5139.058/(T/K)$; temp range 331.913 – $342.277 K$ (Knudsen effusion, Lenchitz & Velicky 1970)

0.0177* ($20^{\circ}C$, gas saturation-GC/ECD, measured range 277.5 – $344.15 K$, Pella 1977)

0.0290 (gas saturation-GC/ECD, interpolated-Antoine eq., measured range 277.5 – $344.15 K$ Pella 1977)

$\log (P/mmHg) = (13.08 \pm 0.19) - (4992 \pm 59)/(T/K)$; temp range 277.5 – $344.15 K$ (gas saturation, Pella 1977)

0.0147 ($20^{\circ}C$, Spangord et al. 1980)

0.6800 (quoted, Mabey et al. 1982)

$\log (P/kPa) = 5.06336 - 1216.523/(76.54 + t/^{\circ}C)$; temp range 100 – $199^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.0296, 0.0032 (extrapolated-Antoine eq.-I, eq.-II, Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.27361 - 5009.432/(T/K)$; temp range 277 – $343 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.7426 - 5139.058/(T/K)$; temp range 331 – $342 K$ (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.1423 - 3039/(T/\text{K})$; temp range 473–572 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04898 - 1956.095/(-108.183 + T/\text{K})$; temp range 344–572 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 5.798 - 1118/(61.8 + t/^\circ\text{C})$; temp range 200–299°C (Antoine eq., Dean 1992)

$\log (P/\text{mmHg}) = 11.5966 - 3.0079 \times 10^3/(T/\text{K}) - 1.6468 \cdot \log (T/\text{K}) + 1.5949 \times 10^{-3}(T/\text{K}) - 1.8722 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 343–814 K (vapor pressure eq., Yaws 1994)

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

0.0160 (calculated-P/C, Smith et al. 1981)

0.4560 (calculated-P/C, Mabey et al. 1982)

0.0878 (Smith et al. 1983; quoted, Howard 1989)

32.23 (quoted from WERL Treatability database, Ryan et al. 1988)

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

1.98 (shake flask, Hansch & Leo 1985)

2.04 (HPLC- k' correlation, Deneer et al. 1987)

1.98 (recommended, Sangster 1993)

1.98 (recommended, Hansch et al. 1995)

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

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

1.59 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

1.11, 1.76 (*daphnia magna*, *lumbriculus variegatus*, Liu et al. 1983)

> 3.30 (*selanastrum capricornutum*, Liu et al. 1983)

1.89, 0.602 (bluegill sunfish in viscera, bluegill sunfish in muscle, Liu et al. 1983)

2.31 \pm 0.03 (guppy-fat basis, Deneer et al. 1987)

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

1.65 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.68 (calculated- K_{OW} , Kolliig 1993)

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

Volatilization: half-life of approximately 100 d (Mills et al. 1982).

Photolysis: direct photolysis rate constant $k = 1.6 \times 10^{-2} \text{ h}^{-1}$ for summer at 40°N latitude in water (Mabey et al. 1982);

aqueous photolysis $t_{1/2} = 23\text{--}72 \text{ h}$, based on measured photolysis rates in water (Mill & Mabey 1985; Simmons & Zepp 1986; quoted, Howard et al. 1991);

atmospheric transformation lifetime $\tau \sim 1\text{--}5 \text{ d}$ (Kelly et al. 1994).

Hydrolysis:

Oxidation: aqueous oxidation rate constants $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 144 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 284\text{--}2840 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 3\text{--}33 \text{ h}$, based on measured photooxidation rates in natural waters (Spanggord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991).

Biodegradation: aqueous anaerobic $t_{1/2} = 48\text{--}240 \text{ h}$, based on anaerobic natural water die-away test data (Spanggord et al. 1980; quoted, Howard et al. 1991); aqueous aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).

Biotransformation: rate constant of $1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 284\text{--}2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime $\tau \sim 1\text{--}5$ d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2} = 3\text{--}33$ h, based on measured photooxidation rates in natural waters (Spangord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991);
estimated $t_{1/2} = 1.7$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
sunlight photolysis $t_{1/2} \sim 42$ h in pure water but ranged from 3 h to 10 h in three natural waters (Mabey et al. 1982).

Groundwater: $t_{1/2} = 48\text{--}8640$ h, based on estimated unacclimated aqueous anaerobic and aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

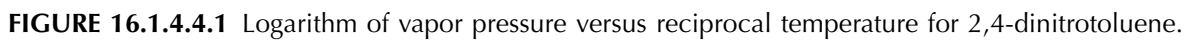
Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

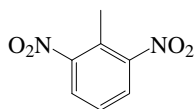
TABLE 16.1.4.4.1

Reported aqueous solubilities and vapor pressures of 2,4-dinitrotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Aqueous solubility		Vapor pressure			
Phelan & Barnett 2001		Lenchitz & Velicky 1970		Pella 1977	
shake flask-HPLC/UV		Knudsen effusion		gas saturation-GC	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
12.4	129	58.765	0.1731	4.0	0.00164
22.0	188	59.927	0.2073	10.0	0.0038
21.7	182	59.927	0.2138	20.0	0.0177
32.0	269	60.883	0.2328	30.0	0.0453
42.0	410	62.926	0.2568	40.0	0.171
51.0	608	62.824	0.3192	50.0	0.695
61.8	975	64.002	0.3450	60.0	1.663
41.2	397	65.115	0.3836	71.0	5.295
25.2	199	67.023	0.4380		
		68.10	0.4952	mp/°C	69.75–70.95
		69.127	0.5202		
				eq. 1	P/mmHg
				A	13.08
				B	4992
		enthalpy of sublimation: ΔH _{subl} = 98.324 kJ mol ⁻¹ (at 25°C)		enthalpy of sublimation: ΔH _{subl} = 95.81 kJ mol ⁻¹	
		eq. 1	P/mmHg		
		A	12.6177		
		B	5139.058		



16.1.4.5 2,6-Dinitrotoluene



Common Name: 2,6-Dinitrotoluene

Synonym: dinitrotoluol, 1-methyl-2,6-dinitrobenzene, 2-methyl-1,3-dinitrobenzene

Chemical Name: 2,6-dinitrotoluene, 1-methyl-2,6-dinitrobenzene

CAS Registry No: 606-20-2

Molecular Formula: $C_7H_6N_2O_4$, $CH_3C_6H_3(NO_2)_2$

Molecular Weight: 182.134

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

66.0 (Weast 1982–83; Howard 1989; Lide 2003)

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

285 (Verschuereen 1977; Callahan et al. 1979; Howard 1989; Lide 2003)

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

1.2833 ($111^{\circ}C$, Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

141.9 ($111^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.396 (mp at $66.0^{\circ}C$)

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

180 ($20^{\circ}C$, estimated, Mabey et al. 1982)

300 (selected, Mills et al. 1982)

182; 155 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

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

2.40 ($29^{\circ}C$, Mabey et al. 1982)

0.0756* (gas saturation-GC/ECD, fitted to Antoine eq., temp range 277.5–323.15 K, Pella 1977)

$\log(P/mmHg) = (13.99 \pm 0.18) - (5139 \pm 52)/(T/K)$, temp range 277.5–323.15 K (gas saturation, Pella 1977)

0.0756 (Howard et al. 1986; quoted, Banerjee et al. 1990)

0.0767 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.9436 - 4446.22/(-21.279 + T/K)$; temp range 277–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.329 - 2971/(T/K)$; temp range 423–523 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.70024 - 2160.968/(-93.282 + T/K)$; temp range 330–533 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

0.0756, 1.008 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/mmHg) = 4.372 - 380/(-43.6 + t/^{\circ}C)$; temp range 150–260 $^{\circ}C$ (Antoine eq., Dean 1992)

$\log(P/mmHg) = -14.5673 - 4.2746 \times 10^3/(T/K) + 12.904 \cdot \log(T/K) - 2.380 \times 10^{-2} \cdot (T/K) + 9.4513 \times 10^{-6} \cdot (T/K)^2$; temp range 339–770 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$)

0.800 (calculated-P/C, Mabey et al. 1982)

32.23 (quoted from WERL Treatability database, Ryan et al. 1988)

0.022 (SOGC 1987; quoted, Howard 1989)

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

1.72	(shake flask, Hansch & Leo 1985)
2.02	(HPLC- k' correlation, Deneer et al. 1987)
2.02	(shake flask-HPLC, Leggett et al. 1992)
2.07	(shake flask-UV, Nakagawa et al. 1992)
2.06	(recommended, Sangster 1993)
2.10	(recommended, Hansch et al. 1995)

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

3.72	(algal biomass, Davis et al. 1981)
1.71	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
1.08	(calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
2.44 ± 0.04	(guppy-fat basis, Deneer et al. 1987)

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

1.96	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
2.31	(soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
1.40	(calculated- K_{OW} , Kollig 1993)

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

Volatilization: $t_{1/2} \sim 100$ d (Mills et al. 1982).

Photolysis: aqueous photolysis $t_{1/2} = 17\text{--}25$ h, based on measured photolysis rates in water (Simmons & Zepp 1986; Mill & Mabey 1985; quoted, Howard et al. 1991)

89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).

Hydrolysis:

Oxidation: aqueous oxidation rate constants $k \ll 360 \text{ M}^{-1} \pm \text{h}^{-1}$ for singlet oxygen and $k = 144 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 2\text{--}17$ h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 284\text{--}2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous anaerobic $t_{1/2} = 48\text{--}300$ h, based on anaerobic natural water die-away test data for 2,4-dinitrotoluene; aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982)

Biotransformation in marine sediments: all broken down in 28 d when incubated at 10°C , and in 7 d when incubated at 20°C in the sandy sediment; degraded by days 7 and 3 for incubation at 10 and 20°C , respectively, in fine-grained sediment (Nipper et al. 2004).

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

Half-Lives in the Environment:

Air: estimated atmospheric $t_{1/2} = 8$ h, based on the vapor phase reaction with hydroxyl radical in air (GEMS 1985; quoted, Howard 1989); photooxidation $t_{1/2} = 284\text{--}2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: midday $t_{1/2} \sim 12$ min in Aucilla river due to indirect photolysis using experimentally determined rate constant $k = 3.6 \text{ h}^{-1}$ (Zepp et al. 1984);

photooxidation $t_{1/2} = 2\text{--}17$ h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991)

89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).

Ground water: $t_{1/2} = 48\text{--}8640$ h, based on estimated unacclimated aqueous anaerobic biodegradation half-life 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: degraded by days 28 and 7 for incubation at 10 and 20°C, respectively, in sandy marine sediment; degraded by days 7 and 3 for incubation at 10 and 20°C, respectively, in fine-grain sediment (Nipper et al. 2004)

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

TABLE 16.1.4.5.1
Reported vapor pressures of 2,6-dinitrotoluene at various temperatures

Pella 1977

gas saturation-GC	
t/°C	P/Pa
4.0	0.00342
10.0	0.0107
20.0	0.0383
30.0	0.147
40.0	0.483
50.0	1.718
mp/°C	57.25–57.75
eq. 1	P/mmHg
$\log P = A - B/(T/K)$	
A	13.99
B	5139
enthalpy of sublimation:	
$\Delta H_{\text{subl}} = 98.324 \text{ kJ mol}^{-1}$	

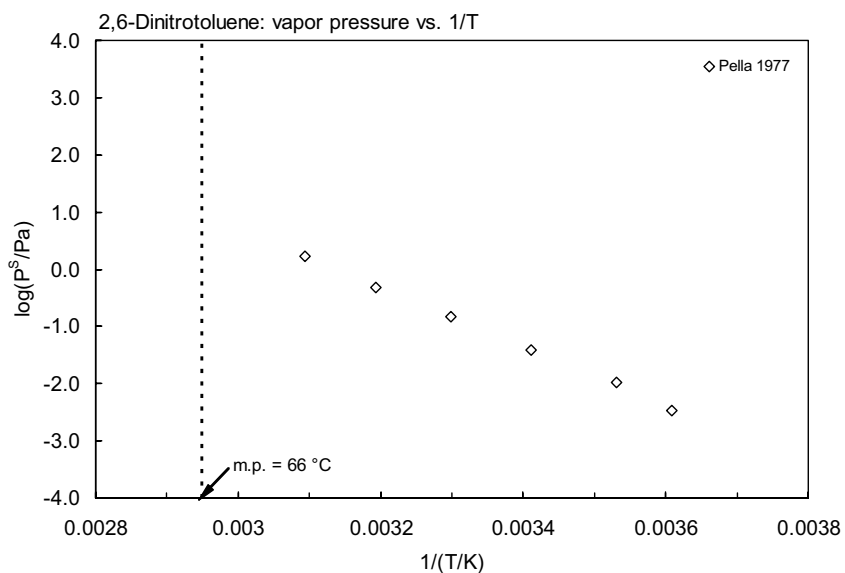
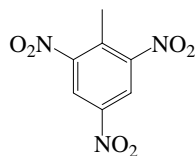


FIGURE 16.1.4.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dinitrotoluene.

16.1.4.6 2,4,6-Trinitrotoluene (TNT)



Common Name: 2,4,6-Trinitrotoluene

Synonym: TNT

Chemical Name: 2,4,6-trinitrotoluene

CAS Registry No: 118-96-7

Molecular Formula: $C_7H_5N_3O_6$, $(NO_2)_3C_6H_2CH_3$

Molecular Weight: 227.131

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

80.5 (Lide 2003)

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

240 explodes (Weast 1982–83; Dean 1992; Lide 2003)

Density (g/cm^3):

1.654 ($20^{\circ}C$, Weast 1982–83; Dean 1992)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

137.3 ($20^{\circ}C$, calculated-density)

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

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.285 (mp at $80.5^{\circ}C$)

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

120* ($20^{\circ}C$, shake flask, measured range 0.30 – $99.5^{\circ}C$, Taylor & Rinkenbach 1923)

85.8 ($21^{\circ}C$, Hale et al. 1979)

104* ($20^{\circ}C$, temp range 10 – $30^{\circ}C$, Spanggard et al. 1983)

200 ($15^{\circ}C$, Verschueren 1983)

100 (Dean 1992)

101.5* (average value at $pH < 9.1$, shake flask-HPLC/UV, measured range 6 – $42^{\circ}C$, Ro et al. 1996)

101.6, 100.5, 110.5 (pH 3.5, pH 6.8, pH 9.1, shake flask-HPLC/UV spectrophotometry, Ro et al. 1996)

$\ln [S/(mg\ L^{-1})] = 16.12 - 3413/(T/K)$, temp range 6 – $42^{\circ}C$, ($pH < 8$, shake flask-HPLC/spec., Ro et al. 1996)

115* ($23.02^{\circ}C$, shake flask-HPLC/UV, measured range 13.6 – $61^{\circ}C$, Phelan & Barnett 2001)

99.85* 97.7* 99.9* ($20^{\circ}C$, pH 4.2, 5.7, 6.2, shake flask-HPLC/UV, measured range 2.3 – $38^{\circ}C$, Lynch et al. 2001)

$\ln [S/(mg\ L^{-1})] = 16.981 - 3607.5/(T/K)$; temp range 2.3 – $38^{\circ}C$ (composite solubility prediction correlation, shake flask-HPLC/UV measurements, Lynch et al. 2001)

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

0.352* ($53^{\circ}C$, Knudsen effusion, measured range 50 – $143^{\circ}C$, Edwards 1950)

$\log (P_s/cmHg) = 14.34 - 6180/(T/K)$; range 50 – $81^{\circ}C$ (solid, Knudsen effusion, Edwards 1950)

$\log (P_L/cmHg) = 10.90 - 4960/(T/K)$; range 81 – $143^{\circ}C$ (liquid, Knudsen effusion, Edwards 1950)

0.0568* ($54.756^{\circ}C$, Knudsen effusion, measured range 55 – $76^{\circ}C$, Lenchitz & Velicky 1970)

$\log (P/mmHg) = 13.0776 - 5400.536/(T/K)$; temp range 55 – $76^{\circ}C$ (Knudsen effusion, Lenchitz & Velicky 1970)

0.00107* (gas saturation-GC/ECD, measured range 287.15 – 329.65 K, Pella 1977)

$\log (P/mmHg) = (12.31 \pm 0.34) - (5175 \pm 105)/(T/K)$, temp range 287.15 – 329.65 K (gas saturation, Pella 1977)

$\log (P/kPa) = 7.36331 - 3199.923/(248.004 + t/^{\circ}C)$; temp range 230 – $250^{\circ}C$ (liquid, Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.00078 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_g/\text{kPa}) = 13.596 - 5874.238/(T/K)$; temp range 293–353 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_g/\text{kPa}) = 12.2025 - 5400.536/(T/K)$; temp range 337–350 K (solid, Antoine eq.-II., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.40336 - 2191.85/(-121.43 + T/K)$; temp range 353–523 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 7.67152 - 2669.4/(205.6 + t/^\circ\text{C})$; temp range 230–250°C (Antoine eq., Dean 1992)

$\log (P/\text{mmHg}) = 6.3156 - 2.6756 \times 10^3/(T/K) - 4.6215 \cdot \log (T/K) + 6.1747 \times 10^{-9} \cdot (T/K) - 2.3743 \times 10^{-12} \cdot (T/K)^2$; temp range 354–518 K (vapor pressure eq., Yaws 1994)

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

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

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

1.8 (shake flask-HPLC, Leggett et al. 1992)

1.73 (recommended, Sangster 1993)

2.05 (estimated-SPARC, Elovitz & Weber 1999)

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

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

1.09 (aquatic oligochaete *Tubifex tubifex*, Conder et al. 2004)

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

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

Volatilization:

Photolysis: $t_{1/2} = 14$ h in summer, $t_{1/2} = 22$ –84 h in winter in pure water and photolyzed very rapidly in natural waters (Mabey et al. 1983)

photocatalytic degradation rates of TNT in a circular photocatalytic reactor using a UV lamp as a light source and TiO_2 as a photocatalyst: 1) at different initial TNT concns: $k = 0.0989 \text{ min}^{-1}$ with $t_{1/2} = 7.07$ min at initial concn of 10 mg/L; $k = 0.0644 \text{ min}^{-1}$ with $t_{1/2} = 10.76$ min at initial concn of 20 mg/L; $k = 0.0405 \text{ min}^{-1}$ with $t_{1/2} = 17.11$ min at initial concn of 30 mg/L; $k = 0.0269 \text{ min}^{-1}$ with $t_{1/2} = 25.77$ min at initial concn of 50 mg/L; and $k = 0.0165 \text{ min}^{-1}$ with $t_{1/2} = 42.01$ min at initial concn of 100 mg/L. 2) at different pH: $k = 0.0173 \text{ min}^{-1}$ with $t_{1/2} = 27.6$ min at pH 3.0; $k = 0.0422 \text{ min}^{-1}$ with $t_{1/2} = 20.1$ min at pH 7.0 and $k = 0.0451 \text{ min}^{-1}$ with $t_{1/2} = 21.5$ min at pH 11.0 (Son et al. 2004)

Photooxidation:

Hydrolysis:

Biodegradation: 95% disappearance within 2 h under aerobic conditions, and complete loss within 10 min under anaerobic conditions in sediment-water systems (Elovitz & Weber 1999)

Biotransformation: 100 % biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)

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

Half-Lives in the Environment:

Air:

Surface water: photolysis $t_{1/2} = 14$ h in summer, $t_{1/2} = 22$ –84 h in water in pure water, less than 1/2 h in some natural waters (Mabey et al. 1983)

photocatalytic degradation $t_{1/2} = 7.07$ min to 42.1 min for different initial concn of TNT from 10–100 mg/L, and $t_{1/2} = 27.1$ –21.5 min at pH 3.0–7.0 in a circular reactor, using a UV lamp as a light source and TiO_2 as a photocatalyst (Son et al. 2004)

Ground water:

Sediment: rapid disappearance 95% within 2 h, of TNT in an aerobic sediment-water system; under anaerobic conditions, TNT loss was complete within 10 min (Elovitz & Weber 1999)

100 % biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)

Soil:

Biota: steady-state concn reached within 1-h in uptake experiments, and TNT depuration after a 24-h exposure occurred completely by 3 h (aquatic oligochaete, Conder et al. 2004)

TABLE 16.1.4.6.1

Reported aqueous solubilities of 2,4,6-trinitrotoluene (TNT) at various temperatures

$$\ln S = A - B/(T/K)$$

(1)

1.

Taylor & Rinkenbach '23		Spanggord et al. 1983		Ro et al. 1996			Phelan & Barnett 2001	
shake flask				shake flask-HPLC/UV			shake flask-HPLC/UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	pH	S/g·m ⁻³	t/°C	S/g·m ⁻³
	average*							
0.30	110	10	67	6	3.7	52.5	13.9	86
5.9	113	20	104	6	6.9	51.3	23.02	115
20.0	120	30	165	12	6.9	64.0	33.3	191
33.1	203			13	3.7	72.2	42.6	266
44.2	340			13	6.9	64.4	51.8	427
45.0	370			20	4.2	86.2	61.0	641
53.0	534			20	7.3	88.5	33.2	191
57.15	614			20	9.2	96.8	13.6	90
73.25	963			20	9.4	95.7	13.6	92
94.4	1375			20	10.1	91.2		
99.5	1467			21	3.5	74.5		
				21	6.8	82.5		
				21	9.1	88.2		
				25	3.5	101.6		
				25	6.8	100.5		
				25	9	110.5		
				42	4.0	204.9		
				42	6.8	204.5		
				42	9.3	167.6		
average of 3 sets of data								
$\ln [S/(\text{mg/L})] = 16.12 - 3413/(T/K)$								
for pH < 8								

2.

Lynch et al. 2001					
shake flask-HPLC/UV					
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
	pH 4.2		pH 5.7		pH 6.2
2.3	49.5	2.3	54.5	2.4	55.0
2.3	50.5	2.2	54.2	2.4	56.4
2.6	54.9	2.3	47.5	2.4	54.9
2.6	55.7	2.3	47.3	2.4	55.4
4.2	57.6	4.1	47.9	4.7	56.7

TABLE 16.1.4.6.1 (Continued)

Lynch et al. 2001					
shake flask-HPLC/UV					
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.2	57.7	4.1	48.2	4.7	57.4
4.2	45.7	4.6	58.1	5.2	56.7
4.2	48.4	4.6	59.1	5.2	56.1
20	100.7	20	96.7	20	99.6
20	99.0	20	98.7	20	100.2
20	99.2	20.1	98.9	20.1	99.5
20	101.7	20.1	100.6	20.1	96.3
20.1	96.3	20.2	98.8	20.1	99.5
20.1	95.9	20.2	99.8	20.1	99.8
20.1	96.0	20.2	97.5	20.2	94.6
20.1	97.8	20.2	100.4	20.2	97.2
36	211.7	35.7	208.5	35.9	216.5
36	213.1	35.7	213.5	35.9	213.9
36	208.5	36	215.2	36	212.2
36	211.6	36	214.3	36	215.3
37.7	219.6	37.7	229.7	37.6	229.4
37.7	219.4	37.7	230.6	37.6	231.4
37.8	218.2	37.7	226.2	38	234.4
37.8	214.8	37.7	228.3	38	235
eq. 1	S/(mg L ⁻¹)	eq. 1	S/(mg L ⁻¹)	eq. 1	S/(mg L ⁻¹)
A	22.741	A	22.399	A	23.244
B	6332	B	6230	B	6506.8

composite correlation eq. : ln [S/(mg L⁻¹) = 16981 – 3607.5/(T/K); temp range 2.3–38°C

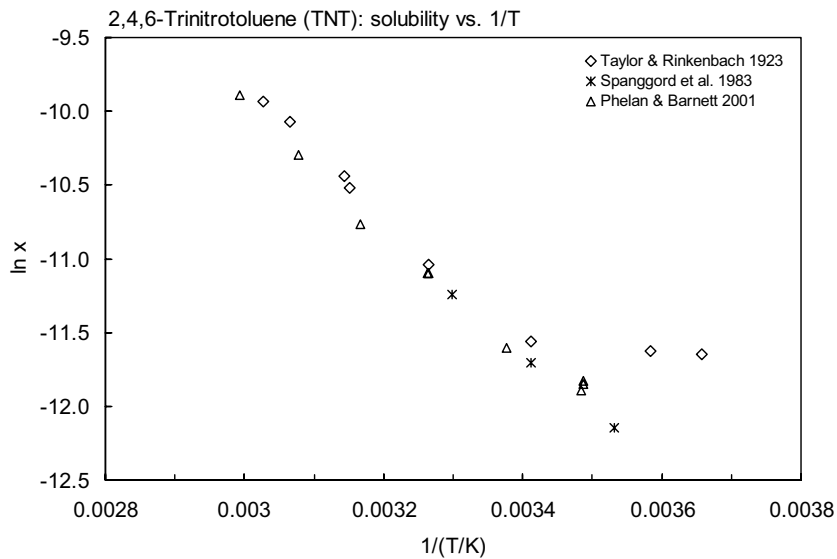


FIGURE 16.1.4.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2,4,6-trinitrotoluene.

TABLE 16.1.4.6.2

Reported vapor pressures of 2,4,6-trinitrotoluene (2,4,6-TNT) 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)			
Edwards 1950		Lenchitz & Velicky 1970		Pella 1977	
Knudsen method		Knudsen effusion		gas saturation-GC	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
53.0	0.0352	54.756	0.0568	14.0	0.000302
60.1	0.0724	59.704	0.0935	19.0	0.000412
60.8	0.0843	64.853	0.1613	25.0	0.00107
61.5	0.0915	70.02	0.3118	25.3	0.00128
61.0	0.0829	72.469	0.3665	26.5	0.00170
72.1	0.4146	72.493	0.3409	35.0	0.00676
72.1	0.4186	75.065	0.5142	40.0	0.00887
78.5	0.8586	65.91	0.1811	45.0	0.0143
78.5	0.7839	68.933	0.2342	50.0	0.0243
78.3	0.8293	73.981	0.4453	55.0	0.0446
79.8	0.8733	76.057	0.5796	56.5	0.05406
80.2	0.9546				
82.4	1.0612	mp/ $^{\circ}\text{C}$	81.1	mp/ $^{\circ}\text{C}$	80.15–81.25
86.9	1.5865				
99.5	5.2529	enthalpy of sublimation: $\Delta H_{\text{subl}} = 120.92 \text{ kJ mol}^{-1}$ (at 25 $^{\circ}\text{C}$)		eq. 2	P/mmHg
99.5	5.4262			A	12.31
110.6	11.012			B	5175
110.5	10.612				
131.5	46.396	eq. 1	P/mmHg	enthalpy of sublimation: $\Delta H_{\text{subl}} = 99.161 \text{ kJ mol}^{-1}$	
141.4	82.793	A	13.0776		
142.0	87.728	B	5400.536		
142.5	82.260				
For solid:					
eq. 1	P/cmHg				
A	14.34				
B	6180				
$\Delta H_{\text{subl}} = 118.41 \text{ kJ mol}^{-1}$					
For liquid:					
eq. 1	P/cmHg				
A	10.90				
B	4960				
$\Delta H_{\text{subl}} = 94.98.34 \text{ kJ mol}^{-1}$					

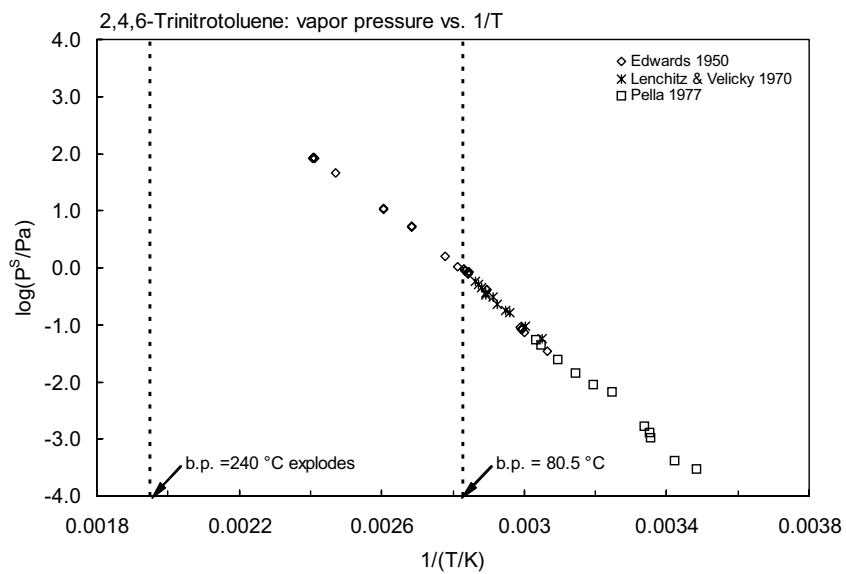
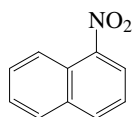


FIGURE 16.1.4.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trinitrotoluene.

16.1.4.7 1-Nitronaphthalene (α -Nitronaphthalene)

Common Name: 1-Nitronaphthalene

Synonym: α -nitronaphthalene

Chemical Name: 1-nitronaphthalene, α -nitronaphthalene

CAS Registry No: 86-57-7

Molecular Formula: $C_{10}H_7NO_2$

Molecular Weight: 173.169

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

61 (Lide 2003)

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

304.0 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987)

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

1.3320 (Weast 1982–83)

1.2230 (Dean 1985)

Molar Volume (cm^3/mol):

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

135.8 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.99 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

54.39 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.443 (mp at $61^{\circ}C$))

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

50.0 (Aqueous Solubility Database, Yalkowsky et al. 1987)

9.82 (generator column-HPLC/UV, Yu & Xu 1992)

9.83 (calculated-molar concentration, Yu & Xu 1992)

50; 34.6 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.202 (effusion method-fitted to Antoine eq., Radchenko & Kitiagorodskii 1974)

0.202 (solid, extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

0.184 (liquid, extrapolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.31261 - 3579.698/(T/K)$; temp range 309–326 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 13.223 - 5584/(T/K)$; temp range 325–332 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.8959 - 3468.4/(T/K)$; temp range 332–580 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

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

3.463 (calculated-P/C with selected values)

0.178 (gas stripping-GC, Altschuh et al. 1999)

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

3.19 (Hansch & Leo 1979)

3.19 (shake flask, Hansch & Leo 1987)

- 3.19 (shake flask-UV, Debnath & Hansch 1992)
 3.19 (recommended, Sangster 1993)

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis: measured photolysis rate constant are: $15.9 \times 10^{-4} \text{ s}^{-1}$ in a 6400-L indoor all-Teflon chamber under blacklamp irradiation and $1.37 \times 10^{-4} \text{ s}^{-1}$ outdoor in a 1000-L all-Teflon chamber under natural solar irradiation (Atkinson et al. 1989);

photolysis rate $k_{\text{phot}} = 1.5 \times 10^{-4} \text{ s}^{-1}$ with a half-life of 1.7 h (Arey et al. 1990)

Hydrolysis:

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:

$k_{OH} = (5.4 \pm 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{NO_3} \leq 7.2 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} < 6.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{N_2O_5} = 1.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 and at $298 \pm 2 \text{ K}$ in the atmosphere (Atkinson et al. 1989)

$k_{OH} = 5.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetime of 2.9 d; $k_{NO_3} \leq 7.2 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetime of -13 d, $k_{O_3} < 6.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of > 28 d and $k_{N_2O_5} = 1.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 a calculated lifetime of 2.4 yr at $298 \pm 2 \text{ K}$ in the atmosphere (Arey et al. 1990)

Biodegradation:

Biotransformation:

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

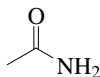
Half-Lives in the Environment:

Air: calculated lifetime of ~2 h based on measured outdoor photolysis rate and rate constants the gas-phase reactions (Atkinson et al. 1989);

photolysis $t_{1/2} = 1.7 \text{ h}$ using an average 12-h daytime NO_2 photolysis rate $k = 5.2 \times 10^{-3} \text{ s}^{-1}$ – a dominant atmospheric loss process; calculated lifetimes of 2.9 d, -13 d, > 28 d and 2.4 yr due to reactions with OH radical, NO_3 radical, O_3 and N_2O_5 (Arey et al. 1990)

16.1.5 AMIDES AND UREAS

16.1.5.1 Acetamide



Common Name: Acetamide

Synonym: ethanamide

Chemical Name: acetamide, acetic acid amine

CAS Registry No: 60-35-5

Molecular Formula: C_2H_5NO , CH_3CONH_2

Molecular Weight: 59.067

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

80.16 (Lide 2003)

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

221 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.9986 ($78^{\circ}C$, Weast 1982–83)

1.159 (Verschueren, 1983)

Molar Volume (cm^3/mol):

59.2 (calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant pK_a : 7.62Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.1 (at bp, Riddick et al. 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):78.66 ($25^{\circ}C$, Riddick et al. 1986)Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.707 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.288 (mp at $80.16^{\circ}C$)Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):975000 ($20^{\circ}C$, Verschueren 1983)408000 ($20^{\circ}C$, Riddick et al. 1986)Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):8.61 (extrapolated-regression of tabulated data, temp range 65 – $222^{\circ}C$, Stull 1947) $\log(P/mmHg) = [-0.2185 \times 14025.3/(T/K)] + 9.088352$; temp range 65.0 – $222^{\circ}C$ (Antoine eq., Weast 1972–73)

100 (Riddick et al. 1986)

 $\log(P/kPa) = 8.24516 - 3282.80/(T/K)$; temp range 65 – $150^{\circ}C$ (Antoine eq., Riddick et al. 1986) $\log(P/kPa) = 7.93409 - 2936.07/(T/K)$; temp range 65 –bp (Antoine eq., Riddick et al. 1986)

2.44 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

 $\log(P_g/kPa) = 10.9717 - 4050.1/(T/K)$; temp range 298 – $349 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987) $\log(P_l/kPa) = 7.97079 - 1998.3/(-89.32 + T/K)$; temp range 381 – $492 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987) $\log(P/mmHg) = -413.1683 + 8.1328 \times 10^3/(T/K) + 172.9 \cdot \log(T/K) - 0.16059 \cdot (T/K) + 5.3892 \times 10^{-5} \cdot (T/K)^2$; temp range 354 – $761 K$ (vapor pressure eq., Yaws 1994)Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$): 3.53×10^{-4} (calculated-P/C with selected values)Octanol/Water Partition Coefficient, $\log K_{ow}$:

-1.09 (shake flask-radiochemical method, Cornford 1982)

- 1.26 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.26 (shake flask-GC, Sotomatsu et al. 1987)
- 1.26 (recommended Sangster 1989, 1993)
- 1.23 (calculated-QSAR, Kollig 1993)
- 1.26 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

- 1.55 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 3.2\text{--}32$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Hydrolysis: overall rate constant $k_h = 5.5 \times 10^{-12} \text{ s}^{-1}$ with $t_{1/2} = 3950$ yr; acid rate constant $k_A = 8.36 \times 10^{-6} \text{ s}^{-1}$ and base rate constant $k_B = 5.5 \times 10^{-5} \text{ s}^{-1}$ at 25°C and pH 7 (Mabey & Mill 1978) acid rate constant $k = 0.03 [\text{M} \pm (\text{H}^+) \pm \text{h}]^{-1}$ at pH 5 and base rate constant $k = 0.17 [\text{M} \pm (\text{OH}^-) \pm \text{h}]^{-1}$ at pH 9 with first-order hydrolysis $t_{1/2} = 3950$ yr at pH 7 and 25°C , (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 24\text{--}168$ h, based on aerobic aqueous screening test data (Malaney & Gerhold 1962, 1969; Urano & Kato 1986; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2} = 96\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 3.2\text{--}32$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

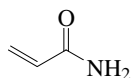
Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.5.2 Acrylamide



Common Name: Acrylamide

Synonym: 2-propenamide

Chemical Name: acrylamide

CAS Registry No: 79-06-1

Molecular Formula: C_3H_5NO , $CH_2=CHCONH_2$

Molecular Weight: 71.078

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

84.5 (Lie 2003)

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

192.5 (Lide 2003)

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

1.122 ($30^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

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

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.261 (mp at $84.5^{\circ}C$)

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

2050000 (quoted, Verschueren 1983)

2150000 ($30^{\circ}C$, Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.616 (average, extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.395 - 3213/(T/K)$, temp range 357–413 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 10.31055 - 3994.667/(T/K)$, temp range 373–413 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 17.0034 - 4.4434 \times 10^3/(T/K) - 1.7158 \cdot \log(T/K) + 2.0063 \times 10^{-6} \cdot (T/K) - 8.0394 \times 10^{-10} \cdot (T/K)^2$; temp range 358–477 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

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

-0.90 (shake flask, Fujisawa & Masuhara 1980, 1981)

-1.24 (calculated-HPLC-RT correlation, Fujisawa & Masuhara 1981)

-0.67 (shake flask, Log P Database, Hansch & Leo 1987)

-0.78 (recommended, Sangster 1989)

-0.67 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

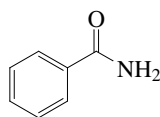
-0.969 (calculated- K_{OW} , Kollig 1993)

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

Half-Lives in the Environment:

Surface water: measured rate constant $k = (1.0 \pm 0.1) \times 10^5 M^{-1} s^{-1}$ for direct reaction with ozone in water at pH 5.4–5.8 and $22 \pm 1^{\circ}C$, with $t_{1/2} = 0.3$ s at pH 7 (Yao & Haag 1991).

16.1.5.3 Benzamide



Common Name: Benzamide

Synonym: benzoylamide

Chemical Name: benzamide

CAS Registry No: 55-21-0

Molecular Formula: C_7H_7NO , $C_6H_5CONH_2$

Molecular Weight: 121.137

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

127.3 (Lide 2003)

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

290 (Lide 2003)

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

Molar Volume (cm^3/mol):

112.2 ($130^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0992 (mp at $127.3^{\circ}C$)

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

13500 ($20-25^{\circ}C$, shake flask-gravimetric method, Dehn 1917)

13499 (Tsonopoulos & Prausnitz 1971)

13490 (Windholz 1983)

13515 (1 g in 74 mL, Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00522 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.69847 - 5062.899/(T/K)$, temp range 325–342 K (solid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

4.52×10^{-5} (calculated-P/C, this work)

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

0.64 (shake flask-UV, Fujita et al. 1964)

0.65 (shake flask, Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1987)

0.66 (shake flask-UV, Yaguzhinskii et al. 1973)

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

0.64 (shake flask-UV, Sotomatsu et al. 1987)

0.50 (centrifugal partition chromatography CPC, Berthod et al. 1988)

0.81 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

0.64 (recommended, Sangster 1989, 1993)

0.65 (counter-current chromatography, Vallat et al. 1990)

0.65 (CPC-RV correlation, El Tayar et al. 1991)

0.64 (shake flask-GC, Alcorn et al. 1993)

0.64 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

- 0.954; 1.301; 1.756 (sediment; Alfisol soil; Podzol soil, von Oepen et al. 1991)
- 1.46 (soil, quoted exptl., Meylan et al. 1992)
- 1.71 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.46 (soil, mean value, Kördel et al. 1993)
- 1.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.46; 1.71 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 1.87, 2.17, 1.12, 1.36, 1.645 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 1.46, 1.22; 2.18, 1.75, 1.88, 1.83, 1.31 (soil: quoted lit., calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)
- 1.747, 1.358, 1.236 (second generation of European reference soil set, Eurosoils ES-1, ES-3, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

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

Volatilization:

Photolysis:

Oxidation: aqueous photooxidation $t_{1/2} = 960 - 7.4 \times 10^4$ h, based on measured rates for reaction with OH radical in water (Anbar et al. 1966; Dorfman and Adams 1973; selected, Howard et al. 1991);
photooxidation $t_{1/2} = 3.1 - 31$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson et al. 1987; selected, Howard et al. 1991).

Hydrolysis: not expected to be significant based on estimated half-lives for hydrolysis of acetamide of 261, 3950, and 46 yr at pH 5, 7, 9, respectively, which were calculated using experimental acid and base hydrolysis rate constants for acetamide (Mabey & Mill 1978; selected, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 48 - 360$ h, and aqueous anaerobic biodegradation $t_{1/2} = 192 - 1400$ h, both based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 3.1 - 31$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson et al. 1987; selected, Howard et al. 1991).

Surface water: $t_{1/2} = 48 - 360$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

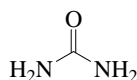
Ground water: $t_{1/2} = 96 - 720$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 48 - 360$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Biota:

16.1.5.4 Urea



Common Name: Urea

Synonym: carbamide, carbonyldiamide, Aquacare, Aqiadrate, Basodexam, Keratinamin, Nutraplus, Onychomal, Pastaron, Ureaphil, Ureophil, Ureaparl

Chemical Name: urea, carbamide, carbonyldiamide

CAS Registry No: 57-13-6

Molecular Formula: $\text{CH}_4\text{N}_2\text{O}$, H_2NCONH_2

Molecular Weight: 60.055

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

133 (Lide 2003)

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

decompose (Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.323 (Weast 1982–83)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

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

Enthalpy of Fusion, ΔH_fus (kJ/mol):

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

Fugacity Ratio at 25°C (assuming $\Delta S_\text{fus} = 56 \text{ J}/\text{mol} \pm \text{K}$), F : 0.0872 (mp at 133°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

975000* (shake flask, measured range 0 – 69.5°C , Speyers 1902)

790000 (20 – 25°C , shake flask-gravimetric method, Dehn 1917)

1047000* (20°C , shake flask, measured range 0 – 70°C , Pinck & Kelly 1925)

53.97 wt %* (23.85°C , synthetic method, measured range 18.72 – 73.11°C , Shnidman & Sunier 1932)

$\log x = -609.8/(T/\text{K}) + 1.468$; temp range 20 – 70°C (synthetic method, Shnidman & Sunier 1932)

0.4388* (60°C , mole fraction solubility, synthetic method, measured range 60 – 100°C , Kakinuma 1941)

997400 (W indholz 1983)

1000000 (Dean 1985; Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

1.61×10^{-3} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (\text{P}_\text{s}/\text{kPa}) = 9.565 - 4579/(T/\text{K})$; temp range 345 – 368 K (solid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pam^3/mol):

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

−1.09 (Hansch & Leo 1979)

−3.00 (Kenaga & Goring 1980)

−1.21, −1.79 to −0.62 (shake flask method: mean, range of mean values, OECD 1981)

−1.54 (shake flask-radiochemical method, Cornford 1982)

−1.57 (HPLC-RT correlation, Harnish et al. 1983)

−1.56 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)

−1.66, −2.11 (shake flask, Log P Database, Hansch & Leo 1987)

−1.60 (shake flask-UV, pH 7.4, Huang 1990)

−2.11 (from Medchem software value, Chessells et al. 1992)

−2.11 (recommended, Sangster 1993)

−1.66 (Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

4.068 (alga *chlorella fusca*, wet wt. basis, Geyer et al. 1984)
 -0.10 (alga *chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)

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

0.50, 0.62 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 0.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Half-Lives in the Environment:

TABLE 16.1.5.4.1
Reported aqueous solubilities of urea at various temperatures

Speyers 1902		Shnidman & Sunier 1932						Kakinuma 1941	
re-calcd by Pinck & Kelly		synthetic method-heating -shake flask						synthetic method	
t/°C	S/g·m ⁻³	t/°C	wt %	x	t/°C	wt %	x	t/°C	x
		urea 1#			urea 2#				
0	674000	18.72	51.10	0.2387	21.59	52.80	0.2513	60	0.4388
11.0	875000	26.80	55.37	0.2712	23.85	53.97	0.2602	65	0.4610
19.8	975000	27.31	55.83	0.2740	30.38	57.51	0.2888	70	0.4903
31.7	1310000	35.42	59.94	0.3099	35.15	59.97	0.3102	75	0.5204
51.4	1930000	37.36	60.87	0.3183	41.11	62.95	0.3377	80	0.6617
69.5	2530000	43.94	64.19	0.3489	43.85	64.31	0.3510	85	0.5843
		46.56	65.39	0.3618	54.97	69.53	0.4065	90	0.6190
		54.77	69.33	0.4041	55.88	70.10	0.4131	95	0.6542
		67.02	70.38	0.4163	69.13	71.49	0.4294	100	0.6910
$\Delta H_{sol}/(kJ\ mol^{-1})$		61.76	72.59	0.4428	63.79	73.64	0.4561		
25°C		73.11	77.57	0.5093	70.49	76.60	0.4956	$\log x = A - B/(T/K)$	
								A	1.5314
								B	631.86
		mp/°C	132.7		mp/°C	132.6			
Pinck & Kelly 1925		mole fraction solubility expressed as:							
shake flask		$\log x = -609.8/(T/K) + 1.468$; temp range 20–70°C							
t/°C	S/g·m ⁻³								
0	670000								
10.0	840000								
20.0	1047000								
30.0	1360000								
39.7	1654000								
50.0	2050000								
50.6	2064000								
60.0	2460000								
68.5	2950000								
70.0	3146000								

urea 1# – urea made by synthetic $NH_3 + CO_2$ process—re-crystallized from water

urea 2# – urea made from calcium-cyanamid — re-crystallized from water and methanol

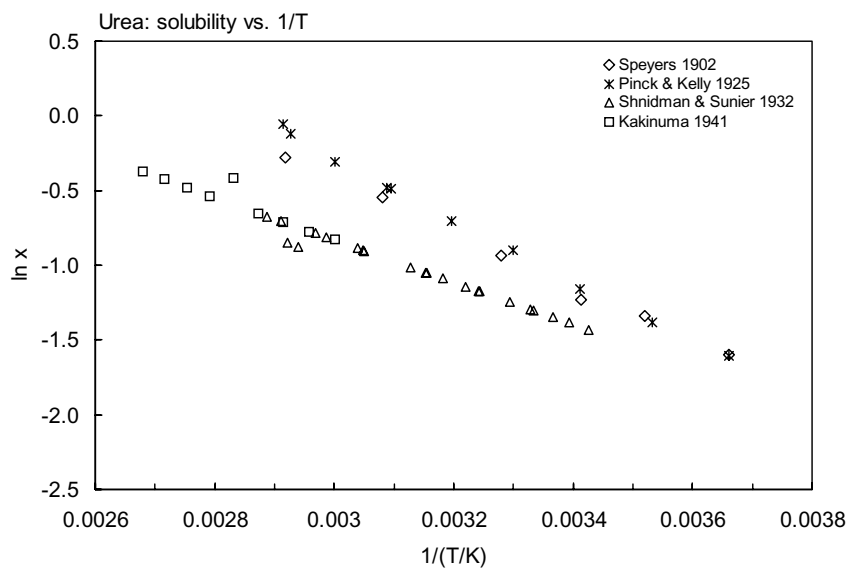


FIGURE 16.1.5.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for urea.

16.1.6 NITROSAMINES

16.1.6.1 *N*-Nitrosodimethylamine

Common Name: Dimethylnitrosoamine

Synonym: *N*-nitrosodimethylamine, *N*-methyl-*N*-nitrosomethanamine, nitrous dimethylamine

Chemical Name: dimethylnitrosoamine, *N*-nitrosodimethylamine

CAS Registry No: 62-75-9

Molecular Formula: $C_2H_6N_2O$, $CH_3N(NO)CH_3$

Molecular Weight: 74.081

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

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

152 (Lide 2003)

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

1.005 ($18^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

73.7 ($10^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant pK_a :

< 1.0 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

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

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

miscible (Mirvish et al. 1976)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

1080 (Mabey et al. 1982)

730 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.10632 - 2159.476/(T/K)$, temp range 309–423 K (Antoine eq., Stephenson & Malanowski 1987)

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

3.344 (calculated, Mabey et al. 1982)

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

0.06 (Radding et al. 1977)

−0.57 (shake flask-UV, Singer et al. 1977)

−0.68 (calculated-f const., Mabey et al. 1982)

0.46 ($30.5^{\circ}C$, shake flask-HPLC, Vera et al. 1992)

0.76 (calculated, Kollig 1993)

−0.57 (recommended, Sangster 1993)

−0.57 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

−0.96 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

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

−1.00 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

0.448 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis: both aqueous and atmospheric photolysis $t_{1/2} = 0.5\text{--}1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).

Hydrolysis:

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 constants $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, and $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

$k_{\text{OH}} = 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{O}_3} \leq 1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Tuazon et al. 1984); photooxidation $t_{1/2} = 25.4\text{--}254$ h in air, based on measured rate constant for the reaction with OH radical in air (Howard et al. 1991);

$k_{\text{OH}} = (2.53 - 3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at 296–298 K (Atkinson 1989).

Biodegradation: aqueous aerobic $t_{1/2} = 504\text{--}4320$ h, based on aerobic soil die-away test data; and aqueous anaerobic $t_{1/2} = 2016\text{--}17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived from results of Tate & Alexander 1975; and Oliver et al. 1979; Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^{-12} \text{ mL} \pm \text{cell}^{-1} \pm \text{h}^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: $t_{1/2} = 0.5\text{--}1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991);

estimated photolysis $t_{1/2} \sim 5$ min, $t_{1/2} = 3$ d for reaction with OH radical and $t_{1/2} > 2$ yr for reaction with O_3 (Tuazon et al. 1984);

photooxidation $t_{1/2} = 25.4\text{--}254$ h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.5\text{--}1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).

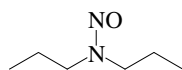
Groundwater: $t_{1/2} = 1008\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2} \sim 3$ wk in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)

$t_{1/2} = 504\text{--}4320$ h, based on aerobic soil die-away test data (derived from data of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota:

16.1.6.2 *N*-Nitrosodipropylamine

Common Name: Di-*n*-Propylnitrosoamine

Synonym: N-nitrosodi-*n*-propylamine, N-nitroso-N-propyl-1-propanamine

Chemical Name: di-*n*-propylnitrosoamine, N-nitrosodi-*n*-propylamine

CAS Registry No: 621-64-7

Molecular Formula: $C_6H_{14}N_2O$, $CH_3CH_2CH_2N(NO)CH_2CH_2CH_3$

Molecular Weight: 130.187

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

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

206 (Lide 2003)

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

Molar Volume (cm^3/mol):

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

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

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

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

9900 (Mirvish et al. 1976)

Vapor Pressure (Pa at $25^{\circ}C$):

53.33 ($37^{\circ}C$, calculated-Troutin's rule, Mabey et al. 1982)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

0.638 (calculated-P/C, Mabey et al. 1982)

0.355 (calculated-P/C, this work)

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

1.31 (calculated as per Leo et al. 1971 from Mirvish et al. 1976 data, Callahan et al. 1979)

1.36 (shake flask-UV, Singer et al. 1977)

1.49 (calculated-f const., Mabey et al. 1982)

2.35 ($30.5^{\circ}C$, shake flask-HPLC, Vera et al. 1992)

2.45 (recommended, Sangster 1993)

1.35 (Kollig 1993)

1.36 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

0.99 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

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

1.18 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.09 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis: both aqueous and atmospheric photolysis $t_{1/2} = 0.17$ – 1.0 h, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: rate constants in water for singlet oxygen $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 2.66\text{--}26.6 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 504\text{--}4320 \text{ h}$, based on aerobic soil die-away test data, and aqueous anaerobic $t_{1/2} = 2016\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived from results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biotransformation: rate constant for bacterial biotransformation $k \sim 3 \times 10^{-12} \text{ mL} \pm \text{cell}^{-1} \pm \text{h}^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.66\text{--}26.6 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Surface water: $t_{1/2} = 0.17\text{--}1.0 \text{ h}$, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 1008\text{--}8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

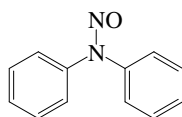
Sediment:

Soil: degradation $t_{1/2} \sim 3 \text{ wk}$ in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)

$t_{1/2} = 504\text{--}4320 \text{ h}$, based on aerobic soil die-away test data (derived from results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota

16.1.6.3 Diphenylnitrosoamine



Common Name: Diphenylnitrosoamine

Synonym: N-nitrosodiphenylamine, N-nitroso-N-phenylbenzamine

Chemical Name: diphenylnitrosoamine, N-nitrosodiphenylamine

CAS Registry No: 86-30-6

Molecular Formula: $C_{12}H_{10}N_2O$, $C_6H_5N(NO)C_6H_5$

Molecular Weight: 198.219

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

66.5 (Weast 1982–83; Lide 2003)

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

151–153 (Windholz 1976; Callahan et al. 1979)

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

Molar Volume (cm^3/mol):

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

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.392 (mp at $66.5^{\circ}C$)

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

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

40.0 (calculated-S, Mabey et al. 1982)

Vapor Pressure (Pa at $25^{\circ}C$):

13.33 (estimated, Mabey et al. 1982)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

66.87 (calculated-P/C, Mabey et al. 1982)

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

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

3.13 (recommended, Sangster 1993)

3.13 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

2.63 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

2.34 (quoted, Isnard & Lambert 1988)

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

2.81 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

2.84 (calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constants in water for singlet oxygen $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical $k < 3600 \text{ M}^{-1} \pm \text{h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 0.70 - 7.0 \text{ h}$ in air, based on measured rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 240 - 816 \text{ h}$, based on data from one soil-die-away test; a range was bracketed around the reported $t_{1/2} = 22 \text{ d}$ (Mallik & Tesfai 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 960 - 3264 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 1 \times 10^{-10} \text{ mL} \pm \text{cell}^{-1} \pm \text{h}^{-1}$ in water (Mabey et al. 1982).

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

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.70 - 7.0 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radicals in air (quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 240 - 816 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 480 - 1632 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 240 - 816 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.7 HETEROCYCLIC COMPOUNDS

16.1.7.1 Pyrrole



Common Name: Pyrrole

Synonym: 1H-pyrrole

Chemical Name: pyrrole, 1H-pyrrole

CAS Registry No: 109-97-7

Molecular Formula: C_4H_4NH

Molecular Weight: 67.090

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

−23.39 (Lide 2003)

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

129.79 (Lide 2003)

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

0.9691 (Weast 1982–83; Dean 1985)

0.96985, 0.96565 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

69.2 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK_a :

−4.40 (Perrin 1972)

−3.80 (Riddick et al. 1986)

−4.10 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.15, 38.75 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.908 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

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

47000 (Dean 1985)

45000 (Riddick et al. 1986)

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

358285* ($176.67^{\circ}C$, static-Bourdon gauge, measured range 176.67 – $271.11^{\circ}C$, Kobe et al. 1956)

1102* (ebulliometry, extrapolated-Antoine eq., measured range 65.67 – $166^{\circ}C$, Scott et al. 1967; Osborn & Douslin 1968)

$\log (P/mmHg) = 7.30295 - 1507.015/(t/^{\circ}C + 211.010)$; temp range 65.67 – $166^{\circ}C$ (Antoine eq., ebulliometry, Scott et al. 1967)

$\log [(P/atm) = [1 - 402.914 \pm (T/K)] \times 10^{\{0.870073 - 5.43768 \times 10^{-4} \pm (T/K) + 4.16086 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 65.67 – $166^{\circ}C$ (ebulliometric method, Cox eq., Scott et al. 1967)

$\log (P/mmHg) = 7.30275 - 1506.877/(t/^{\circ}C + 210.995)$, temp range 65.57 – $166^{\circ}C$ (ebulliometric method, Antoine eq., Scott et al. 1967; Osborn & Douslin 1968)

$\log [(P/atm) = [1 - 402.915 \pm (T/K)] \times 10^{\{0.872196 - 5.54923 \times 10^{-4} \pm (T/K) + 4.30369 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 65.57 – $166^{\circ}C$ (ebulliometric method, Cox eq., Osborn & Douslin 1968)

8386* ($60.3^{\circ}C$, isotenoscope method, measured range 60.3 – $100.3^{\circ}C$, Eon et al. 1971)

1136 (calculated-Cox eq., Chao et al. 1983)

$\log (P/atm) = [1 - 402.916/(T/K)] \times 10^{\{0.880256 - 6.05913 \times 10^{-4} \pm (T/K) + 5.02726 \times 10^{-7} \pm (T/K)^2\}}$; temp range: 250.0 – $635.0\ K$ (Cox eq., Chao et al. 1983)

1100 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.42113 - 1502.586/(129.775 + t/^{\circ}\text{C})$; temp range 65.67–166°C (Antoine eq. from exptl. data of Scott et al. 1967, Boublik et al. 1984)

1100 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/\text{mmHg}) = 7.29470 - 1501.56/(210.42 + t/^{\circ}\text{C})$; temp range 66–166°C (Antoine eq., Dean 1985, 1992)

1100 (quoted lit., Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.42765 - 1506.877/(210.995 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

1103 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.42263 - 1504.171/(-62.39 + T/\text{K})$; temp range 338–440 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 54.1597 - 4.2745 \times 10^3/(T/\text{K}) - 15.873 \cdot \log(T/\text{K}) - 4.5171 \times 10^{-10} \cdot (T/\text{K}) + 4.2338 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 250–640 K (vapor pressure eq., Yaws 1994)

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

1.640 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated

0.75 (shake flask-AS, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Leo 1979)

0.62 (HPLC-RV correlation, Garst 1984)

0.82 (23°C, shake flask-HPLC, De Voogt et al. 1988)

0.80 (23°C, TLC-RT correlation, De Voogt et al. 1990)

0.75 (recommended, Sangster 1989, 1993)

0.75 (recommended, Hansch et al. 1995)

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

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

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

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

Volatilization:

Photolysis:

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

$k_{\text{OH}} = (1.22 \pm 0.04) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson et al. 1984)

$k_{\text{O}_3} = 1.6 \times 10^{-17} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with loss rate of 1.0 d^{-1} , $k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 10 d^{-1} and $k_{\text{NO}_3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 1000 d^{-1} (review, Atkinson & Carter 1984)

$k_{\text{O}_3} = 1.6 \times 10^{-17} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with loss rate of 1.0 d^{-1} , $k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 5.2 d^{-1} and $k_{\text{NO}_3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate $k = 1000 \text{ d}^{-1}$ (review, Atkinson 1985)

$k_{\text{NO}_3} = (4.9 \pm 1.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1985)

$k_{\text{O}_3} = 1.6 \times 10^{-17} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 24 \text{ h}$, $k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 2.3 \text{ h}$ during daylight hours, $k_{\text{NO}_3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 1.4 \text{ min}$ during nighttime hours at room temp. (Atkinson et al. 1985)

$k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 5.2 d^{-1} at room temp. (Atkinson 1985)

$k_{\text{OH}}^* = (1.03 \pm 0.06) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)

$k_{\text{OH}}^* = 9.31 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Atkinson 1989)

$k_{\text{OH}} = 1.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 287.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated lifetimes of 2.3 h, 1.4 min and 24 h due to gas-phase reactions with OH radical (concn of $1 \times 10^6 \text{ cm}^{-3}$ during daylight hours), NO_3 radical (concn of $2.4 \times 10^6 \text{ cm}^{-3}$ during nighttime hours) and O_3 (clean tropospheric concn of $7.2 \times 10^{11} \text{ molecule cm}^{-3}$), respectively, at room temp. (Atkinson et al. 1985)

TABLE 16.1.7.1.1

Reported vapor pressures of pyrrole 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)			
Kobe et al. 1956		Scott et al. 1967		Eon et al. 1971	
static-Bourdon gauge		ebulliometry		isoteniscope/manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
176.67	358285	65.671	9582	60.3	8386
182.22	399626	68.522	10884	70.3	13025
187.78	454747	71.374	12335	80.3	19732
193.33	509867	77.098	15740	90.3	29198
198.89	571878	79.970	17725	100.3	42263
204.44	647669	82.847	19920	$\Delta H_v/(\text{kJ mol}^{-1}) = 41.84$	
210.00	730351	88.622	25007		
215.56	806142	94.422	31160		
221.11	895713	100.244	38547		
226.67	992174	106.096	47359		
232.22	1081746	111.972	57803		
237.78	1185097	117.875	70109		
243.33	1309119	123.806	84525		
248.89	1440031	129.764	101325		
254.44	1564053	135.753	120798		
260.00	1715635	141.768	143268		
265.56	1867217	147.812	169052		
271.11	2032580	153.884	198530		
		159.984	232087		
		166.109	270110		
		eq. 2	P/mmHg		
		A	7.30295		
		B	1507.015		
		C	210.010		
		bp/°C	129.764		
		$\Delta H_v/(\text{kJ mol}^{-1})$	45.10		

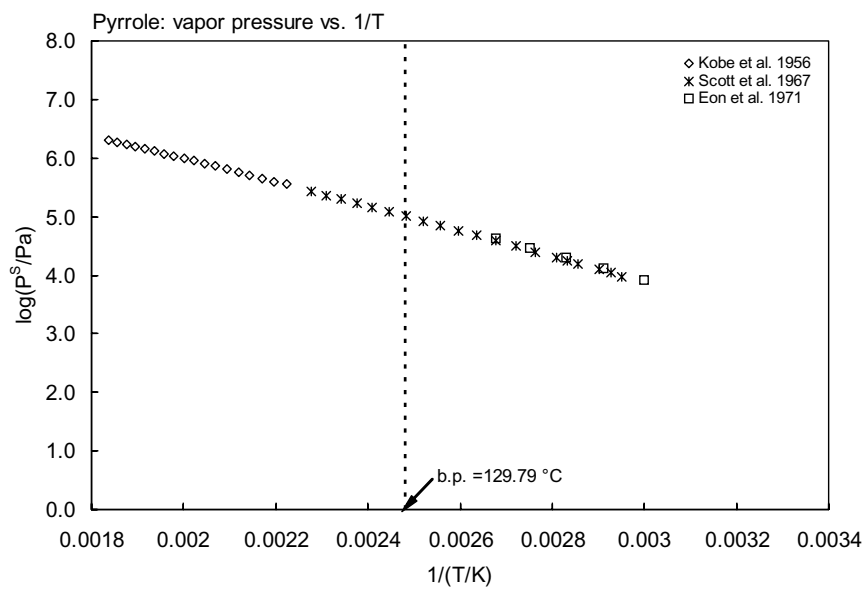
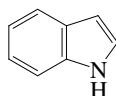


FIGURE 16.1.7.1.1 Logarithm of vapor pressure versus reciprocal temperature for pyrrole.

16.1.7.2 Indole



Common Name: Indole

Synonym: benzo[*b*]pyrrole, 1-benzo[*b*]pyrrole, 1H-indole

Chemical Name: indole

CAS Registry No: 120-72-9

Molecular Formula: C₈H₇N

Molecular Weight: 117.149

Melting Point (°C):

52.5 (Weast 1982–83; Lide 2003)

Boiling Point (°C):

254.0 (Weast 1982–83; Stephenson & Malanowski 1987)

253.6 (Lide 2003)

Density (g/cm³ at 20°C):

1.2200 (Weast 1982–83)

1.0643 (Dean 1985)

Molar Volume (cm³/mol):

133.4 (calculated-Le Bas method at boiling point)

Dissociation Constant, pK_a:

–3.5, –3.62 (Perrin 1972)

–3.17 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} J/mol K:

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.537 (mp at 52.5°C)

Water Solubility (g/m³ or mg/L at 25°C):

3558 (shake flask-GC, Price 1976)

1874 (Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

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

log (P/kPa) = 6.369 – 1933.005/(254.707 + t/°C); temp range 193.3–254.7°C (Antoine eq., Boublik et al. 1984)

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

log (P_s/kPa) = 10.3289 – 3916/(T/K); temp range 291–319 K, (solid, Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 94.1625 – 6.9431 × 10³/(T/K) – 30.613 · log (T/K) + 9.928 × 10^{–3} · (T/K) + 1.7461 × 10^{–13} · (T/K)²; temp range 274–790 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pam³/mol at 25°C):

0.14 (calculated-P/C with selected values)

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

1.14 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

2.14 (shake flask-UV, Hansch & Anderson 1967)

2.25 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)

2.00 (unpublished result, Leo et al. 1971)

2.00, 2.25, 2.13 (Hansch & Leo 1979)

1.66 (RP-HPLC-RT correlation, Veith et al. 1979a)

2.17 (RP-HPLC-RT correlation, Hanai & Hubert 1982)

2.14 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)

1.92	(inter-laboratory studies, HPLC average, Eadsforth & Moser 1983)
2.16 ± 0.03	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.81	(HPLC-k' correlation, Eadsforth 1986)
2.16	(HPLC-RT correlation, Minick et al. 1988)
2.14	(recommended, Sangster 1989; 1993)
2.27	(23°C, shake flask-HPLC, De Voogt et al. 1988, 1990)
2.07	(HPLC-RT correlation, De Voogt et al. 1990)
2.19	(HPLC-RT correlation, Ritter et al. 1994)
2.14	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

16.1.7.3 Pyridine



Common Name: Pyridine

Synonym:

Chemical Name: pyridine

CAS Registry No: 110-86-1

Molecular Formula: C_5H_5N

Molecular Weight: 79.101

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

−41.7 (Lide 2003)

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

115.23 (Lide 2003)

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

0.9819 (Weast 1982–83)

Molar Volume (cm^3/mol):

80.6 (calculated-density, Rohrschneider 1973)

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

Dissociation Constant, pK :

5.23 (pK_a , Leo et al. 1971; Jori et al. 1983; Zachara et al. 1987)

5.198, 5.21, 5.22, 5.229 (Perrin 1972)

5.54 (UV, Yeh & Higuchi 1976)

5.23, 5.16 (quoted, shake flask-TN, Clarke 1984)

5.17 (pK_{BH}^+ , Dean 1985; Riddick et al. 1986)

5.21 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.41, 36.39 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.414 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

miscible (Andon & Cox 1952; Andon et al. 1954; Jori et al. 1983; Riddick et al. 1986)

miscible (Dean 1985; Zachara et al. 1987; Stephenson 1993a)

miscible (Yaws et al. 1990)

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

2666* ($24.8^{\circ}C$, summary of literature data, temp range -18.9 to $115.4^{\circ}C$, Stull 1947)

2520 (interpolated-regression of tabulated data, Stull 1947)

620, 2109 (0 , $20^{\circ}C$, static method-tensimeter, Brown & Barbaras 1947)

2775* (ebulliometry, measured range 47.3 – $115.5^{\circ}C$, extrapolated-Antoine eq., Herington & Martin 1953)

$\log (P/mmHg) = 7.05811 - 1384.991/(216.296 + t/^{\circ}C)$; temp range 47.3 – $115.5^{\circ}C$ (Antoine eq., ebulliometric measurements, Herington & Martin 1953)

2774* (gas saturation, measured range 20 – $40^{\circ}C$, Andon et al. 1954)

461637* ($176.67^{\circ}C$, static-Bourdon gauge, measured range 176.67 – $343.33^{\circ}C$, Kobe et al. 1956)

19920* ($67.299^{\circ}C$, comparative ebulliometry, measured range 67.299 – $152.886^{\circ}C$, McCullough et al. 1957)

$\log (P/mmHg) = 7.04162 - 1374.103/(215.014 + t/^{\circ}C)$; temp range 67.3 – $152.9^{\circ}C$ (Antoine eq. ebulliometry, McCullough et al. 1957)

2763* (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

- log (P/mmHg) = $7.04144 - 1373.990/(t/^{\circ}\text{C} + 215.001)$; temp range 67.3–152.9°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)
- log [(P/atm) = $[1 - 399.384 \pm (T/K)] \times 10^{\{0.856586 - 6.60597 \times 10^{-4} \pm (T/K) + 5.93625 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 67.3–152.9°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)
- 2789 (calculated-Antoine eq., Cabani et al. 1971)
- log (P/mmHg) = $[-0.2185 \times 9649.4/(T/K)] + 8.347670$; temp range –18.9 to 115.4°C (Antoine eq., Weast 1972–73)
- 2767 (calculated-Cox eq., Chao et al. 1983)
- log (P/atm) = $[1 - 388.399/(T/K)] \times 10^{\{0.848882 - 6.09810 \times 10^{-4} \pm (T/K) + 5.15399 \times 10^{-7} \pm (T/K)^2\}}$; temp range: 235.0–620.0 K (Cox eq., Chao et al. 1983)
- 2775, 2763 (extrapolated-Antoine equations, Boublik et al. 1984)
- log (P/kPa) = $6.18358 - 1385.39/(115.256 + t/^{\circ}\text{C})$; temp range 47.3–115.47°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)
- log (P/kPa) = $6.16609 - 1373.826/(115.235 + t/^{\circ}\text{C})$; temp range 67.3–152.9°C (Antoine eq. from reported exptl. data of McCullough et al. 1957, Boublik et al. 1984)
- 2763 (extrapolated-Antoine eq., Dean 1985, 1992)
- log (P/mmHg) = $7.04115 - 1373.80/(214.98 + t/^{\circ}\text{C})$; temp range 67–153°C (Antoine eq., Dean 1985, 1992)
- 2773 (Howard et al. 1986; quoted, Banerjee et al. 1990)
- 2700 (selected, Riddick et al. 1986)
- log (P/kPa) = $6.18595 - 1386.683/(216.469 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
- 2770 (interpolated-Antoine eq. II, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.17372 - 1379.953/(-57.436 + T/K)$; temp range 323–426 K (Antoine eq. I, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.30308 - 1448.781/(-50.948 + T/K)$; temp range 296–353 K (Antoine eq. II, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.16446 - 1373.263/(-58.18 + T/K)$; temp range 348–434 K (Antoine eq. III, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.284 - 1455.584/(-48.272 + T/K)$; temp range 431–558 K (Antoine eq. IV, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $7.25663 - 2578.625/(115.604 + T/K)$; temp range 552–620 K (Antoine eq. V, Stephenson & Malanowski 1987)
- 2773, 1653 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
- 2573* (24.82°C, ebulliometry, measured range 23.55–116.23°C, Lencka 1990)
- ln (P/kPa) = $14.1480 - 3132.3/[(T/K) - 59.179]$; temp range 295.7–388.4 K (ebulliometric measurements, Antoine eq., Lencka 1990)
- log (P/mmHg) = $33.5541 - 3.1318 \times 10^3/(T/K) - 8.8646 \cdot \log (T/K) + 7.1293 \times 10^{-12} \cdot (T/K) + 2.2813 \times 10^{-6} \cdot (T/K)^2$; temp range 232–620 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 0.895 (volatility ratio-transpiration method, Andon et al. 1954)
- 0.900 (exptl., Hine & Mookerjee 1975)
- 0.595, 0.766 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 1.114 (modified gas-stripping, Hawthorne et al. 1985)
- 1.120 (computed, Yaws et al. 1991)
- 0.305 (calculated-molecular structure, Russell et al. 1992)
- 27.78 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
- log K_{AW} = $-1.508 - 128/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 0.65 (shake flask-UV, Iwasa et al. 1965)
- 0.64 (Gehring et al. 1967)
- 0.65, 0.64 (Leo et al. 1971; Hansch & Leo 1979)
- 0.66 (HPLC-RT correlation, Mirrlees et al. 1976)
- 0.63 ± 0.02 (shake flask at pH 7, Unger et al. 1978)
- 0.63 (shake flask-titration, Clarke 1984; Clarke & Cahoon 1987)

0.63 ± 0.06	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
0.62	(shake flask-UV at pH 7.4, El Tayar et al. 1984)
0.63	(shake flask-potentiometric titration, Clarke 1984)
0.54	(calculated- activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
1.28	(HPLC- k' correlation, Eadsforth 1986)
0.79	(calculated- γ from UNIFAC, Banerjee & Howard 1988)
0.70	(shake flask-CPC, Berthod et al. 1988)
0.63	(shake flask-HPLC at pH 7, De Voogt et al. 1988, 1990)
0.65	(recommended, Sangster 1989, 1993)
0.70	(RP-TLC-RT correlation, De Voogt et al. 1990)
0.65	(shake flask-UV, Yamagami et al. 1990)
0.60	(pH 7.2, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

-1.805	(estimated of Anvil Points subsurface materials, Zachara et al. 1987)
-2.541	(estimated of Loring subsurface materials, Zachara et al. 1987)
0.340	(calculated- K_{OW} , Kollig 1993)

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

Volatilization:

Photolysis:

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

photooxidation $t_{1/2} = 14.7\text{--}24.4$ yr in water, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{OH} = (4.9 \pm 0.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere; $k_{O_3} < 1.1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere at room temp. (relative rate method, Atkinson et al. 1987)

$k_{OH} = (0.494 - 0.256) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296–297 K (review, Atkinson 1989)

$k_{OH}(\text{calc}) = 0.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 168\text{--}672$ h, based on anaerobic acclimated screening test data (Naik et al. 1972; selected, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp. and > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere, based on the gas-phase reaction with O_3 (calculated rate constant) in air at room temp. (Atkinson et al. 1987);

photooxidation $t_{1/2} = 128\text{--}1284$ h, based on measured rate data for the reaction with hydroxyl radical in air (selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 14.7\text{--}24.4$ yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: disappears in less than 7 d in soil suspensions (Sims & O'Loughlin 1989);

$t_{1/2} = 24\text{--}168$ h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; selected, Howard et al. 1991).

Biota:

TABLE 16.1.7.3.1

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

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \\ \log P = A[1 - B/(T/K)] & (5) & \text{where } \log A = a - b(T/K) + c(T/K)^2 & \end{array}$$

1.

Stull 1947		Herington & Martin 1953		Andon et al. 1954		Kobe et al. 1956	
summary of literature data		ebulliometry		gas saturation		static-Bourdon gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−18.9	133.3	47.327	8506	20	2109	176.67	461637
2.50	666.6	52.71	10820	25	2774	182.22	502988
13.2	1333	58.349	13806	40	6013	187.78	564988
24.8	2666	68.403	20805			193.33	633889
38.0	5333	75.77	27592			198.89	702790
46.8	7999	82.43	35246			204.44	778581
57.8	13332	82.728	35597			210.00	868153
75.0	26664	88.459	43472			215.56	950834
95.6	53329	92.749	50279			221.11	1047295
115.4	101325	100.994	65759			226.67	1157537
		105.356	75351			232.22	1267778
mp/°C	−42	107.169	79679			237.78	1378020
		110.028	86860			243.33	1495152
		113.222	95488			248.89	1632954
		113.232	95536			254.44	1763866
		113.374	95905			260.00	1908558
		114.015	97713			265.56	2067030
		114.699	99692			271.11	2232392
		115.112	100914			276.67	2397755
		115.287	101402			282.22	2590678
		115.407	101758			287.78	2790491
		115.473	101977			293.33	2997194
						298.89	3183226
		bp/°C	115.256			304.44	3438160
		$\Delta H_v/(\text{kJ mol}^{-1}) = 36.39$				310.00	3672423
		Antoine eq.				315.56	3941137
		eq. 2	P/mmHg			321.11	4216741
		A	7.05811			326.67	4478565
		B	1384.991			332.22	4774839
		C	216.296			337.78	5084894
						343.33	5429399

(Continued)

TABLE 16.1.7.3.1 (Continued)

2.

McCullough et al. 1957		Osborn & Douslin 1968		Lencka 1990	
comparative ebulliometry		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
67.299	19920	67.299	19920	23.55	2394
75.154	25007	73.154	25007	24.82	2573
79.045	31160	79.054	31160	27.0	2902
84.847	38547	84.974	38547	29.26	3290
90.946	47359	90.946	47359	31.63	3720
96.958	57803	96.958	57803	35.86	4626
103.008	70109	103.008	70109	41.0	6035
109.101	84525	109.101	84525	48.51	8525
115.234	101325	115.234	101325	54.17	10999
121.408	120789	121.408	120798	60.65	14321
127.622	143268	127.622	143268	69.25	20650
133.878	169052	133.878	169053	76.97	27794
140.174	198530	140.174	198517	83.45	35213
146.509	232067	146.509	232088	88.70	42359
152.886	270110	152.886	270111	91.76	47951
				96.68	55423
mp/°C	115.23	Antoine eq		100.01	61720
Antoine eq		eq. 2	P/mmHg	102.18	66148
eq. 2	P/mmHg	A	7.04144	106.03	74603
A	7.04162	B	1373.990	112.70	91299
B	1374.103	C	215.001	116.23	101277
C	215.014				
		data also fitted to Cox eq.		eq. 3	cP/kPa
data also fitted to Cox eq.				A	14.1480
eq. 5	P/atm			B	3132.30
A				C	59.719
a	0.858631				
10 ⁻⁴ b	6.7114				
10 ⁻⁷ c	6.0722				
B	388.394				

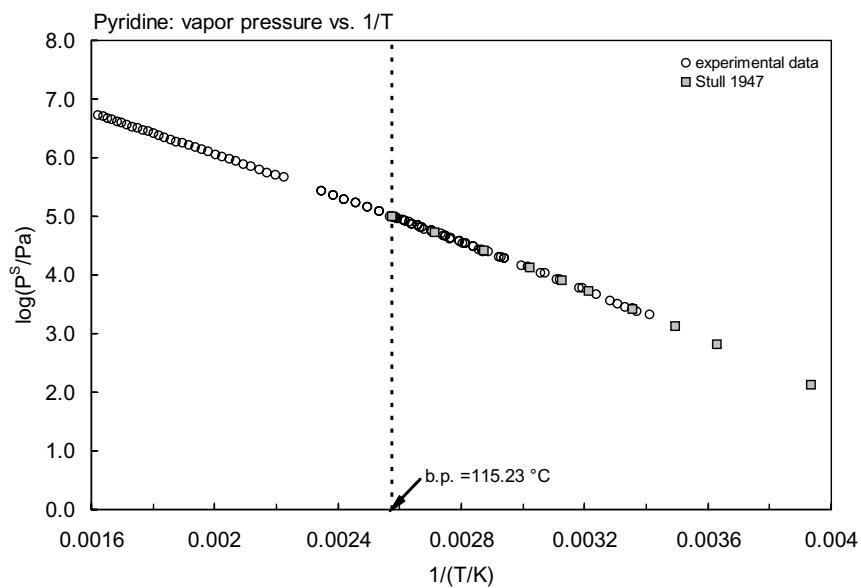


FIGURE 16.1.7.3.1 Logarithm of vapor pressure versus reciprocal temperature for pyridine.

16.1.7.4 2-Methylpyridine



Common Name: 2-Methylpyridine

Synonym: α -picoline, 2-picoline

Chemical Name: 2-methylpyridine, α -picoline

CAS Registry No: 109-06-8

Molecular Formula: $C_5H_4NCH_3$

Molecular Weight: 93.127

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

−66.68 (Lide 2003)

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

129.38 (Lide 2003)

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

0.9443 (Weast 1982–83)

0.9444, 0.93981 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

98.6 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK :

5.957, 6.06 (Perrin 1972)

5.97 (pK_a , $20^{\circ}C$, Weast 1982–83)

6.00 (pK_{BH}^+ , Riddick et al. 1986; quoted, Howard 1990)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

42.919, 36.271 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.724 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

miscible (Andon & Cox 1952)

miscible (Riddick et al. 1986; Yaws et al. 1990)

miscible (Stephenson 1993a)

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

1370* (interpolated-regression of tabulated data, temp range -11.0 to $128.8^{\circ}C$, Stull 1947)

308, 1140 (0 , $20.3^{\circ}C$, static method-tensimeter, Brown & Barbaras 1947)

1277 (manometry, calculated-Antoine eq., Hopke & Sears 1951)

1496* (ebulliometry, extrapolated-Antoine eq., measured range 64.3 – $130^{\circ}C$, Herington & Martin 1953)

$\log (P/mmHg) = 7.03450 - 1417.578/(211.874 + t/^{\circ}C)$; temp range 64.3 – $130^{\circ}C$ (ebulliometric measurements, Antoine eq., Herington & Martin 1953)

1496 (calculated-Antoine eq., Andon et al. 1954)

19920* ($79.794^{\circ}C$, comparative ebulliometry, measured range 79.8 – $168^{\circ}C$, Scott et al. 1963a)

$\log (P/mmHg) = 7.03202 - 1415.494/(t/^{\circ}C + 211.589)$; temp range 79.8 – $168^{\circ}C$ (ebulliometric measurements, Antoine eq., Scott et al. 1963a)

1493 (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

$\log (P/mmHg) = 7.03192 - 1415.424/(t/^{\circ}C + 211.589)$; temp range 79.8 – $168^{\circ}C$ (ebulliometric measurements, Antoine eq., Osborn & Douslin 1968)

$\log [(P/atm) = [1 - 402.536 \pm (T/K)] \times 10^{\{0.866637 - 6.80114 \times 10^{-4} \pm (T/K) + 6.00534 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 79.8 – $168^{\circ}C$ (ebulliometric method, Cox eq., Osborn & Douslin 1968)

$\log (P/\text{mmHg}) = [-0.2185 \times 9933.2/(T/K)] + 8.290910$; temp range -11.0 to 128.8°C (Antoine eq., Weast 1972–73)

1500 (calculated-Cox eq., Chao et al. 1983)

$\log (P/\text{atm}) = [1 - 402.320/(T/K)] \times 10^4 \{0.887914 - 7.70705 \times 10^{-4} \pm (T/K) + 6.85261 \times 10^{-7} \pm (T/K)^2\}$; temp range: 215.0 – 620.0 K (Cox eq., Chao et al. 1983)

1067 (20°C , Verschuere 1983)

1494, 1498 (extrapolated-Antoine equations, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.16509 - 1421.237/(212.286 + t/^\circ\text{C})$; temp range 64.363 – 130.04°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.15718 - 1415.663/(211.617 + t/^\circ\text{C})$; temp range 79.79 – 168.36°C (Antoine eq. from reported exptl. data of Scott et al. 1963, Boublik et al. 1984)

1494 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.0324 - 1415.73/(211.63 + t/^\circ\text{C})$, temp range: 80 – 168°C (Antoine eq., Dean 1985, 1992)

1333 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.15940 - 1417.578/(211.874 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

1386 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.2309 - 1164.1/(-71.0 + T/K)$; temp range 209 – 245 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1558 - 1415.29/(-61.521 + T/K)$; temp range 352 – 442 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15522 - 1414.906/(-61.566 + T/K)$; temp range 352 – 442 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.32356 - 1546.248/(-44.271 + T/K)$, temp range: 429 – 537 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.32144 - 2667.496/(107.978 + T/K)$; temp range 521 – 621 K (Antoine eq.-V, Stephenson & Malanowski 1987)

1500* (ebulliometry, interpolated-Antoine eq., measured range 295.7 – 388.4 K, Ľencka 1990)

$\ln (P/\text{kPa}) = 14.1560 - 3249.15/[T(K) - 61.863]$; temp range 295.7 – 388.4 K (ebulliometric measurements, Antoine eq., Ľencka 1990)

$\log (P/\text{mmHg}) = 34.3728 - 3.2825 \times 10^3/(T/K) - 9.0927 \cdot \log (T/K) - 3.6324 \times 10^{-10} \cdot (T/K) + 2.1425 \times 10^{-6} \cdot (T/K)^2$; temp range 206 – 621 K (vapor pressure eq., Yaws 1994)

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

1.010 (measured volatility ratio-transpiration method, Andon et al. 1954)

1.010 (exptl., Hine & Mookerjee 1975)

0.821, 0.749 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.90 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

30.22 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = -0.700 - 354/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

0.52 (HPLC-RT correlation, Schultz & Moulton 1985)

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

1.11 (shake flask-UV, Yamagami et al. 1990)

1.11 (recommended, Sangster 1989; 1993)

1.11 (recommended, Hansch et al. 1995)

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

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

0.602 (calculated- K_{OW} , Lyman et al. 1982)

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

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

Volatilization: using Henry's law constant, $t_{1/2} = 88$ h for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Howard 1990).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 11.2$ d in air, based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 11.2$ d, based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).

Surface water: estimated $t_{1/2} = 1.0$ d for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 16.1.7.4.1

Reported vapor pressures of 2-methylpyridine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Stull 1947	Herington & Martin 1953		Scott et al. 1963(a)	Lencka 1990			
summary of literature data	ebulliometry		comparative ebulliometry	ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-11.1	133.3	64.363	10660	79.794	19920	18.49	1015
12.6	666.6	69.916	13459	85.853	25007	22.09	1264
24.4	1333	76.836	17758	91.942	31160	24.58	1463
37.4	2666	82.362	21954	98.074	38547	26.74	1657
51.2	5333	88.566	27600	104.252	47359	30.60	2062
59.9	7999	93.617	33044	110.472	57803	33.71	2446
71.4	13332	101.283	42906	116.736	70109	40.03	3414
89.0	26664	108.594	54434	123.038	84525	48.69	5258
108.4	53329	114.552	65581	129.387	101325	57.60	7942
128.8	101325	117.647	72020	135.773	120798	71.51	14375
		122.132	82297	142.207	143268	80.35	20380
mp/°C	-70.0	126.992	91140	148.683	169052	87.31	26426
		125.664	94663	155.201	198530	94.31	33920
		127.828	96885	161.761	232087	101.18	42854
		128.591	99021	168.356	270110	104.03	47076
		129.290	100985			109.24	55653
		129.608	101879	bp/°C	129.39	113.01	62604
		130.037	103095	Antoine eq.		115.31	67182

TABLE 16.1.7.4.1 (Continued)

Stull 1947		Herington & Martin 1953		Scott et al. 1963(a)		Lencka 1990	
summary of literature data		ebulliometry		comparative ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		bp/°C	129.408	eq. 2	P/mmHg	119.20	75535
		$\Delta H_v/(\text{kJ mol}^{-1}) = 37.76$		A	7.03202	122.93	84296
		eq. 2	P/mmHg	B	1415.494	125.77	92024
		A	7.03450	C	211.598	129.88	102813
		B	1417.578			Antoine eq.	
		C	211.874			eq. 3	P/kPa
						A	14.1560
						B	3249.15
						C	61.383

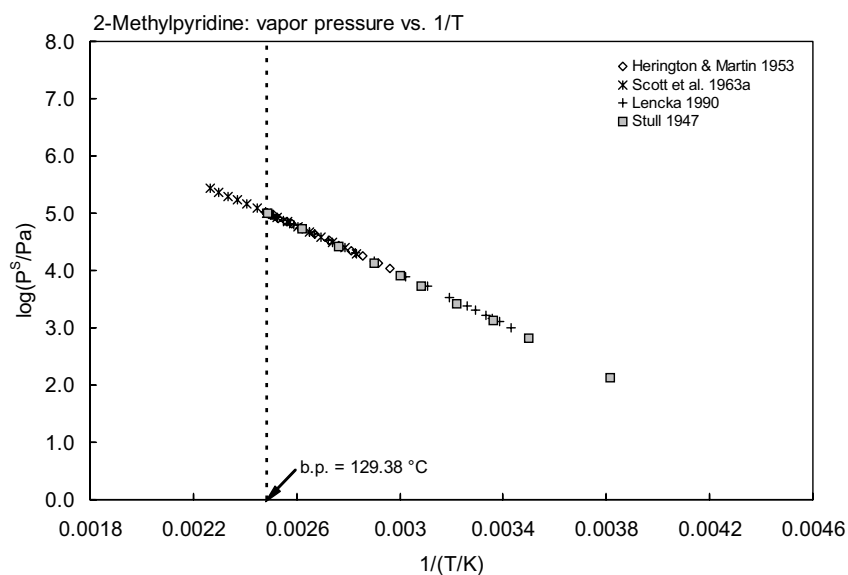


FIGURE 16.1.7.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpyridine.

16.1.7.5 3-Methylpyridine



Common Name: 3-Methylpyridine

Synonym: β -picoline, 3-picoline

Chemical Name: 3-methylpyridine, β -picoline

CAS Registry No: 108-99-6

Molecular Formula: $C_5H_4NCH_3$

Molecular Weight: 93.127

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

-18.14 (Lide 2003)

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

144.14 (Lide 2003)

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

0.9443 (Weast 1982-83)

0.9566 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

97.35 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant, pK:

5.67, 5.703 (Perrin 1972)

5.68 (pK_a , $20^{\circ}C$, Weast 1982-83; pK_a , protonated cation + 1, Dean 1985)

5.75 (pK_{BH^+} , Riddick et al. 1986)

5.65 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.233, 37.323 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.18 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

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

miscible (Andon & Cox 1952; Andon et al. 1954; Yaws et al. 1990)

miscible (Riddick et al. 1986; Howard 1993)

miscible (Stephenson 1993a)

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):

150.7, 594.6 (0, $20^{\circ}C$, static method-tensimeter, Brown & Barbaras 1947)

794* (ebulliometry, extrapolated-Antoine eq., Herington & Martin 1953)

$\log (P/mmHg) = 7.03247 - 1469.894/(209.907 + t/^{\circ}C)$; temp range 81.2 – $145.1^{\circ}C$ (ebulliometric measurements, Antoine eq., Herington & Martin 1953)

794 (calculated-Antoine eq., Andon et al. 1954)

9582* ($74.036^{\circ}C$, comparative ebulliometry, measured range 74.036 – $184.568^{\circ}C$, Scott et al. 1963b)

$\log (P/mmHg) = 7.05375 - 1484.208/(t/^{\circ}C + 211.532)$, temp range 79.8 – $168^{\circ}C$ (ebulliometric measurements, Antoine eq., Scott et al. 1963b)

811 (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

$\log (P/mmHg) = 7.30275 - 1506.877/(t/^{\circ}C + 210.995)$, temp range: 74 – $185^{\circ}C$, (ebulliometric measurements, Antoine eq., Osborn & Douslin 1968)

$\log [(P/atm) = [1 - 417.287 \pm (T/K)] \times 10^{\{0.854256 - 6.02835 \times 10^{-4} \pm (T/K) + 5.00169 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 74 – $185^{\circ}C$ (ebulliometric method, Cox eq., Osborn & Douslin 1968)

806 (calculated-Cox eq., Chao et al. 1983)

$\log (P/\text{atm}) = [1 - 417.217/(T/K)] \times 10^4 \{0.865977 - 6.48542 \times 10^{-4} \pm (T/K) + 5.41256 \times 10^{-7} \pm (T/K)^2\}$; temp range: 255.0–645.0 K (Cox eq., Chao et al. 1983)
 796, 800 (extrapolated-Antoine equations, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.16152 - 1472.639/(210.214 + t/^{\circ}\text{C})$; temp range 81.3–145.1 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.17577 - 1482.229/(211.305 + t/^{\circ}\text{C})$; temp range 74.03–184.6 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data of Scott et al. 1963, Boublik et al. 1984)
 800 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.05021 - 1481.78/(211.25 + t/^{\circ}\text{C})$; temp range 74–185 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)
 1333 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.15737 - 1469.894/(209.907 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 802 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.245 - 3246.9/(T/K)$; temp range 225–255 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.17593 - 1482.943/(-61.705 + T/K)$; temp range 347–458 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.17791 - 1484.285/(-61.554 + T/K)$; temp range 347–458 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.18988 - 1491.897/(-60.745 + T/K)$; temp range 347–381 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.16648 - 1476.25/(-62.502 + T/K)$; temp range 374–458 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.38586 - 1659.184/(-38.176 + T/K)$; temp range 450–570 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.57549 - 3151.52/(161.352 + T/K)$; temp range 561–645 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 35.2679 - 3.4364 \times 10^3/(T/K) - 9.3555 \cdot \log (T/K) - 1.3286 \times 10^{-10} \cdot (T/K) + 2.0461 \times 10^{-6} \cdot (T/K)^2$; temp range 255–645 K (vapor pressure eq., Yaws 1994)

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

0.788 (volatility ratio-transpiration method, Andon et al. 1954)
 0.784; 0.637; 0.749 (exptl.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
 1.836 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 12.69 (20 $^{\circ}\text{C}$, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = -0.826 - 348/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.20 (HPLC-RT correlation, Mirrlees et al. 1976)
 1.20 \pm 0.02 (shake flask at pH 7, Unger et al. 1978)
 1.19 (HPLC-RT correlation, Lewis et al. 1983)
 1.18 \pm 0.01 (HPLC-RV correlation-ALPM, Garst 1984; Garst & Wilson 1984)
 1.20 (shake flask, Log P Database, Hansch & Leo 1985, 1987)
 1.20 (recommended, Sangster 1989, 1993)
 1.20 (recommended, Hansch et al. 1995)

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

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

0.699 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

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

2.029 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

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

Volatilization:

Photolysis:

Oxidation: estimated photooxidation rate constant $k = 1.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/ cm^3 in air at 25 $^{\circ}\text{C}$ which corresponds to an atmospheric half-life of 11 d (Atkinson 1987; quoted, Howard 1993).

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 11$ d from estimated photooxidation rate constant $k = 1.43 \times 10^{-12} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/ cm^3 in air at 25°C (Atkinson 1987; quoted, Howard 1993).

Surface water: estimated $t_{1/2} = 1.0$ d for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.7.5.1

Reported vapor pressures of 3-methylpyridine at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^\circ\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^\circ\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Herington & Martin 1953**Scott et al. 1963(b)****ebulliometry****comparative ebulliometry**

$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
81.282	12871	74.036	9582
85.275	15061	77.115	10884
92.059	19478	80.202	12335
97.519	23773	85.303	13949
103.922	29747	86.403	15740
109.006	35349	89.524	17725
115.583	43796	92.658	19920
121.932	53445	98.946	25007
129.368	66822	105.270	31160
132.163	72471	111.640	38547
137.714	84938	118.052	47359
140.871	92693	124.508	57803
142.132	95948	131.008	70109
142.639	97265	137.551	84525
143.293	99017	144.135	101325
143.577	99782	150.767	120798
143.993	100927	157.441	143268
144.320	101791	164.156	169052
144.659	102725	170.918	198530
145.101	103988	177.821	232087
		184.568	270110
bp/ $^\circ\text{C}$	144.143		
$\Delta H_v/(\text{kJ mol}^{-1}) = 37.76$		bp/ $^\circ\text{C}$	144.14
eq. 2	P/mmHg		
A	7.03247	Antoine	
B	1469.894	eq. 2	P/mmHg
C	209.907	A	7.05375
		B	1484.208
		C	211.532

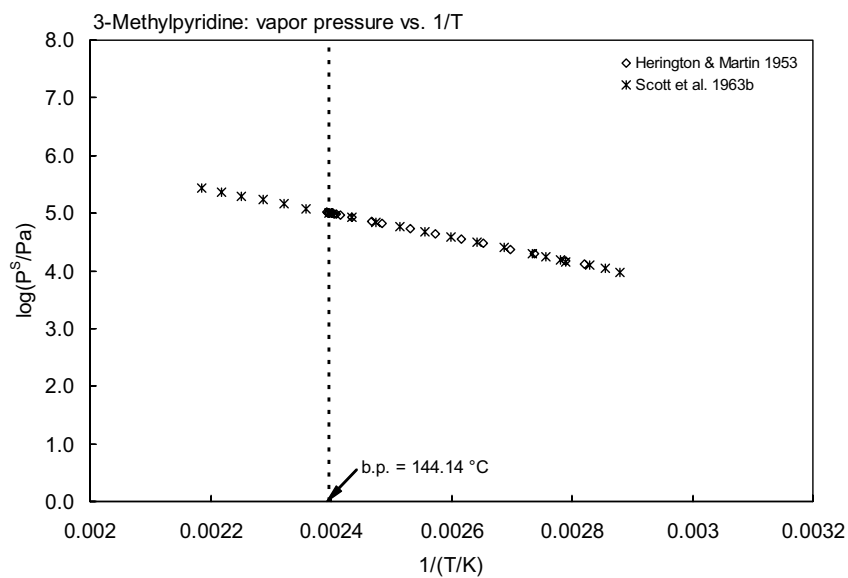


FIGURE 16.1.7.5.1 Logarithm of vapor pressure versus reciprocal temperature for 3-methylpyridine.

16.1.7.6 2,3-Dimethylpyridine



Common Name: 2,3-Dimethylpyridine

Synonym: 2,3-lutidine

Chemical Name: 2,3-dimethylpyridine, 2,3-lutidine

CAS Registry No: 583-61-9

Molecular Formula: C_7H_9N , $C_5H_3N(CH_3)_2$

Molecular Weight: 107.153

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

-15.5 (Stephenson & Malanowski 1987)

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

161.12 (Lide 2003)

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

0.9461, 0.9421 ($20^{\circ}C$, $25^{\circ}C$, Coulson et al. 1959)

0.9319 ($25^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

115.0 (calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK:

6.70 ($20^{\circ}C$, Perrin 1972)

6.57 (pK_a , Weast 1982–83)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

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

104000* ($20^{\circ}C$, shake flask-GC, measured range 16 – $90^{\circ}C$, Stephenson 1993a)

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

366.6, 922.6, 7119 (25 , 40 , $81.2^{\circ}C$, calculated-empirical method with bp and Antoine eq., Andon et al. 1954)

346.4* (ebulliometry, extrapolated-Antoine eq., measured range 99.5 – $162.4^{\circ}C$, Coulson et al. 1959)

$\log (P/mmHg) = 7.05075 - 1528.935/(205.499 + t/^{\circ}C)$; temp range 99.5 – $162.4^{\circ}C$ (Antoine eq., ebulliometry, Coulson et al. 1959)

359.0 (calculated-Cox eq., Chao et al. 1983)

$\log (P/atm) = [1 - 434.216/(T/K)] \times 10^{0.881714 - 6.74484 \times 10^{-4} \pm (T/K) + 5.55055 \times 10^{-7} \pm (T/K)^2}$; temp range: 260.0 – 655.0 K (Cox eq., Chao et al. 1983)

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

$\log (P/kPa) = 6.45509 - 1739.902/(229.887 + t/^{\circ}C)$; temp range 155.3 – $162.4^{\circ}C$ (Antoine eq. from reported exptl. data of Coulson et al. 1959, Boublik et al. 1984)

352.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.18881 - 1538.772/(-66.477 + T/K)$; temp range; 372 – 476 K (Antoine eq., Stephenson & Malanowski 1987)

457 (extrapolated-Antoine eq., Dean 1992)

$\log (P/mmHg) = 7.447 - 1832.6/(240.1 + t/^{\circ}C)$; temp range 155 – $162^{\circ}C$ (Antoine eq., Dean. 1992)

2000* ($54.556^{\circ}C$, comparative ebulliometry, measured range 327.706 – 475.952 K, data fitted to Wagner eq., Steele et al. 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.725 (volatility ratio-transpiration method, Andon et al. 1954)

0.732 (exptl., Hine & Mookerjee 1975)

0.859, 0.732 (calculated.-group contribution, bond contribution, Hine & Mookerjee 1975)
 21.01 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 0.039 - 617/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

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

Bioconcentration Factor, $\log BCF$:

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

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

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 13.0$ d for dimethylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.7.6.1
Reported aqueous solubilities and vapor pressures of 2,3-dimethylpyridine at various temperatures

Aqueous solubility		Vapor pressure			
Stephenson 1993a		Coulson et al. 1959		Steele et al. 1995	
shake flask-GC/TC		ebulliometry		comparative ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	T/K	P/Pa
16.0	171500	99.543	14583	327.706	2000
18.0	121500	107.822	19765	333.396	2666
20.0	104000	116.337	26607	341.852	3999.9
25.0	86000	122.909	33113	348.166	5333
30.0	69100	128.606	39759	357.560	7998.9
35.0	59900	133.429	46191	364.611	10666
40.0	53700	137.704	52572	370.315	13332
50.0	48200	141.757	59255	376.239	16665
60.0	43700	145.829	66652	381.163	19933
70.0	43000	148.764	72421	387.649	25023
80.0	43300	152.203	79677	387.646	25023
90.0	43500	155.326	86769	394.176	31177
		157.94	93067	400.749	38565
		158.603	94703	407.364	47375
		159.141	96085	414.025	57817
		160.125	98614	420.729	70120
		160.668	100030	427.477	84533
		161.199	101438	434.270	101325
		161.682	102701	441.106	120790
		162.077	103788	447.989	143250
		162.412	104696	454.913	169020
				461.885	198490
		mp/°C	−15.22	468.897	232020
		bp/°C	161.157	475.982	270020
ΔH _v = 41.07 kJ/mol					
Antoine eq.				Data fitted to Wagner eq.	
log P = A − B/(C + t/°C)					
			P/mmHg		
A			7.05075		
B			1528.935		
C			205.499		

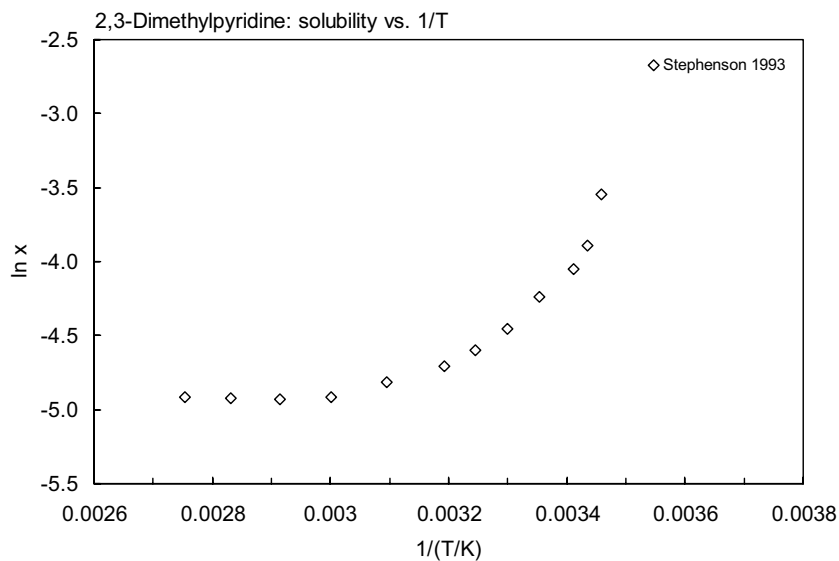


FIGURE 16.1.7.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,3-dimethylpyridine.

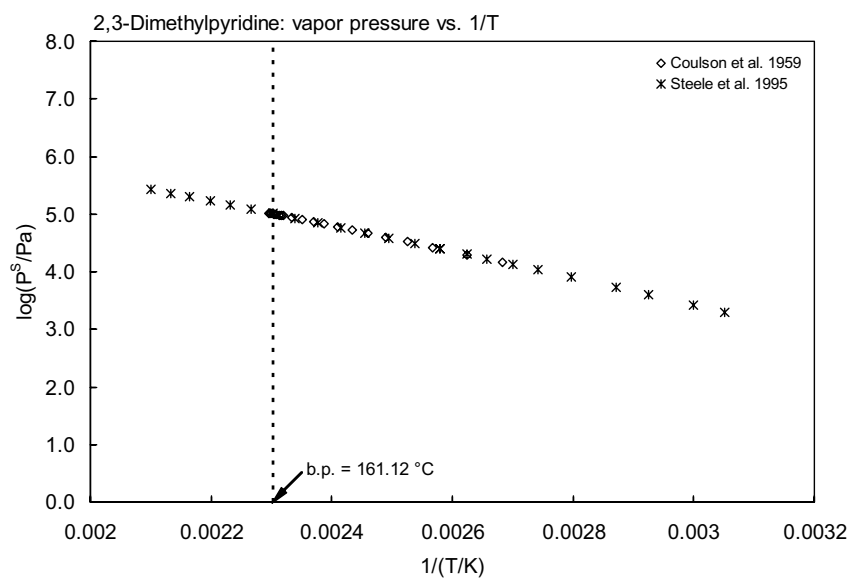
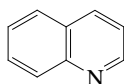


FIGURE 16.1.7.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylpyridine.

16.1.7.7 Quinoline



Common Name: Quinoline

Synonym: benzo[b]-pyridine, 1-benzazine

Chemical Name: quinoline

CAS Registry No: 91-22-5

Molecular Formula: C_9H_7N

Molecular Weight: 129.159

Melting Point (C):

−14.78 (Lide 2003)

Boiling Point (°C):

237.16 (Lide 2003)

Density (g/cm³ at 20°C):

1.0929 (Weast 1982–83)

1.09771, 1.08579 (15, 30°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

118.1 (calculated-density, Rohrschneider 1973)

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

Dissociation Constant, pK:

4.90 (pK_a, 20°C, Weast 1982–83; Zachara et al. 1987; Matzner et al. 1991)

4.80 (pK_a, protonated cation + 1, Dean 1985)

4.94 (pK_{BH}⁺, Riddick et al. 1986)

4.87 (pK_a, Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.71 (at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.79 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6110 (Albersmeyer 1958)

6840 (shake flask-HPLC/UV, Fu & Luthy 1985, 1986)

6386* (20.35°C, equilibrium cell-GC, measured range 20.35–225°C, Leet et al. 1987)

5426 (centrifuge-HPLC at pH 7 and pH 8, Matzner et al. 1991)

8400, 6600 (20°C, 30°C, shake flask-GC, Stephenson 1993a)

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

15.51* (extrapolated-regression of tabulated data, temp range 59.7–237.7°C, Stull 1947)

1.213 (extrapolated, Maczynski & Maczynska 1965)

11.20* (25.16°C, gas saturation-IR, measured range 12.62–35.9°C, Van De Rostyne & Prausnitz 1980)

$\ln(P/\text{mmHg}) = 20.96 - 6993.2/(T/K)$; temp range 12.62–35.9°C (gas saturation-IR, Van De Rostyne & Prausnitz 1980)

11.14 (calculated-bp, Mackay et al. 1982)

12.83 (calculated-Cox eq., Chao et al. 1983)

$\log(P/\text{atm}) = [1 - 510.552/(T/K)] \times 10^4 \{0.897177 - 6.73559 \times 10^{-4} \pm (T/K) + 4.69070 \times 10^{-7} \pm (T/K)^2\}$; temp range: 290.0–780.0 K (Cox eq., Chao et al. 1983)

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

$\log (P/\text{kPa}) = 5.94201 - 1668.355/(186.212 + t/^{\circ}\text{C})$, temp range 164.7–237.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

11.05 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.81759 - 1668.73/(186.26 + t/^{\circ}\text{C})$, temp range 164–238°C (Antoine eq., Dean 1985, 1992)

1.216 (recommended, Neely & Blau 1985)

12.8 (Howard et al. 1986)

11.2 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 5.92679 - 1656.30/(184.78 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

42120* (472.85 K, vapor-liquid equilibrium, measured range 472.85–548.05 K, Klara et al. 1987)

$\log (P/\text{kPa}) = 14.4961 - 4390.0/(65.19 + T/\text{K})$; temp range 472.85–548.05 K (vapor-liquid equilibrium, Klara et al. 1987)

$\log (P_L/\text{kPa}) = 5.92679 - 1656.3/(-88.37 + T/\text{K})$; temp range 433–511 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.15102 - 2846.253/(41.795 + T/\text{K})$; temp range 463–794 K (Antoine eq.-II, Stephenson & Malanowski 1987)

6.145 (calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 76.5432 - 5.7748 \times 10^3/(T/\text{K}) - 24.619 \cdot \log (T/\text{K}) + 8.4666 \times 10^{-3} \cdot (T/\text{K}) + 3.5586 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 258–782 K (vapor pressure eq., Yaws 1994)

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

0.0253 (calculated-P/C, Smith & Bomberger 1980)

0.026 (calculated-P/C, Mackay 1985)

0.168 (calculated-P/C, Meylan & Howard 1991)

0.0697 (estimated-bond contribution, Meylan & Howard 1991)

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

2.03 (shake flask-UV, Iwasa et al. 1965)

2.06 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)

2.03 (Schultz et al. 1970)

2.04 (HPLC-RT correlation, Mirrlees et al. 1976)

2.04 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

2.02 (Hansch & Leo 1979)

2.01 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)

1.88 (HPLC- k' correlation, Haky & Young 1984)

2.20 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

2.10 (shake flask-HPLC, De Voogt et al. 1988, 1990)

2.09 (28°C, shake flask-UV at pH 7.4, Go & Ngiam 1988)

2.03 (recommended, Sangster 1989, 1993)

2.10, 2.15 (HPLC-RT correlation, shake flask-electrometric titration, Slater et al. 1994)

2.03 (recommended, Hansch et al. 1995)

2.17 ± 0.66, 2.33 ± 0.56 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

1.91 (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

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

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

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

1.04 (Coyote Creek sediment with organic content of 1.9%, Smith et al. 1978)

1.96, 2.10, 1.67, 1.72 (estimated- K_{ow} , Karickhoff 1985)

1.42, 1.62 (estimated-S, Karickhoff 1985)

2.20 (best estimate, Karickhoff 1985)

0.251 (estimated Anvil Points subsurface materials, Zachara et al. 1987)

−1.516 (estimated Loring subsurface materials, Zachara et al. 1987)

2.89; 3.05 (humic acid, HPLC- k' correlation; quoted lit., Nielsen et al. 1997)

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

Volatilization: $t_{1/2} = 7000$ h in stream, $t_{1/2} = 35000$ h in eutrophic pond and $t_{1/2} = 28000$ h in eutrophic lake and oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978).

Photolysis:

$k = 7.8 \times 10^{-7} \text{ s}^{-1}$, assuming exposed to 12-h sunlight per day in June, photolysis $t_{1/2} = 1200$ h in stream, $t_{1/2} = 3000$ h in eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

$k(\text{aq.}) = 3.6 \times 10^{-7} \text{ s}^{-1}$ for summer with $t_{1/2} = 535$ h and $k = 5.0 \times 10^{-8} \text{ s}^{-1}$ for winter with $t_{1/2} = 3851$ h both at pH 6.9 and under sunlight at 40°N (Mill et al. 1981; quoted, Howard et al. 1991)

photolytic $t_{1/2} = 550$ h in aquatics (Haque et al. 1980)

$t_{1/2} = 5\text{--}12$ d for disappearance via direct photolysis in aqueous media (Harris 1982)

Oxidation:

$k = 2.8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical with $t_{1/2} > 10^4$ h in stream, eutrophic pond and lake and oligotrophic lake, based on RO_2 concentration of 10^{-9} M on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

$k(\text{aq.}) = 3.5 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 548$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N; $k(\text{aq.}) = 2.8 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 8$ yr for free-radical oxidation in air-saturated water (NRCC 1983) photooxidation $t_{1/2} = 10\text{--}99$ h in air, based on an estimated rate constant for vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991)

first-order photodegradation $k = 8.0 \times 10^{-6} \text{ s}^{-1}$ at 313 nm of in organic-free water with $t_{1/2} = 24.0$ h and $k = 8.4 \times 10^{-6} \text{ s}^{-1}$ in lake water with $t_{1/2} = 23$ h both saturated with air (Kochany & Maguire 1994)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$t_{1/2} = 0.5$ h in stream, eutrophic lake and pond and $t_{1/2} = 10000$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

Biodegradation $k = 7.4 \times 10^{-5} \text{ mL cell}^{-1} \text{ d}^{-1}$ in enrichment culture (Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 72\text{--}240$ h, based on an acclimated fresh water grab sample data (Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 288\text{--}960$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 10\text{--}99$ h, based on an estimated rate constant for vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: half-life for all processes, except for dilution: $t_{1/2} = 0.5$ h in stream, eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

half-life for all processes, including for dilution: $t_{1/2} = 0.28$ h in stream, $t_{1/2} = 0.5$ h in eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

$t_{1/2} = 5\text{--}12$ d for direct photolysis in aqueous media (Harris 1982);

$t_{1/2} = 72\text{--}240$ h, based on an acclimated fresh water grab sample data (Rogers et al. 1984; quoted, Howard et al. 1991);

degrade readily in sunlight in near surface lake water at 40°N latitude in summer with a $t_{1/2} \sim 14$ calendar-d while its $t_{1/2}(\text{calc}) \sim 123$ calendar-d in winter (Kochany & Maguire 1994).

Groundwater: $t_{1/2} = 144\text{--}480$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 72\text{--}240$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Complete mineralization within 7–10 d in batch experiments independent of pH (5.8 and 7.2) (Thomsen et al. 1999)

Biota:

TABLE 16.1.7.7.1

Reported aqueous solubilities and vapor pressures of quinoline at various temperatures and the coefficients for the vapor pressure equations:

Vapor pressure				Aqueous solubility			
Stull 1947		Van De Rostyne & Prausnitz		Klara et al. 1987		Leet et al. 1987	
summary of literate data		gas saturation-IR (1980)		vapor-liquid equilibrium		equilibrium cell-GC	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	S/g·m ⁻³
59.7	133.3	12.62	3.853	472.85	42120	20.35	6386
89.6	666.6	16.71	5.963	504.95	90990	40.05	6458
103.8	1333	21.35	8.159	514.35	112400	64.85	8252
119.8	2666	22.42	9.56	534.35	170300	80.25	10620
136.7	5333	25.16	11.20	548.05	222600	100.05	13920
148.1	7999	28.25	14.80			120.65	20163
163.2	13332	29.10	14.93	eq. 3	P/kPa	145.85	31285
186.2	26664	35.90	24.26	log P = A – B/(C + T/K)		159.65	43555
212.3	53329			A	14.4961	179.85	69602
237.7	101325	eq. 1a	P/mmHg	B	4390.0	199.25	126288
		ln P = A – B/(T/K)		C	65.19	209.05	171494
mp/°C	–15.0	A	20.96			220.25	324333
		B	6993.2			225.05	498697

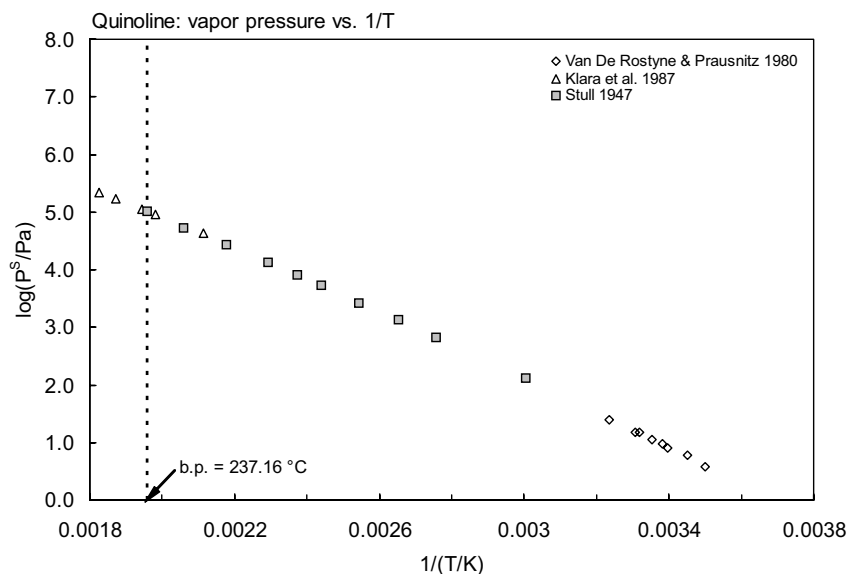
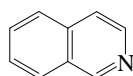


FIGURE 16.1.7.7.1 Logarithm of vapor pressure versus reciprocal temperature for quinoline.

16.1.7.8 Isoquinoline



Common Name: Isoquinoline

Synonym: leucoline

Chemical Name: isoquinoline

CAS Registry No: 119-65-3

Molecular Formula: C_9H_7N

Molecular Weight: 129.159

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

26.47 (Lide 2003)

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

243.22 (Lide 2003)

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

1.0986 (Weast 1982–83)

1.0910 (Dean 1985)

Molar Volume (cm^3/mol):

118.4 ($30^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant, pK :

5.40 (pK_a , Perrin 1972)

5.42 (pK_a , $20^{\circ}C$, Weast 1982–83)

5.40 (pK_a , protonated cation + 1, Dean 1985)

5.38 (pK_{BH}^{+} , Riddick et al. 1986)

5.39 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

48.96 (bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.448 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 0.967 (mp at $26.47^{\circ}C$)

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

4520 (Pearlman et al. 1984)

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

11.8* (extrapolated-regression of tabulated data, temp range 63.5 – $240.5^{\circ}C$, Stull 1947)

7.80 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 516.182/(T/K)] \times 10^4 \{0.91210 - 6.33889 \times 10^{-4} \pm (T/K) + 4.267359 \times 10^{-7} \pm (T/K)^2\}$; temp range: 300.0 – $800.0\ K$ (Cox eq., Chao et al. 1983)

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

$\log(P/kPa) = 6.03709 - 1723.459/(184.268 + t/^{\circ}C)$; temp range 166 – $244^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6.35 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.9122 - 1723.4/(184.3 + t/^{\circ}C)$; temp range 167 – $244^{\circ}C$ (Antoine eq., Dean 1992)

6.70 (Riddick et al. 1986)

$\log(P_L/kPa) = 6.03203 - 1719.5/(-89.12 + T/K)$; temp range 439 – $517\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 45.5737 - 4.4715 \times 10^3/(T/K) - 13.308 \cdot \log(T/K) + 4.0186 \times 10^{-3} \cdot (T/K) - 6.4589 \times 10^{-14} \cdot (T/K)^2$; temp range 299 – $803\ K$ (vapor pressure eq., Yaws 1994)

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

19.14 (calculated-P/C with selected values)

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

2.08 (shake flask-UV, Hansch & Anderson 1967)

2.09 (HPLC-RT correlation, Mirrlees et al. 1976)

2.08 (recommended, Sangster 1989, 1993)

2.30 ± 0.15 , 2.17 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)

2.08 (recommended, Hansch et al. 1995)

2.21 ± 0.66 , 2.26 ± 0.56 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

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

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

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

3.09 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)

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

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

$k_1 = 82.0 \text{ h}^{-1}$, $k_2 = 34.2 \text{ h}^{-1}$ (*daphnia pulex*, 21°C , Southworth et al. 1978)

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 1 \text{ min}$ (*daphnia pulex*, Southworth et al. 1978).

TABLE 16.1.7.8.1
Reported vapor pressures of isoquinoline at
various temperatures

Stull 1947

summary of literature data

$t/^\circ\text{C}$	P/Pa
63.5	133.3
92.7	666.6
107.8	1333
123.7	2666
141.6	5333
152.0	7999
167.6	13332
190.0	26664
214.5	53329
240.5	101325
mp/ $^\circ\text{C}$	24.5

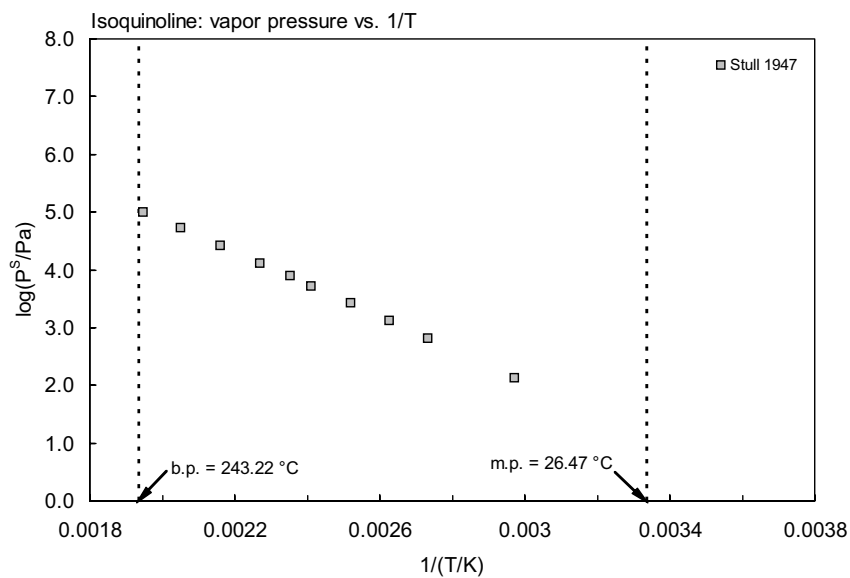
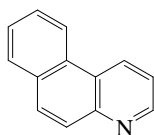


FIGURE 16.1.7.8.1 Logarithm of vapor pressure versus reciprocal temperature for isoquinoline.

16.1.7.9 Benzo[f]quinoline



Common Name: Benzo[f]quinoline

Synonym: 5,6-benzoquinoline, naphthopyridine

Chemical Name: 5,6-benzoquinoline, benzo(f)quinoline

CAS Registry No: 85-02-9

Molecular Formula: $C_{13}H_9N$

Molecular Weight: 179.217

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

94 (Lide 2003)

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

352 (Lide 2003)

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

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK:

5.15 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.210 (mp at $94^{\circ}C$)

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

76.1 (shake flask-GC, Smith et al. 1978)

77.1 (Mill et al. 1981)

176.0 (Steen & Karickhoff 1981)

78.7 (average literature value, Pearlman et al. 1984)

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):

0.00747* ($25.05^{\circ}C$, gas saturation, measured range 288.26–323.15 K, McEachern et al. 1975)

$\log (P/mmHg) = 4339.977/(T/K) + 10.2555$; temp range 288.26–323.15 K (Antoine eq., gas saturation, McEachern et al. 1975)

0.00670 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 9.37682 - 4338.411/(T/K)$; temp range 288–323 K (Antoine eq., Stephenson & Malanowski 1987)

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

0.0096 (calculated-P/C, Smith & Bomberger 1980)

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

3.20 (Steen & Karickhoff 1981)

3.40 (TLC-RT correlation, De Voogt et al. 1988)

3.25 ($23^{\circ}C$, shake flask-HPLC, pH 7, De Voogt et al. 1990)

3.25, 3.40 (lit. values; Sangster 1993)

3.46 ± 0.64 , 3.51 ± 0.53 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

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

Bioconcentration Factor, $\log BCF$:

2.18 (mixed microbial populations, Steen & Karickhoff 1981)

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

- 3.11 (Coyote Creek sediment, Smith et al. 1978)
 4.64, 4.32 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 4.07 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)

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

Volatilization: estimated $t_{1/2} > 10000$ h in river, $t_{1/2} > 100000$ h in eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:

$k = (1.4 \pm 0.7) \times 10^{-4} \text{ s}^{-1}$ for transformation and transport when exposed to 12 h sunlight in mid-June with estimated $t_{1/2} = 2.8$ h in river, $t_{1/2} = 7.0$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 1.4$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)

photolytic $t_{1/2} = 0.52$ h in aquatics (Haque et al. 1980)

$t_{1/2} = 1$ h for disappearance via direct photolysis in aqueous media (Harris 1982)

Oxidation:

laboratory studied $k < 2.8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with the RO_2 radicals and estimated $t_{1/2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

$k(\text{aq.}) = 3.7 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 0.5$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N ; $k(\text{aq.}) < 2.8 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} > 8$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated $t_{1/2} = 190$ h in river, eutrophic pond, eutrophic lake and $t_{1/2} > 10^6$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2} = 0.5$ h in river water, $t_{1/2} = 6.9$ h in pond water, $t_{1/2} = 7.0$ h in eutrophic lake and $t_{1/2} = 1.4$ h in oligotrophic lake predicted by one-compartment for all processes including dilution (Smith et al. 1978)
 $t_{1/2} = 1$ h for disappearance via direct photolysis in aqueous media (Harris 1982).

TABLE 16.1.7.9.1
Reported vapor pressures of benzo[f]quinoline at various temperatures

McEachern et al. 1975

gas saturation	
T/K	P/Pa
288.26	0.00213
293.10	0.00333
298.20	0.00747
303.13	0.0116
308.23	0.0199
313.17	0.0324
318.24	0.0560
323.15	0.0901
P/mmHg	
$\log P = A - B/(T/K)$	
A	10.2555
B	4399.977
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 83.094$	
$\Delta S_{\text{subl}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 196.36$	

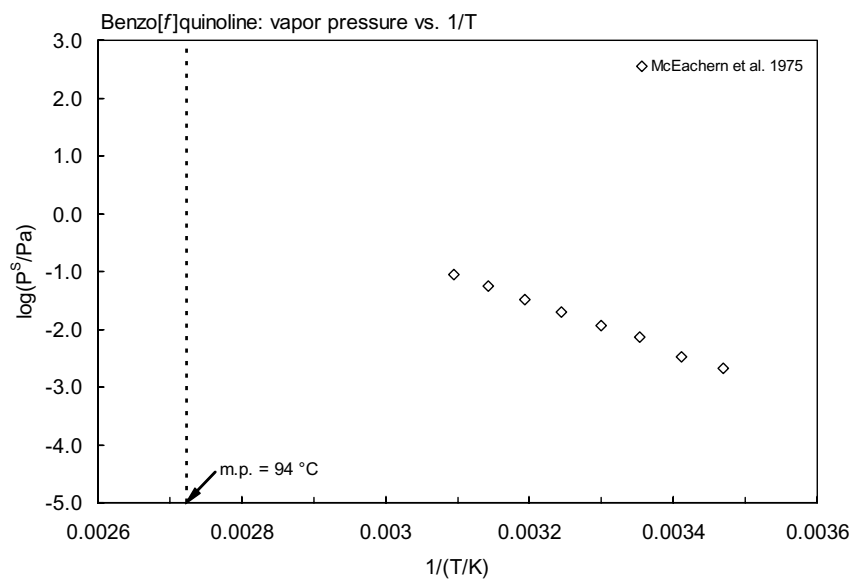
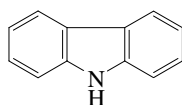


FIGURE 16.1.7.9.1 Logarithm of vapor pressure versus reciprocal temperature for benzo[f]quinoline.

16.1.7.10 Carbazole



Common Name: Carbazole

Synonym: 9H-carbazole, dibenzopyrrole

Chemical Name: carbazole

CAS Registry No: 86-74-8

Molecular Formula: $C_{12}H_9N$, $C_6H_4NHC_6H_4$

Molecular Weight: 167.206

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

246.3 (Lide 2003)

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

354.69 (Lide 2003)

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

1.260 ($25^{\circ}C$, Jiménez et al. 1990)

Molar Volume (cm^3/mol):

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

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.00674 (mp at $246.3^{\circ}C$)

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

1.03 ± 0.05 ($20^{\circ}C$, shake flask-GC, Smith et al. 1978)

1.037 (Mill et al. 1981)

0.428 ($20^{\circ}C$, shake flask-fluorophotometry, Hashimoto et al. 1982)

1.67, 1.03, 0.908; 1.204 (quoted values; lit. average, Pearlman et al. 1984)

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

7999* ($248.2^{\circ}C$, summary of literature data, temp range: 248.2 – $354.8^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 15421.6/(T/K)] + 8.251923$; temp range: 248.2 – $354.8^{\circ}C$ (Antoine eq., Weast 1972–73)

0.0933 ($20^{\circ}C$, Smith et al. 1978)

$\log(P/atm) = [1 - 627.897/(T/K)] \times 10^{[0.924810 - 5.18974 \times 10^{-4} \pm (T/K) + 2.68415 \times 10^{-7} \pm (T/K)^2]}$; temp range: 518.0 – 631.0 K (Cox eq., Chao et al. 1983)

0.00424 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.20101 - 2169.73/(162.465 + t/^{\circ}C)$; temp range 252.6 – $357.3^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 7.0863 - 2179.4/(163.5 + t/^{\circ}C)$; temp range 253 – $368^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.0012 (Antoine eq.-I, Stephenson & Malanowski 1987)

0.0045 (liquid, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.1069 - 4780/(T/K)$; temp range not specified (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.21123 - 2179.424/(-109.636 + T/K)$; temp range 525 – 631 K (liquid, Antoine eq.-II., Stephenson & Malanowski 1987)

0.0002* (extrapolated-Antoine eq., Knudsen effusion, measured range 73.43 – $90.80^{\circ}C$, Jiménez et al. 1990)

$\log(P/Pa) = 14.64 - 5288.4/(T/K)$; temp range 73.43 – $90.80^{\circ}C$ (Knudsen effusion, Jiménez et al. 1990)

$\log(P/mmHg) = -119.857 - 3.2537 \times 10^3/(T/K) + 52.568 \cdot \log(T/K) - 4.6797 \times 10^{-2} \cdot (T/K) + 1.4113 \times 10^{-5} \cdot (T/K)^2$; temp range 518 – 899 K (vapor pressure eq., Yaws 1994)

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

16.0 (calculated-P/C, Smith & Bomberger 1980)

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

3.29 (shake flask-UV at pH 7.4, Rogers 1969)
 3.01 (HPLC- k' correlation, Eadsforth 1986)
 3.50 (calculated, Eadsforth 1986)
 3.72 (recommended, Sangster 1989, 1993)
 3.59 (HPLC-RT correlation, Jenke et al. 1990)
 3.84 (shake flask-HPLC at pH 7, De Voogt et al. 1988)
 3.47 ± 0.63 , 3.22 ± 0.53 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)
 3.72 (recommended, Hansch et al. 1995)

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

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

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

2.24 (Coyote Creek sediment, Smith et al. 1978)
 4.74 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)
 3.80 (soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

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

Volatilization: estimated $t_{1/2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:

$k = 6.6 \times 10^{-5} \text{ s}^{-1}$ for transformation and transport when exposed to midday sunlight in late January with estimated $t_{1/2} = 6.0$ h in river, $t_{1/2} = 15.0$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 3.0$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)

photolytic $t_{1/2} = 1.0$ h in aquatics (Haque et al. 1980)

$t_{1/2} = 3$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation:

laboratory investigated $k = 29 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radicals and estimated $t_{1/2} > 240$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

$k(\text{aq.}) = 1.9 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 1.0$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N ; $k(\text{aq.}) = 29 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 280$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated half-lives of 14 h in river, eutrophic pond, eutrophic lake and $> 10^3$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

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

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 6.0$ h in river, $t_{1/2} = 15.0$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 3.0$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978);

photolytic $t_{1/2} = 1.0$ h in aquatics (Haque et al. 1980); $t_{1/2} = 3$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

TABLE 16.1.7.10.1

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

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Jiménez et al. 1990	
summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
248.2	7999	73.43	0.0610
265.0	13332	78.72	0.101
292.5	26664	81.0	0.129
323.0	53329	83.59	0.167
354.8	101325	86.67	0.219
		87.13	0.227
mp/°C	244.8	90.80	0.329
		ρ (at 25°C)	1.26 g/cm ³
		eq. 1	P/Pa
		A	14.04
		B	5288.4
		enthalpy of sublimation:	
		ΔH _{sub} /(kJ mol ⁻¹) = 103.3	
		at 25°C	

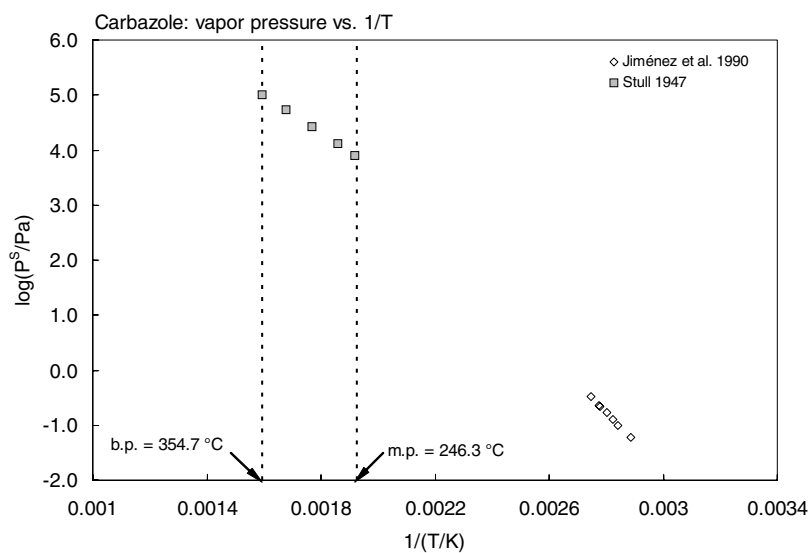
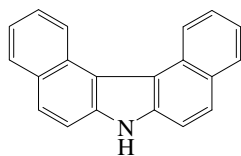


FIGURE 16.1.7.10.1 Logarithm of vapor pressure versus reciprocal temperature for carbazole.

16.1.7.11 Benzo[c,g]carbazole



Common Name: Benzo[c,g]carbazole

Synonym: 7H-dibenzo[c,g]carbazole

Chemical Name: 7H-dibenzo[c,g]carbazole

CAS Registry No: 194-59-2

Molecular Formula: $C_{20}H_{13}N$, $C_{10}H_6NHC_{10}H_6$

Molecular Weight: 267.324

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

158 (Lide 2003)

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

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

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.0496 (mp at $158^{\circ}C$))

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

0.063 ± 0.003 (shake flask-GC, Smith et al. 1978)

0.064 (Mill et al. 1981)

0.064 (Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$):

1.33×10^{-7} (estimated by comparison with benzo[a]pyrene, Smith et al. 1978)

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

0.00048 (calculated-P/C, Smith & Bomberger 1980)

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

5.75 (calculated-S, Steen & Karickhoff 1981)

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

Bioconcentration Factor, $\log BCF$:

4.93 (mixed microbial populations, Steen & Karickhoff 1981)

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

4.31 (Coyote Creek sediment, Smith et al. 1978)

6.03, 6.16 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

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

Volatilization: estimated $t_{1/2} = 15000\ h$ in river, $t_{1/2} = 37000\ h$ in eutrophic pond, $t_{1/2} = 73000\ h$ in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: rate constant

$k = 5.2 \times 10^{-4}\ s^{-1}$ for transformation and transport when exposed to midday sunlight in mid-January with estimated $t_{1/2} = 1.0\ h$ in river, $t_{1/2} = 1.5\ h$ in eutrophic pond and eutrophic lake and $t_{1/2} = 0.5\ h$ in oligotrophic lake assuming winter insulation by the one compartment model (Smith et al. 1978)
photolytic $t_{1/2} = 0.35\ h$ in aquatics (Haque et al. 1980).

Oxidation:

laboratory studied $k = 830 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with the RO_2 radicals and estimated $t_{1/2} > 700 \text{ h}$ in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)
 $k = 5.5 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 0.4 \text{ d}$ under natural sunlight conditions for midday, midsummer at a latitude of 40°N ; $k = 830 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 10 \text{ d}$ for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated half-life to be very long in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model with no acclimated cultures obtained during the screening studies (Smith et al. 1978).

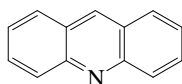
Biotransformation:

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

Half-Lives in the Environment:

Surface water: $t_{1/2} = 0.36 \text{ h}$ in river water, $t_{1/2} = 1.5 \text{ h}$ in pond water, $t_{1/2} = 1.5 \text{ h}$ in eutrophic lake and $t_{1/2} = 0.5 \text{ h}$ in oligotrophic lake for all processes predicted by one-compartment model (Smith et al. 1981);
 $t_{1/2} = 10 \text{ d}$ for free-radical oxidation in air-saturation water (NRCC 1983).

16.1.7.12 Acridine



Common Name: Acridine

Synonym: 2,3,5,6-dibenzopyridine

Chemical Name: acridine, 2,3,5,6-dibenzopyridine

CAS Registry No: 260-94-6

Molecular Formula: $C_{13}H_9N$

Molecular Weight: 179.217

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

110 (Lide 2003)

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

344.86 (Lide 2003)

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

1.005 (Weast 1982–83)

Molar Volume (cm^3/mol):

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

Dissociation Constant, pK_a :

5.60 (Albert 1966; Matzner et al. 1991; Matzner & Bales 1994)

5.58 ($20^{\circ}C$, Weast 1982–83)

5.60 (protonated cation + 1, Dean 1985)

10.65 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.58 ± 0.38 (McEachern et al. 1975)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.147 (mp at $110^{\circ}C$)

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

57.4 (Albert 1966)

38.4 ($24^{\circ}C$, shake flask-LSC, Means et al. 1980)

46.6 (literature average, Pearlman et al. 1984)

54.8 (centrifuge-HPLC at pH 8, Matzner et al. 1991)

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

133.3* ($129.4^{\circ}C$, summary of literature data, temp range 129.4 – $346^{\circ}C$, Stull 1947)

$\log (P/mmHg) = [-0.2185 \times 15174.6/(T/K)] + 8.251980$; temp range 129.4 – $346^{\circ}C$ (Antoine eq., Weast 1972–73)

0.0065* (Langmuir free evaporation, measured range 7.96 – $50^{\circ}C$, McEachern et al. 1975)

$\log (P/mmHg) = 27.076 - 11021.64/(T/K)$; measured range 281.2 – $323.3 K$ (Langmuir free evaporation, McEachern et al. 1975)

0.0075 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/atm) = [1 - 618.827/(T/K)] \times 10^4 \{0.839996 - 4.19344 \times 10^{-4} \pm (T/K) + 3.63487 \times 10^{-7} \pm (T/K)^2\}$; temp range: 402.6 – $619.2 K$ (Cox eq., Chao et al. 1983)

0.2066 (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1983)

0.0065 (Interpolated-Antoine eq.-I, Stephenson & Malanowski 1987; quoted, Ma et al. 1990)

$\log (P_S/kPa) = 8.30838 - 3365.943/(-48.723 + T/K)$; temp range 293–367 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.73664 - 2699.39/(-48.611 + T/K)$; temp range 402–619 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

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

0.030 (calculated-P/C, Ma et al. 1990)

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

3.40 (shake flask-UV, Hansch & Fujita 1964)
 3.39 (HPLC-RT correlation, Mirreles et al. 1976)
 3.39 (shake flask at pH 7.4, Unger et al. 1978)
 3.62 (shake flask-LSC, Means et al. 1980)
 3.29 (shake flask-AS at pH 7.4, Unger & Chiang 1981)
 3.31 ± 0.03 (HPLC-RV correlation-ALPM, Garst 1984)
 3.35 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
 3.32 (shake flask-GC at pH 7.0, Haky & Leja 1986)
 3.40 (recommended, Sangster 1989, 1993)
 3.40 (recommended, Hansch et al. 1995)
 $3.18 \pm 0.64, 3.27 \pm 0.53$ (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

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

Bioconcentration Factor, $\log BCF$:

2.40 (selected, Ma et al. 1990)

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

4.69 (average of sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
 3.32 (calculated, Means et al. 1980)
 -0.157 (estimated of Loring subsurface material, Zachara et al. 1987)
 0.610 (estimated of Anvil Points subsurface material, Zachara et al. 1987)
 3.09–3.41 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987)
 3.16–3.33 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987)
 2.36–2.52 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987)
 2.98–3.30 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987)
 2.19–2.48 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987)
 4.22, 4.26 (soil, quoted, calculated-MCI χ , Sabljic 1987)
 4.11, 3.32 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 4.11, 4.31 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 4.00 (HPLC- k' correlation, Nielsen et al. 1997)
 4.79 (soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

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

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

$k_1 = 109 \text{ h}^{-1}$, $k_2 = 3.68 \text{ h}^{-1}$ (*daphnia pulex*, 21°C, Southworth et al. 1978)

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 11.3 \text{ min}$ (*daphnia pulex*, Southworth et al. 1978).

TABLE 16.1.7.12.1

Reported vapor pressures of acridine 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		McEachern et al. 1975			
summary of literature data		Langmuir free evaporation			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
129.4	133.3	7.96	0.000653	eq. 1a	P/mmHg
165.8	666.6	12.02	0.001027	A	27.076
184.0	1333	16.08	0.002413	B	11021.64
203.5	2666	19.95	0.00329	temp range: 281.2–323.2 K	
224.2	5333	25.05	0.00652	enthalpy of fusion:	
238.7	7999	25.05	0.00656	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.58$	
256.0	13332	29.98	0.01145	enthalpy of sublimation:	
284.0	26664	35.08	0.0213	$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 121.75$	
314.3	53329	40.02	0.0380	temp range: 281.2–323.3 K	
345.0	101325	45.09	0.0640	enthalpy of vaporization:	
		50.0	0.1074	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 72.59$	
mp/°C	110.5				

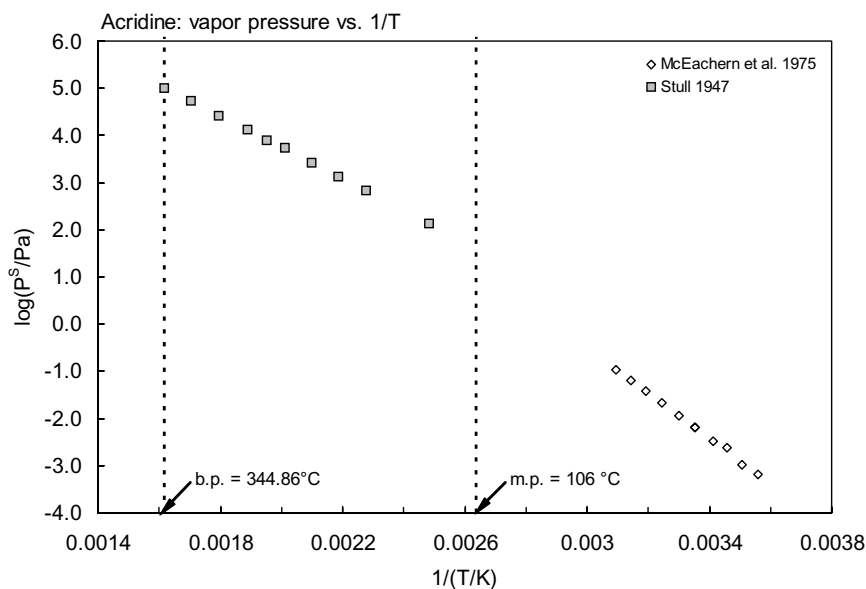


FIGURE 16.1.7.12.1 Logarithm of vapor pressure versus reciprocal temperature for acridine.

16.1.8 SULFUR COMPOUNDS**16.1.8.1 Carbon disulfide**

Common Name: Carbon disulfide

Synonym: carbon disulphide

Chemical Name: carbon disulfide

CAS Registry No: 75-15-0

Molecular Formula: CS₂

Molecular Weight: 76.141

Melting Point (°C):

-112.1 (Lide 2003)

Boiling Point (°C):

46 (Lide 2003)

Density (g/cm³):

1.2632 (20°C, Weast 19820–83)

1.26311, 1.2555 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.522, 26.736 (25°C, bp, Riddick et al. 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.389 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0Water Solubility (g/m³ or mg/L at 25°C):

2100 (20°C, selected, 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):

53329* (28°C, summary of literature data, temp range -73.8 to 46.5°C, Stull 1947)

47359* (24.582°C, comparative ebulliometry, measured range 3.6–80°C, Waddington et al. 1962)

log (P/mmHg) = 6.94194 – 1168.623/(241.534 + t/°C); temp range 3.6–80°C (Antoine eq., comparative ebulliometry, Waddington et al. 1962)

49704* (25.931°C, temp range -17.76 to 45.142°C, Boublik & Aim 1972; quoted, Boublik et al 1984)

log (P/kPa) = 6.86752 – 1169.022/(241.582 + t/°C), temp range 3.6–80°C (Antoine eq. derived from exptl. data of Waddington et al. 1949, Boublik et al. 1984)

log (P/kPa) = 6.03385 – 1151.908/(239.748 + t/°C), temp range -17.76 to 45.14°C (Antoine eq. derived from exptl. data, Boublik et al. 1984)

48210 (selected, Riddick et al. 1986)

log (P/kPa) = 6.06694 – 1168.623/(t/°C + 241.534) temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 6.03694 – 1153.5/(-33.22 + T/K); temp range 256–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)log (P_L/kPa) = 6.07588 – 1174.112/(-30.896 + T/K); temp range 260–353 K (Antoine eq.-II, Stephenson & Malanowski 1987)log (P_L/kPa) = 6 19814– 1231.307/(-26.024 + T/K); temp range 338–408 K (Antoine eq.-III, Stephenson & Malanowski 1987)log (P_L/kPa) = 6 80466– 1278.903/(43.404 + T/K); temp range 388–497 K (Antoine eq.-IV, Stephenson & Malanowski 1987)log (P_L/kPa) = 7.58592 – 2639.181/(165.312 + T/K); temp range 490–533 K (Antoine eq.-V, Stephenson & Malanowski 1987)

39597 (20°C, Howard 1990)

$\log (P/\text{mmHg}) = 25.1475 - 2.0349 \times 10^3/(T/K) - 6.7794 \cdot \log (T/K) + 3.4828 \times 10^{-3} \cdot (T/K) - 1.0105 \times 10^{-14} \cdot (T/K)^2$;
temp range 162–552 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

142 (calculated-P/C, Howard 1990)

1946 (calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

1577 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 3.485 - 1077/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.70–4.60 (Hansch & Leo 1985)

2.14 (recommended, Sangster 1993)

1.94 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

0.90 (calculated-solubility, Howard 1990)

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

1.80 (calculated-solubility, Howard 1990)

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

Volatilization: $t_{1/2} = 2.6$ h in a model river (Howard 1990)

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 1.1$ yr at pH 9 in alkaline solution (Howard 1990)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 9$ d degraded by reacting with atomic oxygen and photochemically produced OH radicals (Howard 1990)

TABLE 16.1.8.1.1

Reported vapor pressures of carbon disulfide 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		Waddington et al. 1962		Boublik & Aim 1972	
summary of literature data		comparative ebulliometry		in Boublik et al. 1984	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
-73.8	133.3	3.588	19920	-17.76	6967
-54.3	666.6	8.772	25007	-12.358	9306
-44.7	1333	13.999	31168	-7.204	12046
-34.3	2666	19.269	38547	-3.286	14549
-22.5	5333	24.582	47359	1.223	17921
-15.3	7999	29.927	57803	5.076	21314

TABLE 16.1.8.1.1 (Continued)

Stull 1947		Waddington et al. 1962		Boublik & Aim 1972	
summary of literature data		comparative ebulliometry		in Boublik et a. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−5.1	13332	35.318	70109	9.448	25780
10.4	26664	40.751	84525	12.981	29923
28.0	53329	46.225	101325	17.168	35493
46.5	101325	51.744	120798	21.087	41470
		57.295	143268	25.931	49704
mp/°C	−110.8	62.885	169052	31.522	61295
		68.531	198530	38.041	77125
		74.218	232087	45.142	97853
		79.927	270110		
				bp/°C	46.217
		bp/°C	46.22		
		Antoine eq.		eq. 2	P/kPa
		eq. 2	P/mmHg	A	6.03385
		A	6.94194	B	1151.908
		B	1168.623	C	239.748
		C	241.534		
		data also fitted to Cox eq.			
		see ref.			

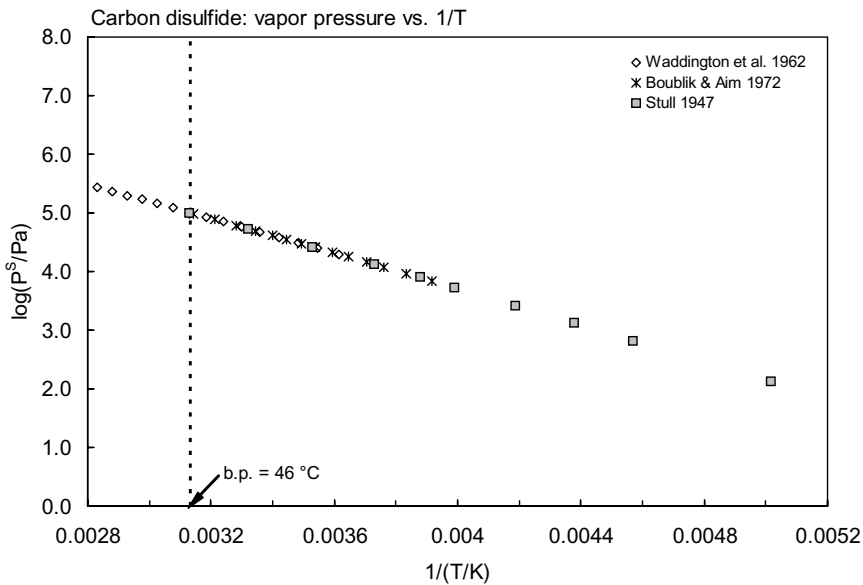


FIGURE 16.1.8.1.1 Logarithm of vapor pressure versus reciprocal temperature for carbon disulfide.

16.1.8.2 Dimethyl sulfide



Common Name: Dimethyl sulfide

Synonym: DMS, methyl sulfide, thiobismethane, 2-thiapropene

Chemical Name: dimethyl sulfide

CAS Registry No: 75-18-3

Molecular Formula: C_2H_6S , $(CH_3)_2S$

Molecular Weight: 62.134

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

−98.24 (Lide 2003)

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

37.33 (Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

0.84825, 0.84230 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

0.8423 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

73.2 (Kamlet et al. 1986)

73.8 ($20^{\circ}C$, calculated-density)

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

Dissociation Constant pK_{BH+} :

−6.99 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.49, 26.82 ($25^{\circ}C$, bp, Dreisbach 1961)

27.65, 27.0 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.99 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

15606 (Hine & Mookerjee 1975)

6300 (Verschueren 1983)

22000 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)

20000 (Riddick et al. 1986)

19600 (selected, Yaws et al. 1990)

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

53174* ($20.087^{\circ}C$, static method, measured range -22.547 to $20.087^{\circ}C$, Osborn et al. 1942)

$\log (P/mmHg) = 16.51798 - 1876.370/(T/K) - 3.04727 \pm \log (T/K)$; temp range -22.547 to $20.087^{\circ}C$ (static method, Osborn et al. 1942)

53329* ($18.7^{\circ}C$, summary of literature data, temp range -75.6 to $36^{\circ}C$, Stull 1947)

64650 (calculated from determined data, Dreisbach 1961)

$\log (P/mmHg) = 6.93138 - 1081.587/(229.746 + t/^{\circ}C)$, temp range -50 to $130^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

64501* (interpolated-Antoine eq., temp range -47.4 to $58.319^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.94879 - 1090.755/(230.799 + t/^{\circ}C)$; temp range -47.4 to $58.319^{\circ}C$ (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

70300 (Hine & Mookerjee 1975)

$\log (P/mmHg) = [-0.2185 \times 6742.3/(T/K)] + 7.589204$; temp range -75 to $224.5^{\circ}C$ (Antoine eq., Weast 1972–73)

56000 ($20^{\circ}C$, Verschueren 1983)

64443 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

64460 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.27843 - 1196.875/(242.81 + t/^{\circ}\text{C})$, temp range -22.55 to 20.09°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

64470 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.1509 - 1195.58/(242.68 + t/^{\circ}\text{C})$; temp range -22 to 20°C (Antoine eq., Dean 1985, 1992)

64650 (quoted, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.07369 - 1090.755/(230.799 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

64520 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.07043 - 1088.851/(-42.594 + T/\text{K})$; temp range 268–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.13042 - 1124.998/(-37.961 + T/\text{K})$; temp range 307–379 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.42655 - 1344.329/(-7.456 + T/\text{K})$; temp range 372–453 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.36327 - 2293.043/(130.243 + T/\text{K})$; temp range 447–503 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 37.2604 - 2.4251 \times 10^3/(T/\text{K}) - 11.384 \cdot \log (T/\text{K}) + 5.8122 \times 10^{-3} \cdot (T/\text{K}) + 8.5893 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 175–503 K (vapor pressure eq., Yaws 1994)

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

278.1 ($1/K_{\text{AW}}$, exptl., Hine & Mookerjee 1975)

298, 366.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

165 (20°C , headspace-GC, Vitenberg et al. 1975)

180.4, 184.7, 173.5 (headspace-GC, concn. of 10, 1.0, 0.1 ppm by weight, Przyjazny et al. 1983)

180.4, 184.7, 173.5 (headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25 – 70°C , data presented in graph, Przyjazny et al. 1983)

$\log (1/K_{\text{AW}}) = 1637.3/(T/\text{K}) - 4.354$; temp range 25 – 70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)

$\log (1/K_{\text{AW}}) = 1635.6/(T/\text{K}) - 4.358$; temp range 25 – 70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)

$\log (1/K_{\text{AW}}) = 1598.2/(T/\text{K}) - 4.205$; temp range 25 – 70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)

163.4 (quoted, Gaffney et al. 1987)

184, 1271 (quoted, calculated-molecular structure, Russell et al. 1992)

138 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)

233.0* (equilibrium headspace-GC, in seawater, measured range 18 – 44°C , Wong & Wang 1997)

61.97 (equilibrium headspace-GC, Marin et al. 1999)

155 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 3.556 - 1394/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

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 , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

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

$k_{\text{OH}}^* = (9.80 \pm 1.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.9 K, measured range 299.9–426.5 K (flash photolysis-resonance fluorescence, Atkinson et al. 1978)

$k_{\text{OH}}^* = (8.28 \pm 0.87) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 273–400 K by flash photolysis-resonance fluorescence, Kurylo 1978)

$k_{\text{O}(^3\text{P})}^* = 57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas-phase reaction with $\text{O}(^3\text{P})$ atom at 296 K, measured range 252–493 K (Slagle et al. 1978)

$k_{\text{OH}}^* = (4.26 \pm 0.56) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 248–363 K (flash photolysis-resonance fluorescence, Wine et al. 1981)

$k_{\text{OH}} = (1.0 \pm 0.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated lifetime $\tau \sim 30$ h in the daytime, $k_{\text{NO}_3} = (5.4 \pm 0.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated $\tau \sim 3$ h in the nighttime hours at 296 ± 2 K (Atkinson et al. 1984)

$k_{\text{O}_3} < 8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.05 \text{ d}^{-1}$, $k_{\text{OH}} = 9.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.8 d^{-1} , and $k_{\text{NO}_3} = 9.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 20 d^{-1} at room temp. (review, Atkinson & Carter 1984)

$k_{\text{O}_3} < 8 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.004 \text{ d}^{-1}$, $k_{\text{OH}} = 6.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.27 d^{-1} , and $k_{\text{NO}_3} = 9.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 20 d^{-1} at room temp. (review, Atkinson 1985)

$k_{\text{OH}}^* = (4.09, 4.44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 267–397 K (flash photolysis-resonance fluorescence, Hynes et al. 1986)

$k_{\text{OH}}^* = (3.60 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–440 K by flash photolysis-resonance fluorescence; $k_{\text{OH}} = 9.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative rate to *n*-hexane, $k_{\text{OH}} = 5.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative rate to cyclohexane at 296 K (Wallington et al. 1986a)

$k_{\text{NO}_3}^* = (8.1 \pm 1.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 280–350 K (flash photolysis-visible absorption, Wallington et al. 1986b)

$k_{\text{OH}}^* = (5.50 \pm 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 260–393 K (discharge flow-resonance fluorescence, Hsu et al. 1987)

$k_{\text{OH}} = (8.0 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Relative rate method, Barnes et al. 1989)

$k_{\text{OH}} = 3.60 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 3.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{\text{NO}_3}^* = (10.6 \pm 1.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 256–376 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)

$k_{\text{OH}}^* = 4.56 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 4.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 9.77 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljić & Güsten 1990; Müller & Klein 1991)

$k_{\text{NO}_3}^* = 1.07 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetime $\tau \sim 30$ h due to reaction with OH radical in the daytime and $\tau \sim 3$ h due to reaction at night with NO_3 radical (Atkinson et al. 1984);

calculated lifetimes, $\tau > 20$ d due to reaction with O_3 in 24-h, $\tau = 28$ h with OH radical during daytime and $\tau = 120$ min with NO_3 radical during nighttime in “clean” atmosphere; $\tau > 3$ d due to reaction with O_3 in 24-h, $\tau = 420$ min with OH radical in daytime and $\tau = 13$ min with NO_3 in nighttime in “moderately polluted” atmosphere (Winer et al. 1984)

estimated tropospheric chemical lifetimes, $\tau = 2$ d, 2 d and > 15 d for reactions with OH, NO_3 and O_3 , respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)

TABLE 16.1.8.2.1

Reported vapor pressures and Henry's law constants of dimethyl sulfide at various temperatures

Vapor pressure						Henry's law constant	
Osborn et al. 1942		Stull 1947		Zwolinski & Wilhoit 1971		Wong & Wang 1997	
static method-manometer		summary of literature data		selected values		equilibrium headspace-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
							in seawater
-22.547	6994	-75.6	-133.3	47.4	1333	18	164.6
-10.028	13699	-58.0	666.6	-37.7	2666	25	233.0
0.096	22437	-49.2	1333	-31.5	4000	35	381.7
4.943	28042	-39.4	2666	-26.9	5333	44	556.4
15.138	43512	-28.4	5333	-23.03	6666		
20.087	53174	-21.4	7999	-19.85	7999	log K _{AW} = A - B/(T/K)	
		-12.0	13332	-14.62	10666		K _{AW}
mp/K	174.855	2.60	26664	-10.39	13332	A	4.806
bp/K	310.49	18.7	53329	-2.258	19998	B	1735
		36.0	101325	3.885	26664		
log P = A - B/(T/K) - C·log (T/K)				8.883	33331		
	P/mmHg	mp/°C	-83.2	13.127	39997		
A	16.51798			20.138	53329		
B	1876.370			25.860	66661		
C	3.04727			30.733	79993		
				35.000	93326		
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 7.985$				35.794	95992		
$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 27.98$				36.572	98659		
at 291.06 K				37.333	101325		
				25	64501		
				Antoine eq.			
				log P = A - B/(C + t/°C)			
					P/mmHg		
				A	6.94879		
				B	1090.755		
				C	230.799		
				bp/°C	37.333		
				$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) =$			
				at 25°C	27.65		
				at bp	26.92		

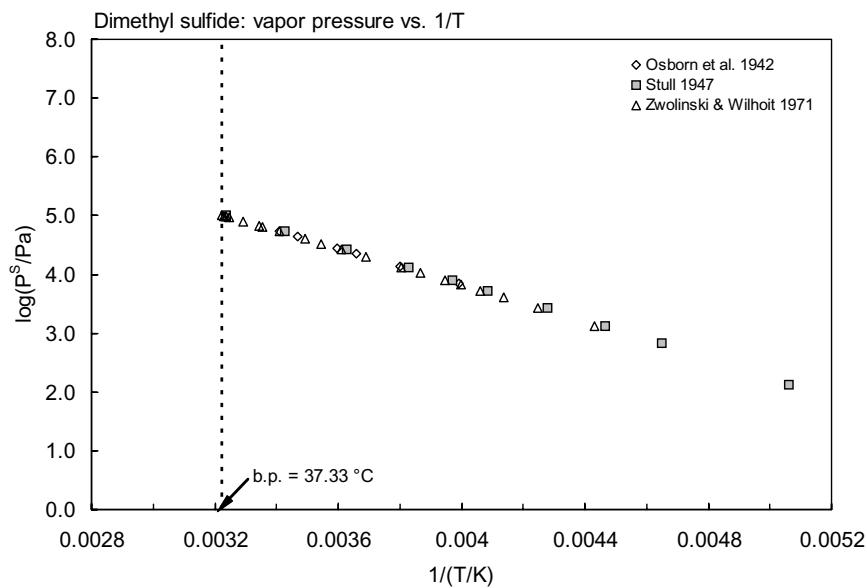


FIGURE 16.1.8.2.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfide.

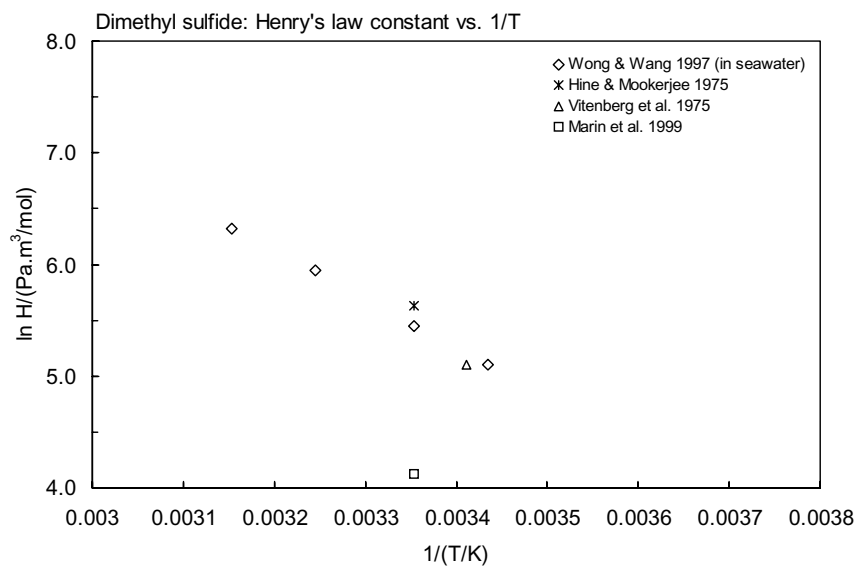


FIGURE 16.1.8.2.2 Logarithm of Henry's law constant versus reciprocal temperature for dimethyl sulfide.

16.1.8.3 Dimethyl disulfide



Common Name: Dimethyl disulfide

Synonym: 2,3-dithiabutane

Chemical Name: dimethyl didisulfide

CAS Registry No: 624-92-0

Molecular Formula: $\text{C}_2\text{H}_6\text{S}_2$, CH_3SSCH_3

Molecular Weight: 94.199

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

−84.67 (Lide 2003)

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

109.74 (Lide 2003)

Density (g/cm^3):

1.6025 (20°C , Weast 1982–83)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

38.37, 33.68 (25, bp, Zwolinski & Wilhoit 1971)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

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

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

3400 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)

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

3825* (static method, measured range 0 – 60°C , Scott et al. 1950)

3813* (interpolated-Antoine eq., temp range 5.356 – 109.745°C , Zwolinski & Wilhoit 1971)

$\log(P/\text{mmHg}) = 6.97792 - 1396.342/(218.863 + t/^{\circ}\text{C})$; temp range 5.356 – 109.745°C (Antoine eq., Zwolinski & Wilhoit 1971)

3850 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

$\log(P/\text{kPa}) = 6.18000 - 1389.151/(223.184 + t/^{\circ}\text{C})$, temp range 0 – 60°C (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.08703 - 1336.665/(217.767 + t/^{\circ}\text{C})$, temp range 61.4 – 128.6°C (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)

$\log(P_L/\text{kPa}) = 6.10018 - 1349.006/(-54.389 + T/\text{K})$, temp range 297 – 402 K , (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 36.232 - 3.1241 \times 10^3/(T/\text{K}) - 9.9328 \cdot \log(T/\text{K}) + 2.2831 \times 10^{-11} \cdot (T/\text{K}) + 3.1730 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 125 – 499 K (vapor pressure eq., Yaws 1994)

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

121 (20°C , headspace-GC, Vitenberg et al. 1975)

112, 101 (headspace-GC, concn. of 10 and 1.0 ppm by weight, measured range 25 – 70°C , data presented in graph, Przyjazny et al. 1983)

$\log(1/K_{\text{AW}}) = 1657.1/(T/\text{K}) - 4.211$; temp range 25 – 70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)

$\log(1/K_{\text{AW}}) = 1854.4/(T/\text{K}) - 4.828$; temp range 25 – 70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)

77.5 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.828 - 1384/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 1.77 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.77 (recommended, Sangster 1993)
- 1.77 (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, $t_{1/2}$, or Lifetimes, τ :

Volatilization:

Photolysis:

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

$k_{OH} = 2.40 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 297 K (relative rate method, Cox & Sheppard 1980)

$k_{OH}^* = (1.84 - 19.8) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 298 K, measured range 255–377 K (flask photolysis-resonance fluorescence, Wine et al. 1984)

$k_{OH}^* = 2.05 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 298 K (tentative recommended, Atkinson 1985)

$k_{NO_3}^* = 4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 280–350 K (flash photolysis-optical absorption, Wallington et al. 1986)

$k_{NO_3}^* = (7.3 \pm 1.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 334–382 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)

$k_{NO_3} = 7.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range ~300–380 K (recommended, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 16.1.8.3.1

Reported vapor pressures of dimethyl disulfide at various temperatures and the coefficients for the vapor pressure equations

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

Scott et al. 1950				Zwolinski & Wilhoit 1971			
static method-manometer		ebulliometric method		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	904	61.411	19920	5.356	1333	106.905	93326
15	2230	67.301	25007	18.299	2666	107.872	95992
20	2936	73.234	31160	25.891	4000	108.819	98659
25	3825	79.201	38547	31.579	5333	109.745	101325
30	4930	85.218	47359	36.177	6666	25.0	3813
35	6301	91.283	57803	40.060	7999	Antoine eq.	
40	7975	97.393	70109	46.435	10666	eq. 2	P/mmHg
45	10007	103.54	84525	51.600	13332	A	6.97792
50	12448	109.738	101325	61.518	19998	B	1396.342
55	15359	115.984	120798	69.008	26664	C	218.863
60	18813	122.273	143268	75.099	33331	bp/°C	109.745
		128.611	169052	80.271	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				88.812	53329	at 25°C	38.37
				95.780	66661	at bp	33.68
				101.712	79993		

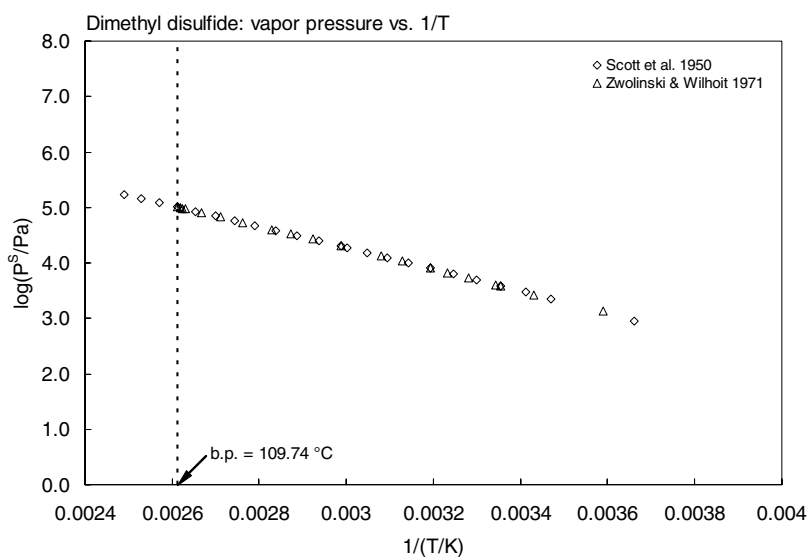


FIGURE 16.1.8.3.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl disulfide.

16.1.8.4 Dimethyl sulfoxide (DMSO)



Common Name: Dimethyl sulfoxide

Synonym: DMSO, sulfinylbismethane, methyl sulfoxide, methylsulfinylmethane, SQ 9453, DMS-70, DMS-90, Deltan, Demasorb, Demavet, Demeso, Dermasorb, Dolicur, Domoso, Dromisol, Gamasol 90, Hyadur, Rimso-50, Sclerosol, Somipront, Somtexan, Topsym

Chemical Name: dimethyl sulfoxide

CAS Registry No: 67-68-5

Molecular Formula: C_2H_6OS , $(CH_3)_2SO$

Molecular Weight: 78.133

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

17.89 (Lide 2003)

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

189.0 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

1.1014 (Weast 1982–83)

Molar Volume (cm^3/mol):

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

Dissociation Constant pK_a :

1.4 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

52.88, 43.14 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.368 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

253000 (Riddick et al. 1986)

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

80.0* (gas saturation, measured range 20 – $50^{\circ}C$, Douglas 1948)

$\log (P/mmHg) = 26.49588 - 3539.32/(T/K) - 6.000 \pm \ln (T/K)$; temp range 20 – $50^{\circ}C$ (gas saturation, Douglas 1948)

460* ($52.35^{\circ}C$, Hg manometer, measured range 325.5 – $442.1 K$, Jakli & van Hook 1972)

$\ln (P/mmHg) = 17.4922 - 4517.79/(T/K - 47.2583)$; temp range 291.7 – $463 K$ (Hg manometer, Antoine eq. with literature data, Jakli & van Hook 1972)

56.0 ($20^{\circ}C$, Verschueren 1983)

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

$\log (P/kPa) = 6.64816 - 1922.32/(223.353 + t/^{\circ}C)$; temp range 52.4 – $168.95^{\circ}C$ (Antoine eq. from reported exptl. data of Jakli & von Hook 1972, Boublik et al. 1984)

80.0 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.72161 - 1962.06/(225.892 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

79.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.72167 - 1962.05/(-47.258 + T/K)$; temp range 305 – $464 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 45.4653 - 4.0439 \times 10^3/(T/K) - 13.21 \cdot \log (T/K) + 1.0981 \times 10^{-7} \cdot (T/K) + 6.4155 \times 10^{-6} \cdot (T/K)^2$; temp range 292 – $465 K$ (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

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

- 1.35 (shake flask, Hansch & Leo 1979, 1987)
- 0.85 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
- 1.35 (recommended, Sangster 1989)
- 1.35 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis:

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

$k_{OH} = (6.2 \pm 2.2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{NO_3} = (1.7 \pm 0.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{O_3} < 5.0 \times 10^{-19} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ at room temp (Barnes et al. 1989)

$k_{OH} = (62 \pm 25) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1989)

$k_{OH} = (1.0 \pm 0.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp (Hynes & Wine 1996)

$k_{OH} = (8.7 \pm 1.6) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Urbanski et al. 1998)

$k_{OH} = (5.9 \pm 1.5) \times 10^{-11} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with tropospheric lifetime $\tau = 5 \text{ h}$, $k_{NO_3} = (5.0 \pm 3.8) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with tropospheric lifetime $\tau = 3 \text{ d}$; $k_{O_3} < 1.0 \times 10^{-19} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with tropospheric lifetime $\tau > 150 \text{ d}$ and $k_{Cl} = (7.4 \pm 1.0) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with Cl atoms with tropospheric lifetime $\tau = 62 \text{ d}$ at room temp and 740 torr (Relative rate method, Falbe-Hansen et al. 2000)

Hydrolysis: $k = 6.60 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ (Buxton et al. 1986)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: estimated tropospheric chemical lifetimes, $\tau = 5 \text{ h}$, 3 d and $> 150 \text{ d}$ for reactions with OH, NO_3 and O_3 , respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)

TABLE 16.1.8.4.1

Reported vapor pressures of dimethyl sulfoxide 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)	$\log P = A - B/(C + T/K)$	(3a)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)	$\ln P = A - B/(T/K) - C \cdot \ln(T/K)$	(4a)		
Douglas 1948	Jakli & van Hook 1972				
gas saturation	mercury manometer				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	55.6	52.35	460	140.15	22905
25	80.0	56.25	573	148.05	29471
30	113.7	61.45	767	162.15	47036
35	159.3	66.15	993	168.95	56342
40	220.8	74.85	1560	eq. 3	P/mmHg
45	302.6	79.95	2000	A	17.4922
50	409.3	85.65	2653	B	4517.79
		90.26	3293	C	47.2583
eq. 4	P/mmHg	96.05	4226		
A	29.49558	100.45	5106		
B	3539.32	100.55	5133		
C	6.0000	104.95	6246		
		111.95	8359		
bp/°C	192	117.95	10452		
$\Delta H_V = 52.89$ kJ/mol		127.45	14745		

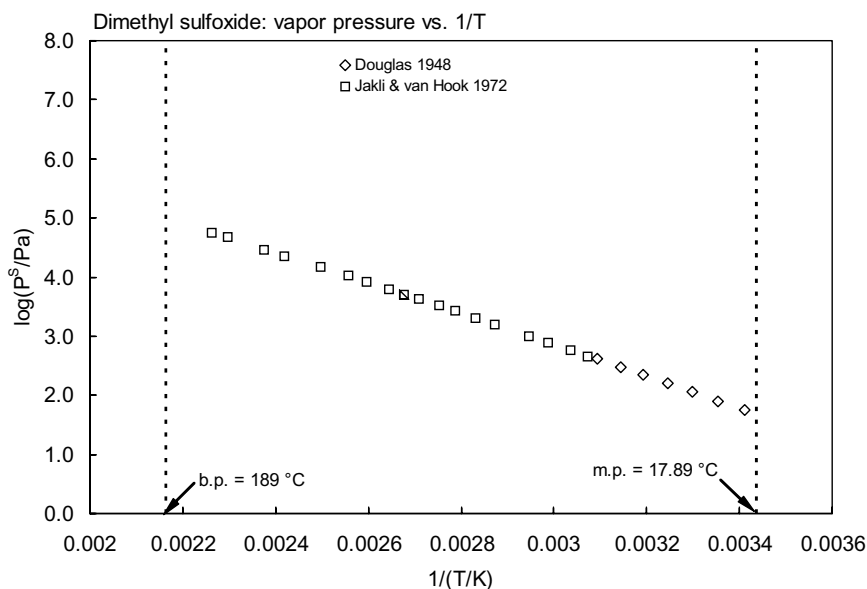
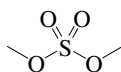


FIGURE 16.1.8.4.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfoxide.

16.1.8.5 Dimethyl sulfate



Common Name: Dimethyl sulfate

Synonym: sulfuric acid dimethyl ester, DMS

Chemical Name: dimethyl sulfate

CAS Registry No: 77-78-1

Molecular Formula: $C_2H_6O_4S$, $CH_3O-SO_2-OCH_3$

Molecular Weight: 126.132

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

-27 (Lide 2003)

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

188 (decomposes, Lide 2003)

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

1.3322 (Dean 1985)

Molar Volume (cm^3/mol):

95.0 ($20^{\circ}C$, Stephenson & Malanowski 1987)

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

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

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

28000 (hydrolyzes, Verschueren 1983; Dean 1985)

28000 ($18^{\circ}C$, Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 133 ($20^{\circ}C$, Verschueren 1983)

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

$\log(P_L/kPa) = 7.28235 - 2437.54/(T/K)$, temp range 340–470 K, (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 33.9406 - 3.853 \times 10^3/(T/K) - 8.5921 \cdot \log(T/K) - 1.1705 \times 10^{-10} \cdot (T/K) + 8.226 \times 10^{-7} \cdot (T/K)^2$;
temp range 241–758 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

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

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2}$ = of 36.5–365 h, based on estimated rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first order hydrolysis rate constant $k = 1.6 \times 10^{-4} s^{-1}$ at pH 7 and $25^{\circ}C$ with $t_{1/2} = 1.2 h$ (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} \sim 168\text{--}672$ h and aqueous anaerobic biodegradation $t_{1/2} \sim 672\text{--}2688$ h (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 36.5\text{--}365$ h, based on photooxidation half-life in air from estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime (reaction with liquid water) estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 1.2\text{--}12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).

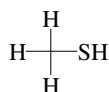
Groundwater: $t_{1/2} = 1.2\text{--}12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 1.2\text{--}12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Howard et al. 1991).

Biota:

16.1.8.6 Methanethiol



Common Name: Methanethiol

Synonym: methyl mercaptan

Chemical Name: methanethiol

CAS Registry No: 74-93-1

Molecular Formula: CH_4S , CH_3SH

Molecular Weight: 48.108

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

−123 (Weast 1982–83; Lide 2003)

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

5.9 (Lide 2003)

Density (g/cm^3):

0.8665 (20°C , Weast 1982–83)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

55.3 (20°C , Stephenson & Malanowski 1987)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

23.8, 24.57 (25, bp, Zwolinski & Wilhoit 1971)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

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

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F: 1.0)

Water Solubility (g/m^3 or mg/L at 25°C):

39000 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

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

101410* (5.977°C , static method-Hg manometer, measured range -51.3 to 5.977°C , Russell et al. 1942)

$\log(P/\text{mmHg}) = 18.27429 - 1769.05/(T/\text{K}) - 3.70248 \pm \log(T/\text{K})$; temp range 221.88–279.137 K (static method, Russell, et al. 1942)

101325* (8.7°C , summary of literature data, temp range -90.7 to 7.8°C , Stull 1947)

202117* (extrapolated, summary of literature data, temp range -70.3 to 5.956°C , Zwolinski & Wilhoit 1971)

$\log(P/\text{mmHg}) = 7.03163 - 1015.547/(238.706 + t/^{\circ}\text{C})$; temp range -70.3 to 24.694°C (Antoine eq., Zwolinski & Wilhoit 1971)

202346 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

$\log(P/\text{kPa}) = 6.18991 - 1030.496/(248.330 + t/^{\circ}\text{C})$, temp range -51.28 to 5.977°C , (Antoine eq. derived from Russell et al. 1942 data, Boublik et al. 1984)

$\log(P_L/\text{kPa}) = 6.19283 - 1031.216/(-32.916 + T/\text{K})$, temp range 221–283 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.19219 - 1030.918/(-32.845 + T/\text{K})$, temp range 222–279 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.13699 - 1006.199/(-35.529 + T/\text{K})$, temp range 267–359 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.53487 - 1278.361/(5.318 + T/\text{K})$, temp range 345–424 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

- 247 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)
 Log (1/K_{AW}) = 1347.1/(T/K) – 3.537; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)
 187 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 300 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 log K_{AW} = 3.249 – 1219/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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}:

Volatilization:

Photolysis:

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

k_{OH}* = 3.39 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 299.8 K, measured range 300–423 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)

k_{OH}* = 3.37 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K, measured range 244–366 K (flash photolysis-resonance fluorescence, Wine et al. 1981)

k_{OH} = 9.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 297 K (relative rate method, Cox & Sheppard 1980)

k_{OH} = 2.01 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 293 K (discharge flow-EPR, Mac Leod et al. 1983)

k_{OH} = 2.56 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 296 K (discharge flow-RF, Lee & Tang 1983)

k_{OH}* = (3.04 – 32.5) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K, measured range 254–430 K ((flash photolysis-resonance fluorescence, Wine et al. 1984)

k_{OH}* = 3.31 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1985)

k_{NO₃} = 9.2 × 10⁻¹³ cm³ ± molecule⁻¹ s⁻¹, independent of temperature over the range 250–370 K (IUPAC recommended, Atkinson et al. 1989)

k_{NO₃} = 9.3 × 10⁻¹³ cm³ ± molecule⁻¹ s⁻¹, independent of temperature over the range 254–367 K (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):

Half-Lives in the Environment:

TABLE 16.1.8.6.1

Reported vapor pressures of methanethiol 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)						
Russell et al. 1942	Stull 1947	Zwolinski & Wilhoit 1971					
static-Hg manometer	summary of literature data	selected values					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−53.28	5484	−90.7	133.3	−70.3	1333	3.869	93326
−23.872	26859	−75.3	666.6	−61.5	2666	4.580	95992
−9.474	53235	−67.5	1333	−55.9	4000	5.275	98659
0.029	79913	−58.8	2666	−51.7	5333	5.956	101325
5.977	101410	−49.2	5333	−48.3	6666	25.0	202117
		−43.1	7999	−45.4	7999	eq. 2	P/mmHg
bp/K	279.12	−34.8	13332	−40.7	10666	A	7.03163
		−22.1	26664	−36.87	13332	B	1015.547
eq. 4	P/mmHg	−7.80	53329	−29.55	19998	C	238.706
A	18.27429	8.70	101325	−24.03	26664	bp/°C	5.956
B	1769.05			−19.54	33331	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
C	3.70248	mp/°C	−	−15.73	39997	at 25°C	23.8
				−9.44	53329	at bp	24.57
				−4.31	66661		
				0.051	79993		

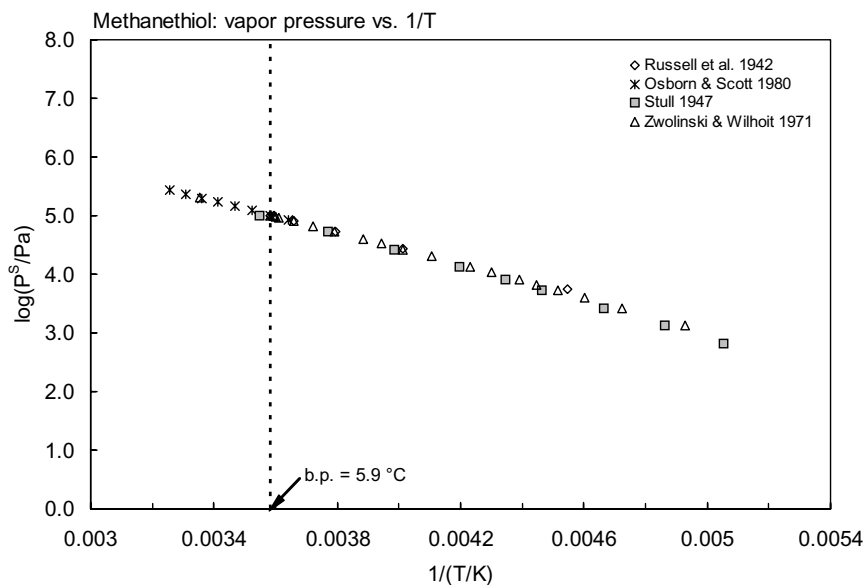


FIGURE 16.1.8.6.1 Logarithm of vapor pressure versus reciprocal temperature for methanethiol.

16.1.8.7 Ethanethiol



Common Name: Ethanethiol

Synonym: ethyl mercaptan, thioethyl alcohol, ethylhydrosulfide

Chemical Name: ethanethiol

CAS Registry No: 75-08-1

Molecular Formula: C_2H_6S , C_2H_5SH

Molecular Weight: 62.134

Melting Point (C):

-147.88 (Lide 2003)

Boiling Point (°C):

35.0 (Stull 1947; Dreisbach 1961; Weast 1982–83; Boublik et al. 1984; Dean 1985; Lide 2003)

Density (g/cm³ at 20°C):

0.83914, 0.83316 (20°C, 25°C, Dreisbach 1961)

0.8391 (Weast 1982–83)

0.8315 (25°C, Dean 1985)

Molar Volume (cm³/mol):

74.0 (20°C, calculated-density)

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

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.30, 26.78 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

15600 (Hine & Mookerjee 1975)

12000 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

15000 (Verschuereen 1983)

6800 (Dean 1985)

6760 (20°C, Budavari 1989)

14800 (selected, Yaws et al. 1990)

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):

74630* (interpolated-regression of tabulated data, temp range -76.7 to 35°C, Stull 1947)

70110* (24.933°C, ebulliometric method, measured range 0.405–66.14°C, McCullough et al. 1952)

$\log(P/\text{mmHg}) = 6.95206 - 1084.531/(231.385 + t/^\circ\text{C})$; temp range 0.405–66.14°C (Antoine eq., ebulliometric method, McCullough et al. 1952)

70300 (calculated from determined data, Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.95206 - 1084.531/(231.385 + t/^\circ\text{C})$; temp range -40 to 100°C (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.95205 - 1084.531/(T/K + 231.385)$ (Antoine eq., Osborn & Douslin 1966)

66660*, 70290 (23.613°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/\text{mmHg}) = 6.95026 - 1084.531/(231.385 + t/^\circ\text{C})$; temp range -49.2 to 55.83°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

70320 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

58660 (20°C, Verschuereen 1983)

70290 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.0768 - 1084.455/(231.374 + t/^\circ\text{C})$, temp range 0.405–66.115°C (Antoine eq. from reported exptl. data of McCullough et al. 1952, Boublik et al. 1984)

70300 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.95206 - 1084.531/(231.39 + t/^{\circ}\text{C})$; temp range -49 to 56°C (Antoine eq., Dean 1985, 1992)
 $\log (P_L/\text{kPa}) = 6.07243 - 1081.984/(-42.085 + T/\text{K})$, temp range 273 – 340 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.08253 - 1086.982/(-41.517 + T/\text{K})$, temp range 273 – 313 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.10279 - 1099.374/(-39.807 + T/\text{K})$, temp range 303 – 375 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.42565 - 1328.598/(-6.231 + T/\text{K})$, temp range 365 – 448 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.84948 - 2874.377/(200.657 + T/\text{K})$, temp range 442 – 499 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 29.2763 - 2.2725 \times 10^3/(T/\text{K}) - 7.7769 \cdot \log (T/\text{K}) - 3.8954 \times 10^{-11} \cdot (T/\text{K}) + 3.517 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 125 – 499 K (vapor pressure eq., Yaws 1994)

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

278.1 (exptl., Hine & Mookerjee 1975)
 298, 366.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 451 (20°C , headspace-GC, Vitenberg et al. 1975)
 360.3 (distilled water, headspace-GC/FID, measured range 25 – 70°C , data in graph, Przyjazny et al. 1983)
 $\log (1/K_{\text{AW}}) = 1486.1/(T/\text{K}) - 4.147$; temp range 25 – 70°C (headspace-GC, Przyjazny et al. 1983)
 292.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 278, 96.44 (quoted, calculated-molecular structure, Russell et al. 1992)
 292.5 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 4.147 - 1486/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

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 , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

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

$k_{\text{O}(3\text{P})}^* = 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas-phase reaction with $\text{O}(^3\text{P})$ atom at 298 K, measured range 257 – 495 K (Slagle et al. 1978)

$k_{\text{OH}} = 3.67 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-RF, Lee & Tang 1983)

$k_{\text{OH}} = 2.70 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 293 K (discharge flow-EPR, Mac Leod et al. 1984)

$k_{\text{OH}}^* = 4.26 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 252 – 425 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

$k_{\text{OH}}^* = 4.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{\text{OH}} = 4.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Barnes et al. 1986)

$k_{\text{OH}}^* = 4.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{NO}_3} = (1.21 \pm 0.28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298K (relative rate method, Mac Leod et al. 1986; quoted, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 16.1.8.7.1

Reported vapor pressures of ethanethiol 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)					
Stull 1947		McCullough et al. 1952		Zwolinski & Wilhoit 1971			
summary of literature data		ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–76.7	133.3	0.405	25007	–49.2	1333	eq. 2	P/mmHg
–59.1	666.6	5.236	31160	–39.5	2666	A	6.95206
–50.2	1333	10.111	38547	–33.3	4000	B	1084.531
–40.7	2666	15.017	47359	–28.7	5333	C	231.385
–29.8	5333	19.954	57803	–24.9	6666	bp/°C	35.003
–22.4	7999	24.933	70109	–21.77	7999	ΔH _v /(kJ mol ^{–1}) =	
–13.0	13332	29.944	84525	–16.58	10666	at 25°C	27.30
1.50	26664	35.000	101325	–12.38	13332	at bp	26.78
17.7	53329	40.092	120798	–4.304	19998		
35.0	101325	45.221	142368	1.796	26664		
		50.390	169052	6.758	33331		
mp/°C	–121	55.604	198530	10.972	39997		
		60.838	232087	17.932	53329		
		66.115	270110	23.613	66661		
				28.451	79993		
		Antoine eq.		32.686	93326		
		eq. 2	P/mmHg	33.475	95992		
		A	6.95206	34.247	98659		
		B	1084.531	35.003	101325		
		C	231.385	25.0	70288		

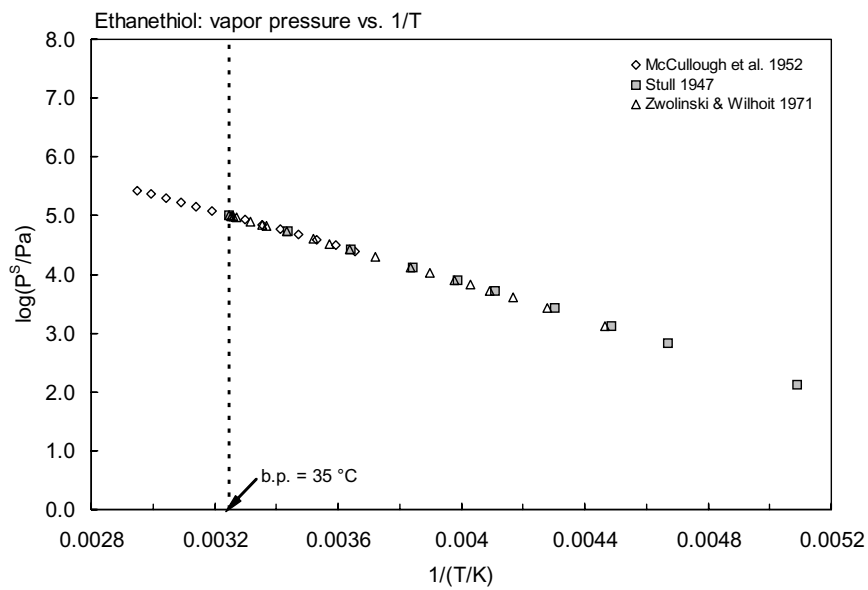
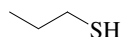


FIGURE 16.1.8.7.1 Logarithm of vapor pressure versus reciprocal temperature for ethanethiol.

16.1.8.8 1-Propanethiol



Common Name: 1-Propanethiol

Synonym: *n*-propyl mercaptan, 1-mercaptopropane

Chemical Name: 1-propanethiol

CAS Registry No: 107-03-9

Molecular Formula: C₃H₈S, CH₃CH₂CH₂SH

Molecular Weight: 76.171

Melting Point (°C):

−113.13 (Lide 2003)

Boiling Point (°C):

67.8 (Lide 2003)

Density (g/cm³):

0.8411 (20°C, Weast 1982–83)

Dissociation Constant, pK_a:

Molar Volume (cm³/mol):

99.6 (calculated-density, Stephenson & Malanowski 1987)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.88, 29.53 (25°C, bp, Zwolinski & Wilhoit 1971)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

3800 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

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

13332* (15.3°C, summary of literature data, temp range −56.0 to 67.4°C, Stull 1947)

19920* (24.275°C, ebulliometry, measured range 24.3–102.088°C, Pennington et al. 1956)

log (P/mmHg) = 6.92846 − 1183.307/(T/K + 224.624); temp range 24.3–102.088°C (Antoine eq., ebulliometry, Pennington et al. 1956; Osborn & Douslin 1966)

20558* (interpolated-Antoine eq., temp range −25 to 90.73°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.92846 − 1183.307/(224.624 + t/°C); temp range −25 to 90.73°C (Antoine eq., Zwolinski & Wilhoit 1971)

20569 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

log (P/kPa) = 6.05331 − 1183.265/(224.618 + t/°C), temp range 24.27–102.088°C (Antoine eq. derived from Pennington et al. 1956 data, Boublik et al. 1984)

log (P_L/kPa) = 6.05019 − 1181.703/(−48.687 + T/K), temp range 296–376 K, (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 6.92846 − 1183.307/(224.62 + t/°C), temp range −25 to 91°C (Antoine eq., Dean 1992)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

414 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)

log (1/K_{AW}) = 1552.2/(T/K) − 4.428; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)

331 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 4.428 − 1552/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

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

1.81 (recommended, Sangster 1993)

1.81 (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, $t_{1/2}$:

Volatilization:

Photolysis:

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

$k_{OH}^* = (4.18-4.56) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 257–419 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 16.1.8.8.1

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

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Pennington et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa
−56.0	133.3	24.275	18820	−25.0	1333
−36.3	666.6	29.563	25007	−14.3	2666
−26.3	1333	34.891	31160	−7.60	4000
−15.4	2666	40.254	38547	−2.50	5333
−3.20	5333	45.663	47359	1.65	6666
4.60	7999	51.113	57803	5.13	7999
15.3	13332	56.605	70109	10.84	10666
31.5	26664	62.139	84525	15.47	13332
49.2	53329	67.719	101325	24.369	19998
67.4	101325	73.341	120798	31.092	26664
		79.004	143268	36.562	33331
mp/ $^{\circ}C$	−112	84.710	169052	41.208	39997
		90.464	198543	48.884	53329
		96.225	232087	55.151	66661
		102.088	270110	60.489	79993
				65.163	93326
		bp/ $^{\circ}C$	67.72	66.034	95992
		Antoine eq.		66.886	98659

TABLE 16.1.8.8.1 (Continued)

Stull 1947		Pennington et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		eq. 2	P/mmHg	67.720	101325
		A	6.92846	25.0	20558
		B	1183.307		
		C	224.824	eq. 2	P/mmHg
				A	6.92846
				B	1193.307
				C	224.624
				bp/°C	67.72
				ΔH_v /(kJ mol ⁻¹) =	
				at 25°C	31.88
				at bp	29.53
		data also fitted to Cox eq.			

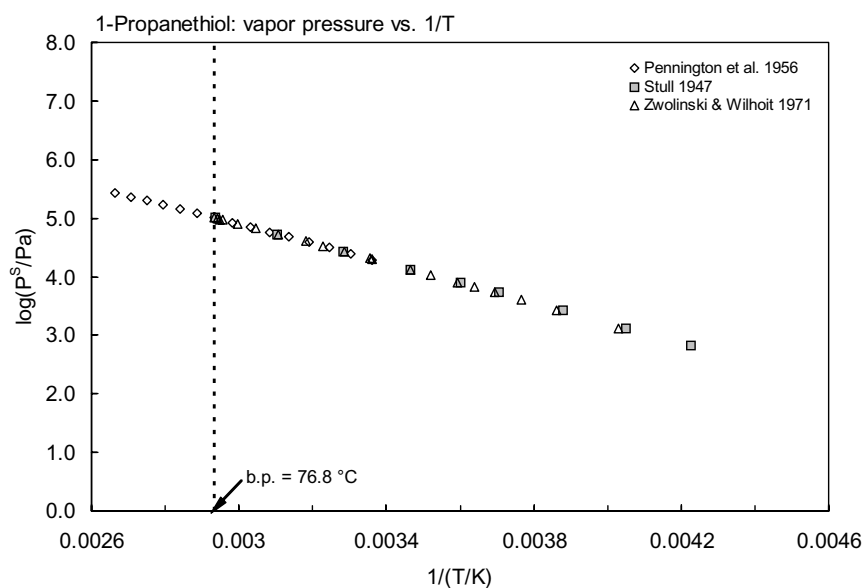
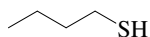


FIGURE 16.1.8.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1-propanethiol.

16.1.8.9 1-Butanethiol (Butyl mercaptan)



Common Name: 1-Butanethiol

Synonym: butyl mercaptan, *n*-butyl mercaptan

Chemical Name: 1-butanethiol

CAS Registry No: 109-79-5

Molecular Formula: $C_4H_{10}S$, $CH_3(CH_2)_3SH$

Molecular Weight: 90.187

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

−115.7 (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

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

98.5 (Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

0.8337 ($20^{\circ}C$, Weast 1982–83)

0.84159, 0.83674 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

107.8 (calculated-density, Stephenson & Malanowski 1987)

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

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

36.53, 32.225 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.46 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

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

597 (Riddick et al. 1986)

600 (selected, Yaws et al. 1990)

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

19920* ($51.409^{\circ}C$, ebulliometry, measured range 51.4 – $135.7^{\circ}C$, Scott et al. 1957)

$\log(P/mmHg) = 6.92754 - 1281.018/(T/K + 218.100)$ (Antoine eq., Osborn & Douslin 1966)

5330*, 6070 ($22.4^{\circ}C$, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.92754 - 1281.018/(218.10 + t/^{\circ}C)$; temp range -2.0 to $123.37^{\circ}C$ (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.05296 - 1281.344/(218.139 + t/^{\circ}C)$, temp range 51.409 – $135.7^{\circ}C$ (Antoine eq. derived from Scott et al. 1957 data, Boublik et al. 1984)

6070 (Riddick et al. 1986)

$\log(P/kPa) = 6.05244 - 1281.018/(218.10 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.05011 - 1279.95/(-55.132 + T/K)$, temp range 323 – 409 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 6.92754 - 1281.018/(218.10 + t/^{\circ}C)$, temp range -2 to $123^{\circ}C$ (Antoine eq., Dean 1992)

$\log(P/mmHg) = 36.2672 - 3.0452 \times 10^3/(T/K) - 9.9743 \cdot \log(T/K) - 9.1432 \times 10^{-11} \cdot (T/K) + 3.2087 \times 10^{-6} \cdot (T/K)^2$; temp range 157 – 569 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):

460.7 (distilled water, headspace-GC/FID, measured range 25 – $70^{\circ}C$, data in graph, Przyjazny et al. 1983)

$\log(1/K_{AW}) = 1655.9/(T/K) - 4.823$; temp range 25 – $70^{\circ}C$ (headspace-GC, Przyjazny et al. 1983)

911.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

363 ($20^{\circ}C$, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.823 - 1656/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 2.28 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.28 (recommended, Sangster 1989)
- 2.28 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, $\log BCF$:

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

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

Volatilization:

Photolysis:

Oxidation: 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:

$k_{OH} = 4.21 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{OH} = 4.55 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

$k_{OH} = 5.82 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Barnes et al. 1986)

$k_{OH} = 5.11 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

TABLE 16.1.8.9.1

Reported vapor pressures of 1-butanethiol 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)			
Scott et al. 1957		Zwolinski & Wilhoit 1971			
ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.409	19920	-2.0	1333	95.687	93326
57.130	25007	9.60	2666	96.630	95992
62.897	31169	16.9	4000	97.553	98659
68.710	38547	22.4	5333	98.456	101325
74.567	47359	26.9	6666	25.0	7399
80.472	57803	30.67	7999	eq. 2	P/mmHg
86.418	70109	36.86	10666	A	6.92854
92.414	84525	41.87	13332	B	1281.018
98.454	101325	51.506	19998	C	218.100
104.544	120798	58.786	26664	bp/°C	98.456
110.682	143268	64.170	33331	$\Delta H_v/(kJ\ mol^{-1}) =$	
116.863	169052	69.742	39997	at 25°C	36.53
123.088	198530	78.056	53329	at bp	32.23
129.362	232087	84.844	66661		
135.678	170110	90.625	79993		

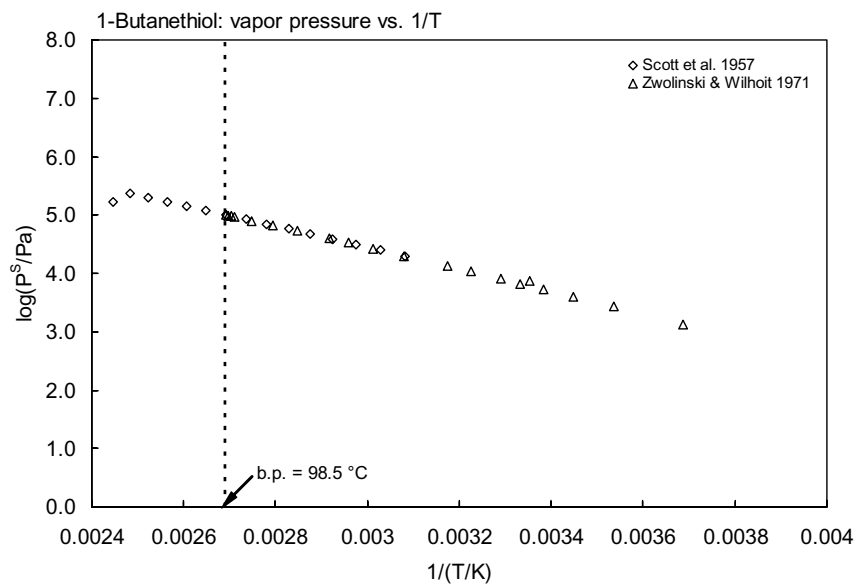
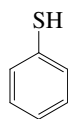


FIGURE 16.1.8.9.1 Logarithm of vapor pressure versus reciprocal temperature for 1-butanethiol.

16.1.8.10 Benzenethiol



Common Name: Benzenethiol

Synonym: thiophenol, phenyl mercaptan, mercaptobenzene

Chemical Name: benzenethiol

CAS Registry No: 108-98-5

Molecular Formula: C_6H_6S , C_6H_5SH

Molecular Weight: 110.177

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

-14.93 (Lide 2003)

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

169.1 (Lide 2003)

Density (g/cm^3):

1.0766 ($20^{\circ}C$, Weast 1982-83)

Dissociation Constant, pK_a :

6.615 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

102.7 (calculated-density, Stephenson & Malanowski 1987)

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

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.35, 36.97 ($25^{\circ}C$, bp, Riddick et al 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.45 (calorimetry at triple pt $258.27\ K$, Scott et al. 1956)

11.447 (Riddick et al. 1986)

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

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

133* ($18.6^{\circ}C$, summary of literature data, temp range 18.6 – $168^{\circ}C$, Stull 1947)

1333* ($51.5^{\circ}C$, ebulliometry, measured range 51.5 – $167.0^{\circ}C$, Vonterres et al. 1955)

19920* ($114.543^{\circ}C$, ebulliometry, measured range 114.543 – $7212.160^{\circ}C$, Scott et al. 1956)

$\log(P/mmHg) = 6.99019 - 1529.454/(230.048 + t/^{\circ}C)$; temp range 114.5 – $212^{\circ}C$ (comparative ebulliometry, data fitted to Antoine eq., Scott et al. 1956)

$\log(P/mmHg) = A \pm [1 - 442.298/(T/K)]$, where $\log A = 0.87370 - 6.4975 \times 10^{-4} \pm (T/K) + 5.2309 \times 10^{-7} \pm (T/K)^2$; measured range 114.5 – $212^{\circ}C$ (data fitted to Cox eq., comparative ebulliometry, Scott et al. 1956)

1333* ($52.28^{\circ}C$, derived from compiled data, temp range 52.3 – $198^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.99019 - 1529.454/(230.048 + t/^{\circ}C)$; temp range 52.3 – $198^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.11539 - 1529.668/(203.074 + t/^{\circ}C)$, temp range 114.54 – $212.16^{\circ}C$ (Antoine eq. derived from Scott et al. 1956 data, Boublik et al. 1984)

397 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.11509 - 1529.46/(t/^{\circ}C + 258.21)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.11531 - 1530.286/(-69.948 + T/K)$; temp range 385 – $486\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -5.4919 - 2.8549 \times 10^3/(T/K) + 8.1770 \cdot \log(T/K) - 1.9494 \times 10^{-2} \cdot (T/K) + 9.2817 \times 10^{-6} \cdot (T/K)^2$; temp range 258 – $69\ K$ (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

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

- 2.52 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.52 (recommended, Sangster 1989)
- 2.52 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

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

Half-Lives in the Environment:

TABLE 16.1.8.10.1

Reported vapor pressures of benzenethiol 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	Vonterres et al. 1955	Scott et al. 1956	Zwolinski & Wilhoit 1971				
summary of literature data	ebulliometry	comparative ebulliometry	selected values				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
18.6	133.3	51.5	1333	114.543	19920	52.28	1333
43.7	666.6	71.5	5333	121.191	25007	65.79	2666
56.0	1333	87.8	6666	127.897	31160	74.38	4000
69.7	2666	97.4	9999	134.649	38547	80.81	5333
84.2	5333	105.5	13332	141.447	47359	86.01	6666
93.9	7999	116.3	19998	148.294	57803	90.40	7999
106.6	13332	124.5	26664	155.194	70109	97.61	10666
125.8	26664	131.3	33330	162.140	84525	103.444	13332
146.7	53329	136.5	39997	176.188	120789	114.655	19998
168.0	101325	141.5	46663	183.278	143268	123.120	26664
		146.0	53329	190.426	169052	130.003	33331
mp/°C	-	149.7	59995	197.623	198530	135.847	39997
		153.0	66661	204.867	232087	145.496	53329
		156.0	73327	212.160	270110	153.367	66661
		159.0	79993			160.067	79993
		162.0	86659	mp/K	258.27	165.932	93326
		165.0	93325	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 11.447$		167.024	95992
		167.0	101325	bp/K	416.9	168.092	98659
						169.138	101325

(Continued)

TABLE 16.1.8.10.1 (Continued)

Stull 1947		Vonterres et al. 1955		Scott et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		comparative ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				eq. 2	P/mmHg	169.653	102658
				A	6.99019	170.163	103991
				B	1529.454	171.167	106658
				C	203.048		
				temp range 114–212°C		eq. 2	P/mmHg
						A	6.99019
						B	1529.454
						C	203.048
						bp/°C	
						$\Delta H_v/(\text{kJ mol}^{-1}) = 40.6$	
						at normal bp	

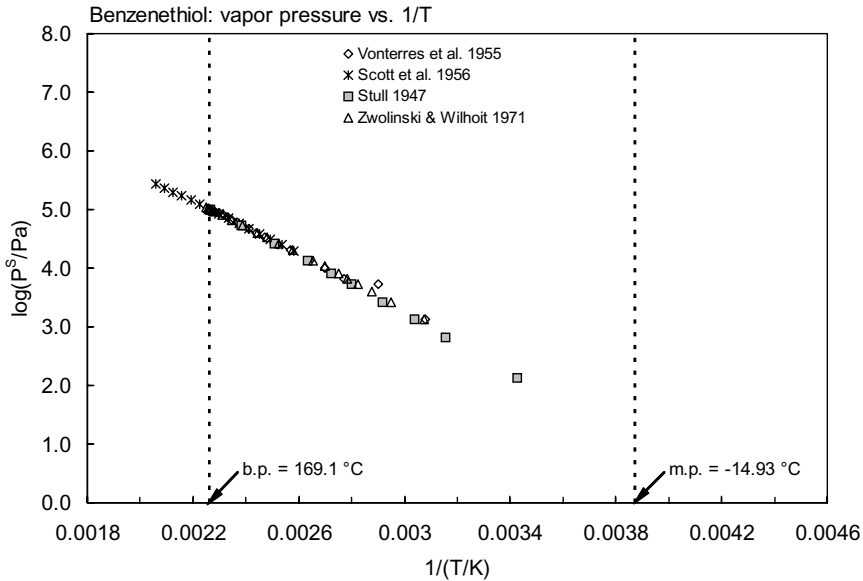


FIGURE 16.1.8.10.1 Logarithm of vapor pressure versus reciprocal temperature for benzenethiol.

16.1.8.11 Thiophene



Common Name: Thiophene

Synonym: thiofuran

Chemical Name: thiophene, thiofuran

CAS Registry No: 110-02-1

Molecular Formula: C_4H_4S

Molecular Weight: 84.140

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

−38.21 (Lide 2003)

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

84.0 (Lide 2003)

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

1.06485, 1.05887 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.0649 (Weast 1982–83)

1.06482, 1.05884 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

79.0 ($20^{\circ}C$, calculated from density)

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

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.6, 31.472 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.088 (Riddick et al. 1986)

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

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

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

3015 (shake flask-GC, Price 1976)

3900 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)

3600 ($18^{\circ}C$, Verschueren 1983)

3020 (selected, Yaws et al. 1990)

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):

9670* (interpolated-regression of tabulated data, temp range -40.7 to $81.4^{\circ}C$, Stull 1947)

7998 ($20.1^{\circ}C$, Stull 1947)

10622* (ebulliometry and manometry, measured range 0 – $84.155^{\circ}C$, Waddington et al. 1949)

10620 (calculated from determined data, Dreisbach 1955)

$\log(P/mmHg) = 6.95926 - 1246.038/(221.354 + t/^{\circ}C)$, temp range 5 – $155^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

482307* ($148.89^{\circ}C$, static-Bourdon gauge, measured range 148.89 – $304.44^{\circ}C$, Kobe et al. 1956)

44930* ($60.3^{\circ}C$, isoteniscope/manometry, measured range 60.3 – $100.3^{\circ}C$, Eon et al. 1971)

10670, 10660* ($25.09^{\circ}C$, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.95926 - 1246.01/(221.35 + t/^{\circ}C)$; temp range -12.3 to $108.1^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 8748.3/(T/K)] + 8.273276$; temp range -40.7 to $84.4^{\circ}C$ (Antoine eq., Weast 1972–73)

2450 (calculated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 394.395/(T/K)] \times 10^4 \{0.901276 - 10.3229 \times 10^{-4} \pm (T/K) + 21.9193 \times 10^{-7} \pm (T/K)^2\}$; temp range: 278.35 – $443.60\ K$ (Cox eq., Chao et al. 1983)

7998, 13330 (20°C, 30°C, quoted, Verschueren 1983)
 10622, 10620 (quoted exptl., calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.1336 - 1260.606/(222.787 + t/^\circ\text{C})$, temp range 0–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.0723 - 1138.803/(220.477 + t/^\circ\text{C})$, temp range 39.9–119.79°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 10620 (calculated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.95926 - 1246.02/(221.35 + t/^\circ\text{C})$, temp range –12 to 108°C (Antoine eq., Dean 1985, 1992)
 10620 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.08416 - 1246.02/(221.35 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 10600 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_S/\text{kPa}) = 9.84733 - 2447.236/(T/\text{K})$, temp range 195–228 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.06132 - 1232.35/(-53.438 + T/\text{K})$, temp range 311–393 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 36.6016 - 2.9794 \times 10^3/(T/\text{K}) - 10.104 \cdot \log(T/\text{K}) + 1.1445 \times 10^{-9} \cdot (T/\text{K}) + 3.2472 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 235–579 K (vapor pressure eq., Yaws et al. 1994)

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

224, 236, 230 (headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983)
 $\log(1/K_{AW}) = 1563.6/(T/\text{K}) - 4.199$; temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)
 $\log(1/K_{AW}) = 1580.0/(T/\text{K}) - 4.277$; temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)
 $\log(1/K_{AW}) = 1661.9/(T/\text{K}) - 4.542$; temp range 25–70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)
 223.3 (calculated-P/C with selected values)
 296 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 182 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 4.542 - 1662/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

1.81 \pm 0.01 (shake flask-UV, Iwasa et al. 1965)
 1.79 (calculated-f const., Rekker 1977)
 1.74 (HPLC-RV correlation, Garst 1984)
 1.82 (shake flask, Log P Database, Hansch & Leo 1987)
 1.81 (recommended, Sangster 1989, 1993)
 1.82 (shake flask-UV, Yamagami & Takao 1992)
 1.81 (recommended, Hansch et al. 1995)

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

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

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

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

Volatilization:

Photolysis:

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

$k_{\text{OH}} = (9.58 \pm 0.38) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated atmospheric lifetime $\tau \sim 28 \text{ h}$; and $k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ and $k_{\text{O}(^3\text{P})} = 4.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O}(^3\text{P})$ atom at room temp. (relative rate method, Atkinson et al 1983)

$k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.004 \text{ d}^{-1}$, $k_{\text{OH}} = 9.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.8 d^{-1} ; $k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.7 d^{-1} at room temp. (review, Atkinson & Carter 1984)

$k_{\text{OH}}^* = (9.37, 9.57) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , measured range $255\text{--}425 \text{ K}$ (flash photolysis-resonance fluorescence, Wine & Thompson 1984)

$k_{\text{OH}} = 9.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.004 \text{ d}^{-1}$, $k_{\text{OH}} = 9.70 \times 10^{-12} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.4 d^{-1} , and $k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.7 d^{-1} at room temp. (review, Atkinson 1985)

$k_{\text{NO}_3} = (3.2 \pm 0.7) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 36 h and a loss rate of 0.7 d^{-1} assuming $2.4 \times 10^8 \text{ NO}_3 \text{ radicals/cm}^3$ in nighttime air at $295 \pm 1 \text{ K}$ in the atmosphere (relative rate technique, Atkinson et al. 1985)

$k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau > 270 \text{ d}$, $k_{\text{OH}} = 9.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 29 h during daytime hours, and $k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 36 h at room temp. (review, Atkinson 1985)

$k_{\text{OH}}^* = 9.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{NO}_3} = 3.93 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range $272\text{--}296 \text{ K}$ (recommended, Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 14.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (molecular orbital calculations, (Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetime of $\sim 28 \text{ h}$ due to reactions with OH radical (Atkinson et al. 1983);

calculated gas-phase lifetime of 29 h for the reaction with OH radical during daytime hours, calculated lifetime of 36 h for reaction with NO_3 radical and a calculated lifetime $> 270 \text{ d}$ for reaction with O_3 at room temp. (Atkinson et al. 1985)

TABLE 16.1.8.11.1

Reported vapor pressures of thiophene 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	Waddington et al. 1949	Kobe et al. 1956	Zwolinski & Wilhoit 1971				
summary of literature data	manometry and ebulliometry	static-Bourdon gauge	selected values				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
static method							
-40.7	133	0	2858	148.89	482307	-12.3	1333
-20.8	666.6	15	6497	154.44	585659	-1.10	2666
-10.9	1333	20	8355	160.00	620109	5.94	4000
0.0	2666	25	10627	165.56	730351	11.24	5333
12.5	5333	30	13398	171.11	813032	15.52	6666
20.1	7999	35	16733	176.67	895713	19.14	7999

(Continued)

TABLE 16.1.8.11.1 (Continued)

Stull 1947		Waddington et al. 1949		Kobe et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		manometry and ebulliometry		static-Bourdon gauge		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.5	13332	40	20736	182.22	992174	25.09	10666
46.5	26664	ebulliometric method		187.78	1088636	29.90	13332
64.7	53329	39.061	19920	193.33	1198877	39.15	19998
81.4	101325	44.560	25007	198.89	1316009	46.14	26664
		50.094	31160	204.44	1440031	51.82	33331
mp/°C	-38.3	55.663	38547	210.00	1584723	56.65	39997
		61.276	47359	215.56	1722525	64.62	53329
		66.931	57903	221.11	1874107	71.12	66661
		72.629	70109	226.67	2039470	76.66	79993
Eon et al. 1971		78.370	84525	232.22	2211722	81.51	93326
isoteniscope-manometer		84.155	101325	237.78	2397755	82.41	95992
t/°C	P/Pa			243.33	2590678	83.30	98659
60.3	44930	mp/°C	-38.1	248.89	2797381	84.16	101325
70.3	64795	bp/°C	84.16	254.44	3010974		
80.3	91459			260.00	3238347	bp/°C	84.16
90.3	126790	eq. 2	P/mmHg	265.56	3472610		
100.3	172519	A	6.95926	271.11	3727544	eq. 2	P/mmHg
		B	1246.038	276.67	3996258	A	6.95926
		C	221.354	282.22	4251192	B	1246.02
$\Delta H_v/(kJ\ mol^{-1}) = 34.77$				287.78	4540576	C	221.35
		$\Delta H_v/(kJ\ mol^{-1}) =$		293.33	4836850		
		at 45.36°C	33.61	298.89	5146905	$\Delta H_v/(kJ\ mol^{-1}) =$	
		at 63.08°C	32.67	304.44	5463849	at 25°C	34.60
		at bp	31.47			at bp	31.47

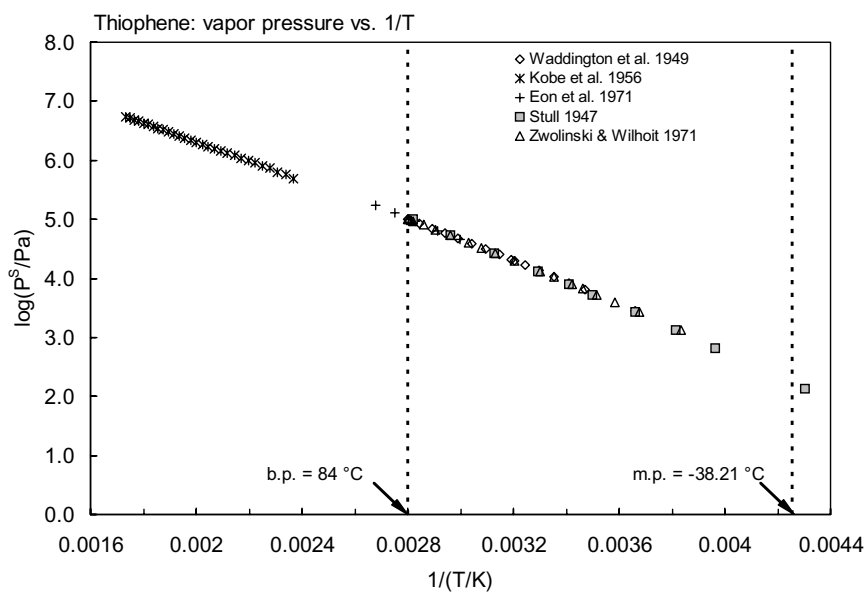
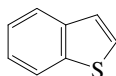


FIGURE 16.1.8.11.1 Logarithm of vapor pressure versus reciprocal temperature for thiophene.

16.1.8.12 Benzo[*b*]thiophene

Common Name: Benzo[*b*]thiophene

Synonym: thianaphthene, thionaphthene, 1-benzothiophene

Chemical Name:

CAS Registry No: 95-15-8

Molecular Formula: C₈H₆S

Molecular Weight: 134.199

Melting Point (°C):

32 (Lide 2003)

Boiling Point (°C):

221 (Lide 2003)

Density (g/cm³ at 20°C):

1.1500 (Verschuieren 1983)

Molar Volume (cm³/mol):

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

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.854 (mp at 32°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

130.0 (20°C, shake flask, Smith et al. 1978)

130.2 (Mill et al. 1981)

216* (59.05°C, equilibrium cell-GC, measured range 332.2–490.5 K, Leet et al. 1987)

Vapor Pressure (Pa at 25°C or as indicated):

26.7 (20°C, estimated from naphthalene, Smith et al. 1978)

14.80 (calculated-bp, Mackay et al. 1982)

$\log(P/\text{mmHg}) = -9.5352 - 2.6947 \times 10^3/(T/K) + 8.8858 \cdot \log(T/K) - 1.5478 \times 10^{-2} \cdot (T/K) + 6.5159 \times 10^{-6} \cdot (T/K)^2$;
temp range 305–754 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

28.0 (calculated-P/C, Smith & Bomberger 1980)

24.1 (calculated-P/C, this work)

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

3.09 (shake flask-UV, pH 7.4, Rogers & Cammarata 1969)

3.05 (HPLC-RT correlation, De Voogt et al. 1988)

3.12 (recommended, Sangster 1989, 1993)

3.26 (shake flask-HPLC, De Voogt et al. 1990)

3.18 (HPLC-RT correlation, Ritter et al. 1994)

3.17 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

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

Bioconcentration Factor, log BCF:

2.08 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log K_{oc}:

1.77 (Coyote Creek sediment, Smith et al. 1978)

2.30 (lab. mixture of microorganisms, Smith et al. 1978)

3.49, 3.0 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

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

Volatilization: estimated $t_{1/2} = 45$ h in river, $t_{1/2} = 230$ h in eutrophic pond, $t_{1/2} = 180$ hours in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7} \text{ s}^{-1}$ exposed to 12 h sunlight per day in late May with estimated $t_{1/2} = 1200$ h in river, $t_{1/2} = 2900$ h in eutrophic pond, $t_{1/2} = 3500$ h in eutrophic lake and $t_{1/2} = 600$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Oxidation:

laboratory investigated $k = 83 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical and estimated $t_{1/2} = 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)
 $k = 5.7 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 34$ h under natural sunlight conditions, $k = 83 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 96$ d for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated $t_{1/2} > 20$ h in river, $t_{1/2} < 20$ h in eutrophic pond, $t_{1/2} = 20$ h in eutrophic lake and very long half-life in oligotrophic lake, based on the biodegradation rate in the presence of alternative carbon sources will be one-half the biodegradation rate of quinoline when quinoline is the only carbon source by the one compartment model (Smith et al. 1978).

Biotransformation:

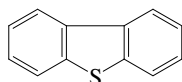
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated volatilization $t_{1/2} = 45$ h in river, $t_{1/2} = 230$ h in eutrophic pond, $t_{1/2} = 180$ h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978);

photolysis rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7} \text{ s}^{-1}$ exposed to 12 h sunlight per day in late May with estimated photolysis $t_{1/2} = 1200$ h in river, $t_{1/2} = 2900$ h in eutrophic pond, $t_{1/2} = 3500$ h in eutrophic lake and $t_{1/2} = 600$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

16.1.8.13 Dibenzothiophene



Common Name: Dibenzothiophene

Synonym:

Chemical Name: dibenzothiophene

CAS Registry No: 132-65-0

Molecular Formula: $C_{12}H_8S$

Molecular Weight: 184.257

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

98.2 (Lide 2003)

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

332.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

191.3 (calculated-Le Bas method at normal boiling point)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.191 (mp at $98.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.11 \pm 0.09 ($28^{\circ}C$, measured, Smith et al. 1978)

1.470 ($24^{\circ}C$, shake flask-LSC, Means et al. 1980)

1.106 (Mill et al. 1981)

1.500 (Steen & Karickhoff 1981)

1.032 (literature average, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.267 ($20^{\circ}C$, estimated, Aubry et al. 1975)

$\log(P/mmHg) = 22.90 - 10910/(T/K)$, temp range $60-00^{\circ}C$ (solid, gas saturation, Edward & Prausnitz 1981)

$\log(P/mmHg) = 21.10 - 8353/(T/K)$, temp range $100-130^{\circ}C$ (liquid, gas saturation, Edward & Prausnitz 1981)

0.263, 0.0083 ($20^{\circ}C$, quoted, calculated-bp, Mackay et al. 1982)

0.893 (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1982)

0.586 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 605.160/(T/K)] \times 10^{0.865373 - 5.51221 \times 10^{-4} \pm (T/K) + 6.05701 \times 10^{-7} \pm (T/K)^2}$; temp range: $424.81-607.53$ K (Cox eq., Chao et al. 1983)

$\log(P_L/kPa) = 7.18577 - 3140.15/(T/K)$, temp range $385-574$ K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

44.3 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.38 (shake flask-LSC, Means et al. 1980)

4.33 (HPLC-RT correlation, De Voogt et al. 1988)

4.38 (recommended, Sangster 1989, 1993)

4.49 (shake flask-HPLC, De Voogt et al. 1990)

4.38 (recommended, Hansch et al. 1995)

4.41 ± 0.19 , 4.43 ± 0.61 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

4.36 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

3.20 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log K_{OC} :

3.14 (Coyote Creek sediment, Smith et al. 1978)
 4.05 (soil, Hassett et al. 1980)
 4.05 (average of 3 sediment/soil samples, equilibrium sorption isotherm, Means et al. 1980)
 4.00 (soil, calculated-MCI χ , Sabljic 1987)
 4.00 (soil, calculated-MCI χ , Sabljic 1987)
 4.17 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987)
 3.75 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987)
 2.92 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987)
 4.00 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987)
 3.60 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987)
 4.59 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)
 3.87 (soil: organic carbon OC $\geq 0.1\%$, average, Delle Site 2001)
 4.02, 4.04 (sediments: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)
 4.07 (Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 140$ h in river, $t_{1/2} = 720$ h in eutrophic pond, $t_{1/2} = 580$ h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: solar photolysis $k = 1.5 \times 10^{-8} \text{ s}^{-1}$ over 24-h day; rate constant of transformation and transport of $(2.04 \pm 0.08) \times 10^{-6} \text{ s}^{-1}$ exposed to 12 h sunlight per day in early March with estimated $t_{1/2} = 380$ h in river, $t_{1/2} = 950$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 190$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978); $t_{1/2} = 4\text{--}8$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation: laboratory investigated $k < 7.5 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical and estimated $t_{1/2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978). $k = 1.5 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 128$ h under natural sunlight conditions, $k < 7.5 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} > 3.5$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: $k = 5.3 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ and the estimated $t_{1/2} = 13$ h in river, eutrophic pond, and eutrophic lake and $t_{1/2} > 10^4$ h in oligotrophic lake by the one compartment model (Smith et al. 1978)

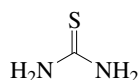
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: $t_{1/2} = 0.5$ h from river water, $t_{1/2} = 13$ h from pond water, $t_{1/2} = 13$ h from eutrophic lake and $t_{1/2} = 140$ h from oligotrophic lake predicted by one-compartment model for all processes; estimated volatilization $t_{1/2} = 140$ h in river, $t_{1/2} = 720$ h in eutrophic pond, $t_{1/2} = 580$ h in eutrophic lake and oligotrophic lake; photolysis rate constant of transformation and transport $k = (2.04 \pm 0.08) \times 10^{-6} \text{ s}^{-1}$ exposed to 12 h sunlight per day in early March with estimated photolysis $t_{1/2} = 380$ h in river, 950 h in eutrophic pond and eutrophic lake and $t_{1/2} = 190$ h in oligotrophic lake; biodegradation $t_{1/2} = 13$ h in river, eutrophic pond water and $t_{1/2} = 140$ h in oligotrophic lake (Smith et al. 1978); $t_{1/2} = 4\text{--}8$ h for disappearance via direct photolysis in aqueous media (Harris 1982).

16.1.8.14 Thiourea



Common Name: Thiourea

Synonym: thiocarbamide

Chemical Name: thiourea

CAS Registry No: 62-56-6

Molecular Formula: $\text{CH}_4\text{N}_2\text{S}$, H_2NCSNH_2

Molecular Weight: 76.121

Melting Point ($^{\circ}\text{C}$):

178 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

decomposes (Verschuereen 1983)

Density (g/cm^3 at 20°C):

1.045 (Weast 1982–83; Verschuereen 1983, Dean 1992)

Dissociation Constant, pK :

2.03 (pK_1 , Dean 1985)

Molar Volume (cm^3/mol):

76.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.42 (Donnelly et al. 1990)

12.55 (Kim et al. 1994)

15.64, 14.92, 15.17 (differential scanning calorimetry in three types of crucibles, Gatta et al. 2000)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

35.2, 33.7, 34.1 (Gatta et al. 2000)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F : 0.0315 (mp at 178°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

91000 (20 – 25°C , shake flask-gravimetric, Dehn 1917)

91800 (13°C , Verschuereen 1983)

89800 (Windholz 1983)

110000 (Budavari 1989)

90000 (Dean 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

−1.02 (Leo et al. 1971)

−0.95 (shake flask, Cornford 1982)

−2.38, −0.95 (calculated, Verschuereen 1983)

−1.17 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)

−1.08, −1.03 (pH 6.5, pH 12, shake flask-HPLC, Govers et al. 1986)

−1.14, −1.02 (shake flask, Log P Database, Hansch & Loe 1987)

−0.99 (recommended, Sangster 1993)

−1.02 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.73 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)

−0.699 (alga *Chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 1.6\text{--}16$ h in air, based on rate constant for the vapor-phase reaction with OH radical and photooxidation $t_{1/2} = 2048\text{--}81927$ h in water, based on estimated rate data for reaction with OH radical in aqueous solution (Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 24\text{--}168$ h, based on aqueous aerobic screening test data and aqueous anaerobic biodegradation $t_{1/2} = 96\text{--}672$ h, based on aqueous aerobic degradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{1/2} = 1.6\text{--}16$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

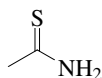
Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota:

16.1.8.15 Thioacetamide



Common Name: Thioacetamide

Synonym: ethanethioamide, acetothioamide

Chemical Name: thioacetamide

CAS Registry No: 62-55-5

Molecular Formula: C_2H_5NS , CH_3CSNH_2

Molecular Weight: 75.133

Melting Point ($^{\circ}C$):

115.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

84.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.129 (mp at $115.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

163000 (Dean 1985)

163000 (Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

-0.46, 0.36 (Verschuere 1983)

-0.26 (shake flask, Log P Database, Hansch & Leo 1987)

-0.26 (recommended, Sangster 1993)

-0.26 (recommended, Hansch & Leo 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric $t_{1/2} = 3.2\text{--}31.7$ h, based on estimated rate data for OH radical in air (Howard et al. 1991).

Hydrolysis: first-order rate constant $k = 8.6 \times 10^{-1} h^{-1}$ at pH 7 and $25^{\circ}C$ (Ellington et al. 1987), corresponding to a $t_{1/2} = 8064$ h (Howard et al. 1991);

acid rate constant $k = 6.0 \times 10^{-2} M^{-1} \pm h^{-1}$, corresponding to a $t_{1/2} = 333$ d and base rate constant $k = 1.4 M^{-1} \pm h^{-1}$, corresponding to a $t_{1/2} = 289$ d (Howard et al. 1991).

Biodegradation: aerobic biodegradation $t_{1/2} = 24\text{--}168$ h, based on aqueous aerobic screening test data and anaerobic biodegradation $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 3.2\text{--}31.7$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}268$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.2 SUMMARY TABLES

TABLE 16.2.1
Summary of physical properties of nitrogen and sulfur containing compounds

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 _M cm ³ /mol		pK _a or pK _b
							MW/ ρ at 20°C	Le Bas	
Nitriles:									
Acetonitrile	75-05-8	CH ₃ CN	41.052	−43.82	81.65	1	52.25	56.3	
Propionitrile	107-12-0	C ₂ H ₅ CN	55.079	−92.78	97.14	1	70.45	78.5	
Butyronitrile	109-74-0	C ₃ H ₇ CN	69.106	−111.9	117.6	1	87.35	100.7	
Acrylonitrile (2-Propenitrile)	107-13-1	C ₂ H ₃ CN	53.063	−83.48	77.3	1	65.83	71.1	
Benzonitrile	100-47-0	C ₆ H ₅ CN	103.122	−13.99	191.1	1		107.9	
Adiponitrile	111-69-3	CN(CH ₂) ₄ CN	108.141	1	295	1		149.6	
Aliphatic amines:									
Methylamine	74-89-5	CH ₃ NH ₂	31.058	−93.5	−6.32	1		43.8	
Dimethylamine	124-40-3	(CH ₃) ₂ NH	45.084	−92.18	6.88	1	68.77	67.5	10.77
Trimethylamine	75-50-3	(CH ₃) ₃ N	59.110	−117.1	2.87	1	93.00	93.3	9.8
Ethylamine	75-04-7	CH ₃ CH ₂ NH ₂	45.084	−80.5	16.5	1	66.02	66.0	10.63
Diethylamine	109-89-7	(C ₂ H ₅) ₂ NH	73.137	−49.8	55.5	1	103.45	111.9	10.8
Triethylamine	121-44-8	(C ₂ H ₅) ₃ N	101.910	−114.7	89	1		154.8	10.78
n-Propylamine	107-10-8	C ₃ H ₇ NH ₂	59.110	−84.75	47.22	1	82.41	88.2	10.568
Dipropylamine	142-84-7	(C ₃ H ₇) ₂ NH	101.190	−63	109.3	1			
Diisopropylamine	108-18-9	i(C ₃ H ₇) ₂ NH	101.190	−61	83.9	1			
Tripropylamine	102-69-2	(C ₃ H ₇) ₃ N	143.270	−93.5	156	1			10.66
n-Butylamine	109-73-9	C ₄ H ₉ NH ₂	73.137	−49.1	77.0	1	98.94	110.4	10.64
Isobutylamine	78-81-9	iC ₄ H ₉ NH ₂	73.137	−86.7	67.75	1		110.4	10.41
tert-Butylamine	75-64-9	(CH ₃) ₃ CNH ₂	73.137	−66.94	44.04	1		110.4	1.685
Di-n-butylamine	111-92-2	(C ₄ H ₉) ₂ NH	129.244	−62	159.6	1		199.2	11.25
Tributylamine	102-82-9	(C ₄ H ₉) ₃ N	185.349	−70	216.5	1		288	9.93
Ethylenediamine	107-15-3	H ₂ NCH ₂ CH ₂ NH ₂	60.098	11.14	117	1			
Ethanolamine	141-43-5	HOCH ₂ CH ₂ NH ₂	61.098	10.5	171	1	60.21	73.4	9.48
Diethanolamine	111-42-2	(HOCH ₂ CH ₂) ₂ NH	105.136	28	268.8	0.934	95.87	126.7	8.88
Triethanolamine	102-71-6	(HOCH ₂ CH ₂) ₃ N	149.188	20.5	335.4	1	132.71	182.1	7.76
Cyclohexylamine	108-91-8	C ₆ H ₁₁ NH	99.174	−17.8	134	1		117.4	10.66

(Continued)

TABLE 16.2.1 (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 _M cm ³ /mol		pK _a or pK _b
							MW/ ρ at 20°C	Le Bas	
Aromatic amines:									
Aniline	62-53-3	C ₆ H ₅ NH ₂	93.127	−6.02	184.17	1	91.15	110.2	4.596
2-Chloroaniline	95-51-2	Cl(C ₆ H ₄)NH ₂	127.572	−1.9	208.8	1	105.21	131.1	2.661
3-Chloroaniline	108-42-9	Cl(C ₆ H ₄)NH ₂	127.572	−10.28	230.5	1	104.91	131.1	3.5
4-Chloroaniline	106-47-8	Cl(C ₆ H ₄)NH ₂	127.572	70.5	232	0.358		131.1	3.982
3,4-Dichloroaniline	95-76-1	Cl ₂ C ₆ H ₃ NH ₂	162.017	72	272	0.346		152.0	
2,4,6-Trichloroaniline	634-93-5	C ₆ H ₄ Cl ₃ N	196.462	78.5	262	0.299		172.9	
<i>o</i> -Toluidine	95-53-4	CH ₃ C ₆ H ₄ NH ₂	107.153	−14.41	200.3	1	107.32	132.4	4.45
<i>m</i> -Toluidine	108-44-1	CH ₃ C ₆ H ₄ NH ₂	107.153	−31.3	203.3	1	108.36	132.4	4.71
<i>p</i> -Toluidine	106-49-0	CH ₃ C ₆ H ₄ NH ₂	107.153	43.6	200.4	0.657	111.40	132.4	5.08
N,N′-Dimethylaniline	121-69-7	C ₆ H ₅ N(CH ₃) ₂	121.180	2.42	194.15	1	126.80	154.6	5.15
2,4-Xylidine	95-68-1	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.180	−14.3	214	1		154.6	4.89
2,5-Xylidine	95-78-3	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.180	15.5	214	1		154.6	4.54
2,6-Xylidine	87-62-7	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.180	11.2	215	1	123.12	154.6	3.95
2-Ethylaniline	578-54-1	C ₂ H ₅ C ₆ H ₄ NH ₂	121.180	−43	209.5	1		139.6	4.42
3-Ethylaniline	587-02-0	C ₂ H ₅ C ₆ H ₄ NH ₂	121.180	−64	214	1		139.6	4.70
4-Ethylaniline	589-16-2	C ₂ H ₅ C ₆ H ₄ NH ₂	121.180	−2.4	217.5	1		139.6	5.00
N,N′-Diethylaniline	91-66-7	C ₆ H ₅ N(C ₂ H ₅) ₂	149.233	−38.8	216.3	1		199.0	6.56
Diphenylamine	122-39-4	(C ₆ H ₅) ₂ NH	169.222	53.2	302	0.529	145.88	200.3	0.90
4-Aminobiphenyl	92-67-1	C ₆ H ₅ C ₆ H ₄ NH ₂	169.222	53.5	302	0.525		168.8	4.27
Benzidine	92-87-5	NH ₂ (C ₆ H ₄) ₂ NH ₂	184.236	120	401	0.117		213.0	4.66
3,3′-Dichlorobenzidine	91-94-1	C ₁₂ H ₁₀ Cl ₂ N ₂	253.126	132.5		0.0882		254.8	11.7
α-Naphthylamine	134-32-7	C ₁₀ H ₇ NH ₂	143.185	49.2	300.7	0.579		161.8	3.92
β-Naphthylamine	91-59-8	C ₁₀ H ₇ NH ₂	143.185	113	306.2	0.137		161.8	4.15
N,N′-Bianiline	122-66-7	(C ₆ H ₅) ₂ (NH) ₂	184.236	131		0.0912		213.0	13.2
2-Nitroaniline	88-74-4	C ₆ H ₆ N ₂ O ₂	138.124	71.0	284	0.354		138.7	−0.28
3-Nitroaniline	99-09-2	C ₆ H ₆ N ₂ O ₂	138.124	113.4	306 dec	0.136		138.7	2.46
4-Nitroaniline	100-01-6	C ₆ H ₆ N ₂ O ₂	138.124	147.5	332	0.0628	97.00	138.7	1.01
2,4-Dinitroaniline	97-02-9	(O ₂ N) ₂ C ₆ H ₃ NH ₂	183.122	180.0		0.0301		167.2	−4.25
2,6-Dinitroaniline	606-22-4	(O ₂ N) ₂ C ₆ H ₃ NH ₂	183.122	141		0.0728		167.2	−5.23
3,5-Dinitroaniline	618-87-1	(O ₂ N) ₂ C ₆ H ₃ NH ₂	183.122	163		0.0443		167.2	0.229

Nitroaromatic compounds:

Nitrobenzene	98-95-3	C ₆ H ₅ NO ₂	123.110	5.7	210.8	1	102.28	112.0
1,2-Dinitrobenzene	528-29-0	C ₆ H ₄ (NO ₂) ₂	168.107	116.5	318	0.127		149.4
1,3-Dinitrobenzene	99-65-0	C ₆ H ₄ (NO ₂) ₂	168.107	90.3	291	0.229		149.4
1,4-Dinitrobenzene	100-25-4	C ₆ H ₄ (NO ₂) ₂	168.107	173.5	297	0.0349		149.4
2-Nitrotoluene	88-72-2	CH ₃ C ₆ H ₄ NO ₂	137.137	-10.4	222	1	117.93	153.0
3-Nitrotoluene	99-08-1	CH ₃ C ₆ H ₄ NO ₂	137.137	15.5	232	1		153.0
4-Nitrotoluene	99-99-0	CH ₃ C ₆ H ₄ NO ₂	137.137	51.63	238.3	0.548		153.0
2,4-Dinitrotoluene (DNT)	121-14-2	CH ₃ C ₆ H ₃ (NO ₂) ₂	182.134	70.5	300 dec	0.358		175.2
2,6-Dinitrotoluene	606-20-2	CH ₃ C ₆ H ₃ (NO ₂) ₂	182.134	66.0	285	0.396		175.2
2,4,6-Trinitrotoluene (TNT)	118-96-7	CH ₃ C ₆ H ₂ (NO ₂) ₃	227.131	80.5	240 exp	0.285	137.32	203.7
1-Nitronaphthalene	86-57-7	C ₁₀ H ₇ NO ₂	173.169	61	304	0.443		176.1
2-Nitronaphthalene	581-89-5	C ₁₀ H ₇ NO ₂	173.169	79	314	0.295		176.1
4-Nitrobiphenyl	92-93-3	C ₁₂ H ₉ NO ₂	199.205	114	340	0.134		211.3
5-Nitro-acenaphthene	602-87-9	C ₁₂ H ₉ NO ₂	199.205	103		0.172		211.3

Amide and ureas:

Acetamide	60-35-5	CH ₃ CONH ₂	59.067	80.16	222	0.288		66.9	7.62
Acrylamide	79-06-1	H ₂ C=CHCONH ₂	71.078	84.5	192.5	0.261		80.8	
Benzamide	55-21-0	C ₆ H ₅ CONH ₂	121.137	127.3	290	0.0992		132.4	
Urea	57-13-6	H ₂ NCONH ₂	60.055	133	dec	0.0872	45.39	58.0	

Nitrosoamines:

<i>N</i> -Nitrosodimethylamine	62-75-9	(CH ₃) ₂ NNO	74.081		152			87.7	
<i>N</i> -Nitrosodiethylamine	55-18-5	(C ₂ H ₅) ₂ NNO	120.134		176.9			130.6	
Di- <i>n</i> -propyl nitrosamine	621-64-7	(C ₃ H ₇) ₂ NNO	130.187		206			176.5	
Diphenylnitrosamine	86-30-6	(C ₆ H ₅) ₂ NNO	198.219	66.5	152	0.392		220.5	

Heterocyclic compounds:

1 <i>H</i> -Pyrrole	109-97-7	C ₄ H ₅ N	67.090	-23.39	129.79	1	69.18	78.2	
1-Methylpyrrole	96-54-8	C ₅ H ₇ N	81.117	-56.32	112.81	1		104.0	
Pyrrolidine	123-75-1	C ₄ H ₈ NH	71.121	-57.79	86.56	1		96.6	4.453
Imidazole	288-32-4	C ₃ H ₄ N ₂	68.077	89.5	257	0.233		78.9	11.305
Indazole	271-44-3	C ₇ H ₆ N ₂	118.136	148	269	0.0621		130.5	
Indole	120-72-9	C ₈ H ₇ N	117.149	52.5	253.6	0.537		133.4	
Indoline	496-15-1	C ₈ H ₉ N	119.164		229			140.8	
Pyridine	110-86-1	C ₅ H ₅ N	79.101	-41.70	115.23	1	80.56	93.0	5.17
2-Methylpyridine	109-06-8	C ₆ H ₇ N	93.127	-66.68	129.38	1	98.61	115.2	5.96
3-Methylpyridine	108-99-6	C ₆ H ₇ N	93.127	-18.14	144.14	1	97.35	115.2	5.68
4-Methylpyridine	108-89-4	C ₆ H ₇ N	93.127	3.67	145.36	1		115.2	6.00

(Continued)

TABLE 16.2.1 (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 _M cm ³ /mol		pK _a or pK _b
							MW/ ρ at 20°C	Le Bas	
2,3-Dimethylpyridine	583-61-9	C ₇ H ₉ N	107.153	-15.5	161.12	1		135.9	6.6
2,4-Dimethylpyridine	108-47-4	C ₆ H ₉ N	107.153	-64	158.38	1		135.9	
2,6-Dimethylpyridine	108-48-5	C ₇ H ₉ N	107.153	-6.1	144.01	1		135.9	6.72
2,4,6-Trimethylpyridine	108-75-8	C ₈ H ₁₁ N	121.180	-46	170.6	1		158.1	7.43
Quinolines:									
Quinoline	91-22-5	C ₉ H ₇ N	129.159	-14.78	237.16	1		144.7	4.90
Isoquinoline	119-65-3	C ₉ H ₇ N	129.159	26.47	243.22	0.967		144.7	5.4
3-Methyl-isoquinoline	1125-80-0	C ₁₀ H ₉ N	143.185	68	249	0.379		166.9	
2,7-Dimethylquinoline	93-37-8	C ₁₁ H ₁₁ N	157.212	61	264.5	0.443		189.1	
Benzo[f]quinoline	85-02-9	C ₁₃ H ₉ N	179.217	94	352	0.210		196.3	
Benzo(h)quinoline	230-27-3	C ₁₃ H ₉ N	179.217	52	339	0.543		196.3	
9H-Carbazole	86-74-8	C ₆ H ₄ NHC ₆ H ₄	167.206	246.3	354.69	0.00674		192.9	
7H-Dibenzo[c,g]carbazole	194-59-2	(C ₁₀ H ₆) ₂ NH	267.324	158		0.0496		296.1	
Acridine	260-94-6	C ₁₃ H ₉ N	179.217	110	344.86	0.147		196.3	5.60
Benz[a]acridine	225-11-6	C ₁₇ H ₁₁ N	229.276					244.8	
Benz[c]acridine	225-51-4	C ₁₇ H ₁₁ N	229.276	132		0.0892		244.8	
Dibenz[a,h]acridine	53-70-3	C ₂₂ H ₁₄	278.346	269.5	524	0.00399		300.0	
Sulfur compounds:									
Carbon disulfide	75-15-0	CS ₂	76.141	-112.1	46	1	60.28	66.0	
Dimethyl sulfate	77-78-1	(CH ₃ O) ₂ SO ₂	126.132	-27	188 dec	1		109.7	
Diethyl sulfate	64-67-5	(C ₂ H ₅ O) ₂ SO ₂	154.185	-24	208	1		138.4	
Dimethyl sulfite	616-42-2	(CH ₃ O) ₂ SO	110.132		126			100.5	
Dimethyl sulfoxide (DMSO)	67-68-5	(CH ₃) ₂ SO	78.133	17.89	189	1		85.7	
Dimethyl sulfone	67-71-0	(CH ₃) ₂ SO ₂	94.133	108.9	238	0.150		94.0	
Dimethyl sulfide	75-18-3	(CH ₃) ₂ S	62.134	-98.24	37.33	1	73.77	77.4	
Dimethyl disulfide	624-92-0	C ₂ H ₆ S ₂	94.199	-84.67	109.74	1	58.78	103.0	
Diethyl sulfide	352-93-2	C ₄ H ₁₀ S	90.187	-103.91	92.1	1		128.1	
Diethyl disulfide	110-81-6	C ₄ H ₁₀ S ₂	122.252	-101.5	154.0	1		147.4	
Thiols:									
Methanethiol	74-93-1	CH ₃ SH	48.108	-123	5.9	1	55.52	55.2	10.7
Ethanethiol	75-08-1	C ₂ H ₅ SH	62.134	-147.88	35.0	1	74.05	77.4	10.61
Propanethiol	107-03-9	C ₃ H ₇ SH	76.161	-113.13	67.8	1	90.55	99.6	
1-Butanethiol (Butyl mercaptan)	109-79-5	CH ₃ (CH ₂) ₃ SH	90.187	-115.7	98.5	1	107.16	121.8	

2-Butanethiol	513-53-1	C ₄ H ₇ SH	90.187	-165	85.0	1		121.8	
Benzenethiol	108-98-5	C ₆ H ₅ SH	110.177	-14.93	169.1	1	102.34	106.8	6.5
2-Methylbenzenethiol	137-06-4	C ₇ H ₈ S	124.204	15	195	1		129.0	
3-Methylbenzenethiol	108-40-7	C ₇ H ₈ S	124.204	-20	195	1		129.0	
4-Methylbenzenethiol	106-45-6	C ₇ H ₈ S	124.204	43	195	0.666		129.0	
Thiophenes:									
Thioazole	288-47-1	C ₃ H ₃ NS	85.128	-33.62	118	1		85.2	
Thiophene	110-02-1	C ₄ H ₄ S	84.140	-38.21	84.0	1	79.02	88.1	
2-Methylthiophene	554-14-3	C ₅ H ₆ S	98.167	-63.4	112.6	1		110.3	
3-Methylthiophene	616-44-4	C ₅ H ₆ S	98.167	-69	115.5	1		110.3	
Benzo[<i>b</i>]thiophene	95-15-8	C ₈ H ₆ S	134.199	32	221	0.854		139.7	
Dibenzothiophene	132-65-0	C ₁₂ H ₈ S	184.257	98.2	332.5	0.191		191.3	
Thianthrene	92-85-3	(C ₆ H ₄) ₂ S ₂	216.322	159.3	365	0.0481		210.9	
Thiobenzamide	2227-79-4	C ₆ H ₅ CSNH ₂	137.203	117		0.125		135.8	
Thiourea	62-56-6	H ₂ NCSNH ₂	76.121	178		0.0315	72.84	76.2	2.03
Thioacetamide	62-55-5	CH ₃ CSNH ₂	75.133	115.5		0.129		84.2	

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$

TABLE 16.2.2

Summary of selected physical-chemical properties of nitrogen and sulfur containing compounds at 25°C.

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility			log K _{OW}	H/(Pa·m ³ /mol)	
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		calcd P/C	exptl
Nitriles:								
Acetonitrile	11840	11840	miscible			−0.34		2.75
Propionitrile	5950	5950	103000	1870.0	1870.0	0.16	3.182	3.8
Butyronitrile	2546	2546	33000	477.5	477.5			5.263
Benzonitrile	100	100	2000	19.39	19.39	1.55	5.156	
Acrylonitrile (2-Propenitrile)	11000	11000	75500	1423	1423	0.25	7.731	11.14
Adiponitrile	0.3066	0.3066	8000	73.96	73.96	−0.32	0.0041	
Aliphatic amines:								
Methylamine	357300	357300	miscible			−0.57		1.125
Dimethylamine	206200	206200	miscible			−0.38		1.8
Trimethylamine	219300	219300	miscible			0.27		6.67
Ethylamine	141650	141650	miscible			−0.13		1.012
Diethylamine	31490	31490	miscible			0.43		2.60
Triethylamine	7610	7610	55000	540	540	1.64	14.099	
<i>n</i> -Propylamine	40740	40740	miscible			0.48		1.274
Dipropylamine			53000	520	520			
Diisopropylamine			12390	122				
Tripropylamine			220	1.536	1.54	2.79		
<i>n</i> -Butylamine	13650	13650	miscible			0.97		1.526
Isobutylamine	18760	18760	miscible			0.73		
<i>t</i> -Butylamine	48260	48260	miscible			0.4		
Di- <i>n</i> -butylamine	304	304	4700	36.37	36.37	2.83	8.359	
Tributylamine	5330	5330	40	0.216	0.216		2.47 × 10 ⁴	
Ethanolamine	34.66	34.66	miscible			−1.31		
Diethanolamine	0.0373	0.0399	miscible			−1.43		
Triethanolamine	4.79 × 10 ^{−4}	4.79 × 10 ^{−4}	miscible			−1.59		
Cyclohexylamine	1173	1173	miscible			1.49		
Diphenylamine	0.0612	0.115	300	1.773	3.338	3.45	0.035	
α-Naphthylamine	0.254	0.45				2.23		
β-Naphthylamine	0.035	0.248	6.4	0.045	0.317	2.34		
4-Aminobiphenyl						2.83		

Aromatic amines:

Aniline	65.19	65.19	36070	387.4	387.35	0.90	0.168	12.16
2-Chloroaniline	22.66	22.66	3800	29.79	29.79	1.90	0.761	
3-Chloroaniline	9.53	9.530	5440	42.64	42.64	1.88	0.223	
4-Chloroaniline	2.33	6.873	3000	23.52	69.37	1.83	0.099	
3,4-Dichloroaniline	1.3	3.746	92.05	0.568	1.637	2.67	2.289	
2,4,6-Trichloroaniline	0.00626	0.021				3.694		
<i>o</i> -Toluidine	13.3	13.30	15000	139.98	139.98		0.095	
<i>m</i> -Toluidine	36	36.0	15030	140.26	140.26	1.44	0.257	
<i>p</i> -Toluidine	45	61.48	7350	68.59	93.70	1.4	0.656	
N,N'-Dimethylaniline	107	107.0	1105	9.119	9.119	2.31	11.734	
2,4-Xylidine	20.5	20.50	5900	48.69	48.69		0.421	
2,5-Xylidine			5000	41.26	41.26			
2,6-Xylidine	670	670.0	4700	38.79	38.79	1.94	17.275	
2-Ethylaniline			7500	61.89	61.89	1.93		
4-Ethylaniline	13.5	13.50	5100	42.09	42.09	1.96	0.321	
N,N'-Diethylaniline	9.7	9.70	670	4.49	4.49		2.161	
Benzidine	1.0×10^{-6}	1.06×10^{-5}	400	2.17	23.1	1.81	4.61×10^{-7}	
3,3'-Dichlorobenzidine	5.6×10^{-5}	6.41×10^{-4}	3.1	0.0122	0.140	3.51	0.005	
N,N'-Bianiline	0.0035		0.252	0.0014	0.0154	3.82	3.45×10^{-4}	
2-Nitroaniline	0.62	1.851	1200	8.687	25.93	1.78		
4-Nitroaniline	0.035	0.589	800	5.792	97.50	1.31		
2,4-Dinitroaniline						4.1		

Nitroaromatic compounds:

Nitrobenzene	20	20.0	1900	15.43	15.43	1.85	1.296	
1,2-Dinitrobenzene	0.0052	0.0433						
1,3-Dinitrobenzene	0.0081	0.0348	546	3.25	13.94	1.49	0.002	
1,4-Dinitrobenzene	13.3	386.63	442	2.63	76.43	2.37	5.059	
2-Nitrotoluene	17.9	17.90	651.42	4.75	4.75	2.30	3.768	
3-Nitrotoluene	27.2	27.20	499.19	3.64	3.64	2.45	7.473	
4-Nitrotoluene	0.653	1.2004	254.4	1.86	3.41	2.37	0.352	
2,4-Dinitrotoluene (DNT)	0.133	0.3705	270	1.48	4.13	2.01	0.090	
2,6-Dinitrotoluene	0.0767	0.1952	200			1.72	0.070	
2,4,6-Trinitrotoluene (TNT)	0.00107	0.0038	210	0.925	3.29			
1-Nitronaphthalene	0.702 0.0312	0.072	9.82	0.057	0.132	3.19	3.50	
2-Nitronaphthalene			9.24	0.053	0.183			
4-Nitrobiphenyl			1.231	6.18×10^{-3}	0.045	3.78		
5-Nitro-acenaphthene			0.91	4.57×10^{-3}	0.026			

(Continued)

TABLE 16.2.2 (Continued)

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility				H/(Pa·m ³ /mol)	
	P ^s /Pa	P _L /Pa	S/(g/m ³)	C ^s /(mol/m ³)	C _L /(mol/m ³)	log K _{OW}	calcd P/C	exptl
Amides: RCONH2								
Acetamide (ethanamide)	2.44	8.3562	408000	6907.1	23650	−1.26	3.53 × 10 ^{−4}	
Acrylamide	0.415	1.5900	2050000	2884	11050	−0.9	1.44 × 10 ^{−4}	
Benzamide	0.00522	0.0544	14000	1692	17630	0.64	4.52 × 10 ^{−5}	
Urea: (NH2)2C=O								
Urea	0.0016	0.0186	1000000	16650	1.93x10 ⁵	−2.11	9.61 × 10 ^{−8}	
Nitrosoamines:								
N-Nitrosodimethylamine			miscible			−0.57		3.343
Di- <i>n</i> -propyl nitrosamine	27		9900	76.04		1.31	0.355	
Diphenyl nitrosamine	13.33	34.27	35.10	0.116	0.299	3.13	114.6	
Heterocyclic compounds:								
1 <i>H</i> -Pyrrole	1100	1100	45000	670.7	670.7	0.75	1.640	
1-Methylpyrrole	3312							
Indazole			827	7.00	100.43			
Indole	2.24	4.187	1874	16.00	29.90	2	0.140	
Indoline			10800	90.63				
Pyridine	2775	2775	miscible			0.65		0.895
2-Methylpyridine	1496	1496	miscible			1.11		1.01
3-Picoline	1333	1333	miscible			1.2–1.24		0.788
4-Picoline	757	757	miscible			1.22		0.601
2,3-Dimethylpyridine	426		104000	970.6				0.725
2,4-Dimethylpyridine	456	456	miscible					0.678
2,6-Dimethylpyridine	746	746	miscible					1.06
2,4,6-Trimethylpyridine	5170	5170	35700	294.6	294.6		17.549	
Quinolines:								
Quinoline	1.21	1.21	6110	47.31	47.31	2.06	0.026	
Isoquinoline	670	693	4521	35.00	36.20	2.08	19.141	
2,7-Dimethylquinoline			1795	11.42	24.77			
Benzo[<i>f</i>]quinoline		0.0067	76.1	0.42	2.02	3.20	0.0096	
Benzo[<i>h</i>]quinoline	0.03	0.0555						
9 <i>H</i> -Carbazole	0.0933	14.976	1.03	0.006	0.989	3.80	15.146	
7 <i>H</i> -Dibenzo[<i>c,g</i>]carbazole	1.3 × 10 ^{−7}	2.5 × 10 ^{−6}	0.063	0.236	4.532	5.75		

Acridine	0.0065	0.0451	38.5	0.215	1.492	3.4	0.030	
Benz[<i>a</i>]acridine						4.45		
Sulfur compounds:								
Carbon disulfide	48210	48210	2100	27.584	27.584		1747.75	
Dimethyl sulfate	128	128						
Diethyl sulfate	49.1	49.1						
Dimethyl sulfoxide (DMSO)	80.0	80.0	253000	354.8	354.8	−1.35	0.225	
Dimethyl sulfone	5.16	34.17				−1.41	200.83	
Dimethyl sulfide	64650	64650	20000	321.9			7.72	
Dimethyl disulfide	4000	4000	6300	66.88	66.88		59.81	
Diethyl sulfide	7782	7782				1.95		
Diethyl disulfide	689	689						
Thiols:								
Methanethiol	201980	201980						
Ethanethiol	70000		15000				289.94	
Propanethiol	20635	20635				1.81		
1-Butanethiol	6070	6070	597	6.62	6.62	2.28	916.94	
2-Butanethiol	10790	10790						
Benzenethiol	397	397				2.52		
2-Methylbenzenethiol	87.4	87.4						
3-Methylbenzenethiol	76.6	76.60						
4-Methylbenzenethiol	85.2	128.3						
Thiophenes:								
Thioazole	2287							
Thiophene	10620	8000	3015	35.833	35.833	1.81	223.3	224
2-Methylthiophene	3318							
3-Methylthiophene	2953							
Benzo[<i>b</i>]thiophene	26.66	26.7	130	0.969	1.107	3.12	24.1	
Dibenzothiophene	0.267		1.11	0.006		4.38	44.3	
Thiourea			90000	1182	36833	−0.99		
Thioacetamide			163000	2170	15722	−0.26		

TABLE 16.2.3

Suggested half-life classes for nitrogen and sulfur containing compounds in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Acetonitrile	6	5	5	6
Propionitrile	6	5	5	6
Acrylonitrile (2-Propenitrile)	3	4	4	5
Dimethylamine	1	3	4	5
Ethylamine	2	3	4	5
Eiethylamine	1	2	2	3
<i>n</i> -Butylamine	2	3	3	4
Ethanolamine	1	3	3	4
Diethanolamine	1	4	4	5
Cyclohexylamine	1	3	3	4
Aniline	1	4	4	6
2-Chloroaniline	3	4	5	6
4-Chloroaniline	1	4	4	5
<i>o</i> -Toluidine	1	3	3	4
<i>N,N'</i> -Dimethylaniline	1	4	5	6
2,6-Xylidine	1	4	5	6
Diphenylamine	1	4	5	6
Benzidine	1	4	4	5
3,3'-Dichlorobenzidine	1	1	5	6
<i>N,N'</i> -Bianiline	1	3	3	4
α -Naphthylamine	1	4	4	6
β -Naphthylamine	1	4	4	6
Nitrobenzene	1	6	6	7
2-Nitrotoluene	2	3	6	7
4-Nitrotoluene	2	3	6	7
2,4-Dinitrotoluene (DNT)	2	3	6	7
2,4,6-Trinitrotoluene (TNT)	1	2	6	7
Acetamide	2	4	4	5
Benzamide	2	4	4	5
<i>n</i> -Nitrosodimethylamine	1	2	6	7
<i>n</i> -Nitrosodiethylamine	1	2	6	7
Di- <i>n</i> -propyl nitrosoamine	1	2	6	7
Diphenyl nitrosoamine	1	2	6	7
Pyridine	5	5	6	7
3-Methylpyridine	5	5	6	7
4-Methylpyridine	5	5	6	7
Quinoline	3	4	5	6
Dimethyl sulfate	4	2	2	3
Diethyl sulfate	2	2	3	4
Thiophene	3	3	6	7
Benzo[<i>b</i>]thiophene	4	5	6	7
Thiourea	1	4	4	5
Thioacetamide	2	4	4	5

TABLE 16.2.3 (*Continued*)

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

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