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# 4 Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

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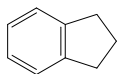
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## 4.1. LIST OF CHEMICALS AND DATA COMPILATIONS

### 4.1.1 POLYNUCLEAR AROMATIC HYDROCARBONS (PAHs)

#### 4.1.1.1 Indan



Common Name: Indan

Synonym: hydroindene, 2,3-dihydroindene, 2,3-dihydro-1H-indene, indane

Chemical Name: indan

CAS Registry No: 496-11-7

Molecular Formula: C<sub>9</sub>H<sub>10</sub>

Molecular Weight: 118.175

Melting Point (°C):

−51.38 (Lide 2003)

Boiling Point (°C):

177.97 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.9639 (Weast 1982–83; Dean 1985; Lide 2003)

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

123.0 (20°C, calculated-density)

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

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

49 ± 1.5 (Ambrose & Sprake 1976)

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

8.60 (exptl., Chickos et al. 1999)

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

38.77, 45.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

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

88.9 (shake flask-GC, Price 1976)

109.1 (shake flask-fluorescence, Mackay & Shiu 1977)

100 (recommended-IUPAC, Shaw 1989)

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):

5523\* (91.68°C, ebulliometry, measured range 91.68–129.05°C, Stull et al. 1961)

204.0\* (comparative ebulliometry, extrapolated from vapor pressure equation derived from exptl data, Ambrose & Sprake 1976)

$\log (P/\text{kPa}) = 6.10462 - 1574.160/[(T/\text{K}) - 67.079]$ ; temp range 355.006–482.437 K (vapor pressure eq., ebulliometry, Ambrose & Sprake 1976)

9585\* (101.124°C, comparative ebulliometry, measured range 101.124–192.408°C, Osborn & Scott 1978)

$\log (P/\text{atm}) = [1 - 451.051/(T/\text{K})] \times 10^4 \{0.859420 - 6.08324 \times 10^{-4} \cdot (T/\text{K}) + 4.77502 \times 10^{-7} \cdot (T/\text{K})^2\}$ ; temp range 355.01–452.24 K (Cox eq., Chao et al. 1983)

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

$\log (P/\text{kPa}) = 6.1012 - 1571.723/(205.798 + t/^\circ\text{C})$ ; temp range 81.86–209.3°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1976, Boublik et al. 1984)

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

$\log (P_L/\text{kPa}) = 6.11622 - 1580.315/(-66.49 + T/\text{K})$ ; temp range 374–466 K (Antoine eq., Stephenson & Malanowski 1987)

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

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

3.33	(Hansch & Leo 1979)
3.30	(calculated-TSA, Yalkowsky & Valvani 1976)
3.57	(calculated-fragment const., Valvani & Yalkowsky 1980)
3.29	(calculated-solubility, Mackay et al. 1980)
3.31	(calculated-fragment const., Yalkowsky et al. 1983)
3.33	(shake flask, Log P Database, Hansch & Leo 1987)
3.36	(calculated-molar volume, Wang et al. 1991)
3.33	(recommended, Sangster 1993)
3.18	(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: photolysis rate  $k < 3 \times 10^{-5} \text{ s}^{-1}$  with  $t_{1/2} > 1 \text{ d}$  (Kwok et al. 1997)

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:

$k_{OH} = 9.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K (Atkinson 1989)

$k_{OH}(\text{exptl}) = (19 \pm 5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{calc}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated lifetime of 8 h;  $k_{NO_3}(\text{exptl}) = (6.6 \pm 2.0) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated lifetime of 7 d; and  $k_{O_3}(\text{exptl}) < 3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated lifetime of  $> 55 \text{ d}$  at  $297 \pm 2 \text{ K}$  (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: photolysis  $t_{1/2} > 1 \text{ d}$ ; calculated tropospheric lifetimes of 8 h, 7 d and  $> 55 \text{ d}$  due to reactions with OH radical,  $NO_3$  radical and  $O_3$ , respectively, at room temp. (Kwok et al. 1997)

**TABLE 4.1.1.1.1**

**Reported vapor pressures of indan 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 et al. 1961		Ambrose & Sprake 1976		Osborn & Scott 1978	
ebulliometry		comparative ebulliometry		comparative ebulliometry	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
91.68	5523	81.856	4343	101.124	9585
107.38	12086	88.012	5650	104.381	10887
128.56	25246	93.482	7069	107.849	12339
152.36	51766	98.033	6471	111.229	13955
176.03	96999	101.96	9860	114.621	15748

(Continued)

TABLE 4.1.1.1.1 (Continued)

Stull et al. 1961		Ambrose & Sprake 1976		Osborn & Scott 1978	
ebulliometry		comparative ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
178.04	101729	109.194	12920	118.027	17735
129.05	104442	116.391	16722	121.442	19933
		120.345	19150	128.315	25023
mp/K	221.77	123.556	21300	135.235	31177
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 8.60$		128.597	25174	142.204	38565
Antoine eq.		134.718	30586	149.224	47375
eq. 2	P/mmHg	139.494	35453	156.300	57817
A	7.05483	146.528	43667	263.418	70120
B	1625.70	152.479	51799	170.590	84432
C	211.645	158.969	61998	177.812	101325
		164.763	72392	177.812	101325
		171.453	86085	177.811	101325
		176.521	97757	185.085	120790
		177.075	99114	192.408	143240
		177.531	100222		
		25.0	204.0	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 39.67$	
				at bp	
		bp/K	451.12 K	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 49.03$	
				at 298.15 K	
		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 39.8$ at bp			
		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 49.0$			
		at 298.15 K			
		eq. 3	P/kPa		
		A	6.10462		
		B	1574.160		
		C	-67.079		

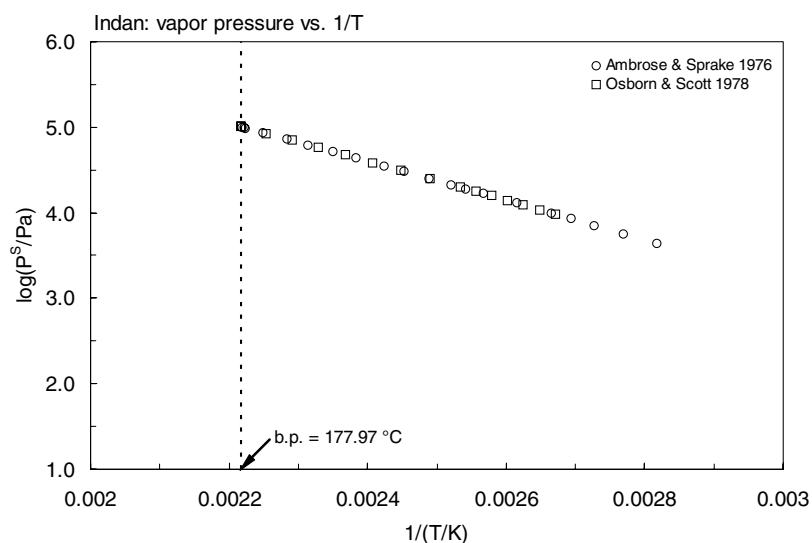
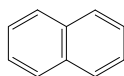


FIGURE 4.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for indan.

## 4.1.1.2 Naphthalene



Common Name: Naphthalene

Synonym: naphthene, tar camphor, moth balls

Chemical Name: naphthalene

CAS Registry No: 91-20-3

Molecular Formula:  $C_{10}H_8$

Molecular Weight: 128.171

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

80.26 (Lide 2003)

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

217.9 (Lide 2003)

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

1.0253 (Weast 1983–84)

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

125.0 ( $20^{\circ}C$ , calculated-from density)

133.2 (from density, Bohon & Claussen 1951)

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

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

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

73.93 (Colomina et al. 1982)

72.92 (Van Ekeren et al. 1983)

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

19.29 (Parks & Huffman 1931)

19.08 (Wauchope & Getzen 1972; Podoll et al. 1989)

19.10 (exptl., Chickos et al. 1999)

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

54.39 (Casellato et al. 1973)

54.81 (Ubbelohde 1978)

53.75, 44.4 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.287 (mp at  $80.26^{\circ}C$ )

0.310 (calculated, Passivirta et al. 1999)

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):

30.0\* (shake flask-gravimetric, measured range  $0$ – $25^{\circ}C$ , Hilpert 1916)

31.5 (shake flask-UV, Andrews & Keefer 1949)

12.5 (shake flask-UV, Klevens 1950)

34.4\* (shake flask-UV, measured range  $2$ – $42^{\circ}C$ , Bohon & Claussen 1951)

30.6 (Stephen & Stephen 1963)

20.4 (shake flask, Sahyun 1966)

33.47 (shake flask-GC, Gordon & Thorne 1967)

38.4 ( $20^{\circ}C$ , shake flask-UV, Eisenbrand & Baumann 1970)

31.2\* (shake flask-UV, measured range  $29$ – $73.4^{\circ}C$ , Wauchope & Getzen 1972)

$R \cdot \ln x = -8690/(T/K) + (0.000408)[(T/K) - 291.15]^2 - 13.4 + 0.0139 \cdot (T/K)$ ; temp range  $29.2$ – $73.4^{\circ}C$  (shake flask-UV, Wauchope & Getzen 1972)

32.17 (shake flask-UV, Vesala 1974)

31.3 (shake flask-GC, Eganhouse & Calder, 1976)

22.0 (fluorescence, Schwarz & Wasik 1976)

31.7 (shake flask-fluorescence, Mackay & Shiu, 1977)

30.0\* ( $25^{\circ}C$ , shake flask-fluorescence, measured range  $8$ – $31^{\circ}C$ , Schwarz & Wasik 1977)

30.25\* ( $25^{\circ}C$ , shake flask-fluorescence, measured range  $8.4$ – $31.8^{\circ}C$ , Schwarz 1977)

- 31.69 (generator column-HPLC/UV, measured temp range 5–30°C, May et al. 1978)  
 $S/(\text{mg/kg}) = 13.66 + 0.2499 \cdot (t/^\circ\text{C}) + 0.0189 \cdot (t/^\circ\text{C})^2$ ; temp range 5–30°C (generator column-HPLC/UV, May et al. 1978)
- 30.64 (generator column-HPLC/UV, Wasik et al. 1983)
- 31.94\* (25°C, generator column-HPLC/UV, measured range 8.2–27°C, May et al. 1983)  
 $R \cdot \ln x = -80.55/(\theta/K) + 28.7/[1/(\theta/K) - 1/(T/K)] + 0.31 \cdot \{(\theta/K)/(T/K) - 1 - \ln [(\theta/K)/(T/K)]\}$ ,  $\theta = 298.15 \text{ K}$ , temp range 8.2–27°C (generator column-HPLC/UV, May et al. 1983)
- 32.2 (average lit. value, Pearlman et al. 1984)
- 32.90 (generator column-HPLC/fluorescence, Walters & Luthy 1984)
- 30.75\* (25.2°C, shake flask-UV, Bennet & Canady 1984)  
 $\ln x = -1767.4601/R \cdot (T/K) + (17.95209/R) \cdot \ln (T/K) + 1$ ; temp range 2–45°C (shake flask-UV, Bennet & Canady 1984)
- 30.6 (shake flask-HPLC/UV, Fu & Luthy 1985)
- 31.12 (vapor saturation-GC, Akiyoshi et al. 1987)
- 31.3, 31.9 (generator column-HPLC/UV, Billington et al. 1988)
- 31\* (recommended, IUPAC Solubility Data Series, Shaw 1989)
- 33.71\* (shake flask-UV, measured range 5–40°C, Perez-Tejeda et al. 1990)  
 $\log [S/(\text{mol/dm}^3)] = -31.24 - 143.5/(T/K) + 4.772 \cdot \ln (T/K)$ ; temp range 5–40°C (shake flask-UV, Perez-Tejeda et al. 1990)
- 30.6 (generator column-HPLC, Vadas et al. 1991)
- 29.9 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
- 34.8 (generator column-HPLC/fluorescence, De Maagd et al. 1998)  
 $\log [S_L/(\text{mol/L})] = 2.992 - 1001/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $\ln x = -1.54117 - 3191.9/(T/K)$ ; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

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

- $\log (P/\text{mmHg}) = 7.091 - 3465/(T/K)$ ; temp range 87–224 (static isotenoscope method, Mortimer & Murphy 1923)
- 8.64\* (20°C, effusion, measured range 10–30°C Swan & Mack 1925)  
 $\log (P/\text{mmHg}) = 29.820/(T/K) - 200.682 \cdot \log (T/K) + 595.642$ ; measured temp range 10–30°C (effusion, Swan & Mack 1925)
- $\log (P/\text{mmHg}) = 10.40 - 3429/(T/K)$ ; temp range 15–33°C (effusion, Zil'berman-Granovskaya 1940)
- 133.3\* (52.6°C, summary of literature data, temp range 52.6–217.9°C, Stull 1947)
- 14.26\* (manometry-Rodebush gauge, Sears & Hopke 1949)  
 $\log (P/\text{mmHg}) = -[108.30/(t/^\circ\text{C} + 27)] + 1.115$ ; temp range 19–35°C (manometry-Rodebush gauge, Sears & Hopke 1949)
- 10.8\* (effusion method, measured range 6.7–20.7°C, Bradley & Cleasby 1953)  
 $\log (P/\text{cmHg}) = 10.597 - 3783/(T/K)$ ; temp range 6.7–20.7°C, (Antoine eq., effusion, Bradley & Cleasby 1953)
- 6815\* (126.325°C, manometry, measured range 126.325–218.638°C, Camin & Rossini 1955)  
 $\log (P/\text{mmHg}) = 6.84577 - 1606.529/(187.227 + t/^\circ\text{C})$ ; temp range 126.3–218.6°C (Antoine eq. Camin & Rossini 1955)
- $\log (P/\text{mmHg}) = 10.75 - 3616/(T/K)$ ; temp range –20 to 10°C (Knudsen effusion method, Hoyer & Peperle 1958)
- 0.1188\* (–13°C, Knudsen effusion, measured range –43 to –13°C, Miller 1963)
- 46.66\* (40.33°C, Hg manometer, measured range 40.33–80.34°C, Fowler et al. 1968)
- 10.98, 32.95 (manometry, extrapolated solid, supercooled liquid  $P_L$ , Fowler et al. 1968)  
 $\log (P_S/\text{mmHg}) = 9.58102 - 2692.92/(t/^\circ\text{C} + 220.651)$ ; temp range 40–80°C (Antoine eq., mercury manometer, Fowler et al. 1968)
- $\log (P_L/\text{mmHg}) = 7.03382 - 1756.91/(t/^\circ\text{C} + 204.931)$ ; temp range 81–180°C (Antoine eq., mercury manometer, Fowler et al. 1968)
- 30.66\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)  
 $\log (P/\text{mmHg}) = 7.01065 - 1733.71/(201.859 + t/^\circ\text{C})$ ; temp range 86.581–250.27°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 11.60 (interpolated-Antoine eq., Weast 1972–73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 17065.2/(T/K)] + 11.450$ ; temp range 0–80.0°C (Antoine eq., Weast 1972–73)
- $\log (P/\text{mmHg}) = [-0.2185 \times 12311.6/(T/K)] + 8.413089$ ; temp range 52.6–217.9°C (Antoine eq., Weast 1972–73)
- 12.26\* (Knudsen effusion method, extrapolated from measured data, Radchenko & Kitiagorodskii 1974)



- $\log(P/\text{mmHg}) = 11.7041 - 3796.574/(T/K)$ ; temp range 9.0–23.91°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)
- 10.93\* (gas saturation, Sinke 1974)
- 11.21\* (Baratron model diaphragm pressure gauge, Ambrose et al. 1975)
- $T \cdot \log(P/\text{Pa}) = \frac{1}{2} a_0 + \sum a_i E_i(x)$ ;  $a_0 = 310.6247$ ,  $a_1 = 791.4937$ ,  $a_2 = -82536$ ,  $a_3 = 0.4043$ ; temp range: 230–344 K, (Chebyshev polynomial, diaphragm pressure gauge, Ambrose et al. 1975)
- $\log(P/\text{Pa}) = 13.70 - 3773/(T/K)$  (Antoine eq. derived from exptl data of Ambrose et al. 1975, Wania et al. 1994)
- 13.5 (effusion method-pressure gauge, DePablo 1976)
- 10.64\* (gas saturation, interpolated-Clapeyron eq., Macknick & Prausnitz 1979)
- $\log(P/\text{mmHg}) = 26.250 - 8575/(T/K)$ ; temp range 7.15–31.85°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
- 11.30\* (effusion method, de Kruif 1980)
- $\log(P/\text{Pa}) = 14.187 - 3907/(T/K)$ ; temp range 253–273 K (torsion effusion, regression, de Kruif 1980)
- $\log(P/\text{Pa}) = 14.053 - 3860/(T/K)$ ; temp range 253–273 K (weighing effusion, regression, de Kruif 1980)
- $\log(P/\text{Pa}) = 14.107 - 3886/(T/K)$ ; temp range 253–273 K (effusion, mean regression, de Kruif 1980)
- 10.42\* (effusion method, de Kruif et al. 1981)
- 11.41\* (Knudsen effusion, extrapolated-Antoine eq. from exptl data, Colomina et al. 1982)
- $\log(P/\text{Pa}) = 14.01 - 3861.8/(T/K)$ ; temp range 271.46–284.63 K (Antoine eq., Knudsen effusion, Colomina et al. 1982)
- 11.33\* (gas saturation-GC, Grayson & Fosbraey 1982)
- $\ln(P/\text{Pa}) = 31.8 - 8753/(T/K)$ ; temp range 302–352 K, (Antoine eq., gas saturation, Grayson & Fosbraey 1982)
- $\log(P/\text{atm}) = [1 - 490.988/(T/K)] \times 10^{0.832267 - 4.41855 \times 10^{-4} (T/K) + 2.89627 \times 10^{-7} (T/K)^2}$ ; (Cox eq., temp range 340.15–751.65 K, Chao et al. 1983)
- 6.53 (20°C, Mackay et al. 1983)
- 10.4\* (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
- $\log(P/\text{Pa}) = 14.299 - 3960.03/(T/K)$ ; temp range 10–50°C (Antoine eq., gas saturation, Sonnefeld et al. 1983)
- 1.63\* (244.19°C, spinning-rotor gauge, measured range 244.19–255.86 K, Van Ekeren et al. 1983)
- 10.4 (generator column-HPLC, Wasik et al. 1983)
- $\log(P_L/\text{kPa}) = 5.93404 - 1579.278/(184.062 + t/^\circ\text{C})$ ; temp range 126.3–218.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log(P_L/\text{kPa}) = 6.1638 - 1760.018/(215.204 + t/^\circ\text{C})$ , temp range 80.3–179.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 22.64, 28.24 ( $P_{GC}$  by GC-RT correlation with BP-1 column, Apolane-87 column, Bidleman 1984)
- $\log(P_L/\text{mmHg}) = 7.01065 - 1733.71/(201.86 + t/^\circ\text{C})$ ; temp range 86–250°C (Antoine eq., Dean 1985, 1992)
- $\log(P_L/\text{mmHg}) = 6.8181 - 1585.86/(184.82 + t/^\circ\text{C})$ ; temp range 125–218°C (Antoine eq., Dean 1985, 1992)
- 10.7\* (25.35°C, gas saturation, temp range 24.85–57.75°C, Sato et al. 1986)
- $\ln(P_S/\text{Pa}) = 22.8929 - 4025.35/(T/K - 102.243)$ ; temp range 298.5–330.9 K (Antoine eq., gas saturation, Sato et al. 1986)
- 11.27 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_S/\text{kPa}) = 8.70592 - 2619.91/(-52.499 + T/K)$ ; temp range 310–353 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_S/\text{kPa}) = 9.45562 - 3069.145/(-29.892 + T/K)$ ; temp range 263–353 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log(P_S/\text{kPa}) = 11.9681 - 4577.47/(30.394 + T/K)$ ; temp range not specified (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.19487 - 1782.509/(-65.637 + T/K)$ ; temp range 352–500 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.14835 - 1751.644/(-68.319 + T/K)$ ; temp range 491–565 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.53231 - 2162.182/(-12.108 + T/K)$ ; temp range 563–665 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 7.74783 - 4042.567/(227.985 + T/K)$ ; temp range 661–750 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
- 11.37\* (pressure gauge, interpolated-Antoine eq., measured range –12.15 to 70.16°C, Sasse et al. 1988)
- $\log(P_S/\text{mmHg}) = 10.05263 - 2907.918/(236.459 + t/^\circ\text{C})$ ; temp range –12.15 to 70.16°C (Antoine eq., pressure gauge, Sasse et al. 1988)

$\log (P_L/\text{mmHg}) = 2.25180 - 76.496/(-25.09 + t/^\circ\text{C})$ ; temp range 80.16–90.15°C (Antoine eq., pressure gauge, Sasse et al. 1988)

22.65 (PGC, GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)

41.88, 38.02 (supercooled liquid  $P_L$  values converted from literature  $P_S$  with different  $\Delta S_{\text{fus}}$  values, Hinckley et al. 1990)

0.7634\* (0°C, gas saturation-GC, measured range –30.6 to 0°C, Wania et al. 1994)

$\log (P/\text{Pa}) = 13.93 - 3851/(T/\text{K})$ ; temp range –30 to 0°C, (Antoine eq., gas saturation, Wania et al. 1994)

24.0 (supercooled liquid  $P_L$ , GC-RT correlation, Donovan 1996)

5.58–12.30; 10.4–14.0; 11.2–14.4; 7.71–17.2; 6.45–8.40 (quoted lit. ranges: effusion method; gas saturation; manometry; calculated; from GC-RT correlation, Delle Site 1997)

11.16 (solid  $P_S$ , van der Linde et al. 1998)

40.0; 12.4 (quoted  $P_L$  from Hinckley et al. 1990; converted to  $P_S$  with fugacity ratio  $F$ , Passivirta et al. 1999)

$\log (P_S/\text{Pa}) = 10.90 - 2927/(T/\text{K})$  (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.06 - 1923/(T/\text{K})$  (supercooled liquid, Passivirta et al. 1999)

$\log (P/\text{Pa}) = 13.59 - 3742/(T/\text{K})$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

37.0 (supercooled liquid  $P_L$ , GC-RT correlation, Lei et al. 2002)

$\log (P_L/\text{Pa}) = -2930/(T/\text{K}) + 11.39$ ;  $\Delta H_{\text{vap.}} = -56.1 \text{ kJ}\cdot\text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

56.0 (gas stripping, Southworth, 1979)

48.9 (gas stripping, Mackay et al. 1979; Mackay & Shiu 1981)

44.6 (gas stripping, Mackay et al. 1982)

36.5 (20°C, EPICS method, Yurteri et al. 1987)

74.3 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

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

47.1 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)

42.6\* (gas stripping-GC, measured range 3.7–35.5°C, Alaee et al. 1996)

$\ln K_{\text{AW}} = 13.95 - 5364.45/(T/\text{K})$ , temp range: 3.7–35.5°C (gas stripping-GC, Alaee et al. 1996)

26.2, 35.5, 48.1, 62.5, 77.7, 108.1 (9.2, 14.5, 20.1, 24.6, 30.5, 34.8°C, seawater with salinity of 35‰ (0.660M NaCl), gas stripping-GC, Alaee et al. 1996)

44.6 (gas stripping-GC; calculated-P/C, Shiu & Mackay 1997)

45.0 (gas stripping-HPLC/fluor., De Maagd et al. 1998)

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

$\log K_{\text{AW}} = 6.058 - 2332/(T/\text{K})$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient,  $\log K_{\text{OW}}$  at 25°C or as indicated:

3.37 (shake flask, Fujita et al. 1964; Hansch et al. 1973)

3.37, 3.01, 3.45 (Leo et al. 1971)

3.37 (calculated-fragment const., Rekker 1977)

3.395 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

3.30, 3.01, 3.37, 3.45, 3.59 (quoted, Hansch & Leo 1979)

3.17 (HPLC-RT correlation, Veith et al. 1979a,b)

3.36 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)

3.21 (HPLC- $k'$  correlation, Hanai et al. 1981)

3.18 (HPLC- $k'$  correlation, D'Amboise & Hanai 1981)

3.35 (generator column-HPLC/UV, Wasik et al. 1981 1983)

3.35 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)

3.45 (HPLC-RT correlation, Hammers et al. 1982)

3.31; 3.35 (shake flask; HPLC correlation, Eadsforth & Moser 1983)

3.36 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)

3.35; 3.42 (shake flask; ALPM, Garst & Wilson 1984)

3.57 (HPLC-RV correlation, Garst & Wilson 1984)

3.38 (RP-HPLC correlation, Chin et al. 1986)

3.43 (HPLC-RT correlation, Eadsforth 1986)

3.29	(HPLC-RT correlation, Wang et al. 1986)
3.29	(HPLC-RT correlation, de Kock & Lord 1987)
3.30	(average, HPLC-RT correlation, Ge et al. 1987)
3.35	(shake flask-GC, Opperhuizen et al. 1987)
3.23	(HPLC-RT correlation, Minick et al. 1988)
3.29	(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
3.35	(recommended, Sangster 1989, 1993)
3.49	(centrifugal partition chromatography, Menges et al. 1990)
3.36	(shake flask-HPLC/UV, Menges & Armstrong 1991)
3.30	(TLC-RT correlation, De Voogt et al. 1990)
3.70	(centrifugal partition chromatography, Berthod et al. 1992)
3.37	(shake flask-UV, pH 7.4, Alcorn et al. 1993)
3.30	(recommended, Hansch et al. 1995)
3.44; 3.68	(26°C; 4°C, quoted, Piatt et al. 1996)
3.47, 3.58; 3.40	(HPLC- $k'$ correlation: ODS column; Diol column; quoted lit. average, Helweg et al. 1997)
3.33	(range 3.24–3.40) (slow stirring method-HPLC/fluor., De Maagd et al. 1998)
3.40	(shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
3.77	(RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

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

5.10	(calculated- $K_{OW}/K_{AW}$ , Wania & Mackay 1996)
5.19	(calculated- $S_{oct}$ and vapor pressure $P$ , Abraham et al. 2001)

## Bioconcentration Factor, log BCF at 25°C:

1.64	(mussel <i>Mytilus edulis</i> , Lee et al. 1972)
4.11	(bile of rainbow trout, Melancon & Lech 1978)
2.12	( <i>Daphnia pulex</i> , Southworth et al. 1978)
2.07	( <i>Daphnia pulex</i> , by kinetic estimation, Southworth et al. 1978)
2.63	(fathead minnow, Veith et al. 1979b, 1980)
2.62	(microorganisms-water, calculated from $K_{OW}$ , Mabey et al. 1982)
4.10, 3.84, 4.25	(average, <i>Selenastrum capricornutum</i> -dosed singly, dosed simultaneously, Casserly et al. 1983)
2.11; 2.43	( <i>Chlorella fusca</i> ; calculated- $K_{OW}$ , Geyer et al. 1984)
1.48, 2.10, 3.0	(fish, algae, activated sludge, Freitag et al. 1985)
2.50	(bluegill sunfish, McCarthy & Jimenez 1985)
2.48	(bluegill sunfish with dissolved humic material, McCarthy & Jimenez 1985)

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

3.11	(natural sediment, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
2.38	(22°C, suspended particulates, Herbes et al. 1980)
2.94	(sediment/soil, sorption isotherm by batch equilibrium, Karickhoff 1981)
3.62, 3.87, 4.23	(soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
3.50; 4.43; 3.21	(Speyer soils: pH 7.0, 0.69% OC; pH 5.8, 2.24% OC; pH 7.1, 1.12% OC at 0.15–0.5 mm, batch equilibrium-sorption isotherm, Rippen et al. 1982)
3.11; 3.16	(soils: Alfisol 0.76% OC at pH 7.5, Entisol 1.11% OC at pH 7.9, batch equilibrium-sorption isotherm, Rippen et al. 1982)
3.30	(Offshore Grand Haven sediment, batch equilibrium-sorption isotherm, Voice & Weber 1985)
2.67, 2.77	(Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
2.95	(sediment, calculated, Pavlou 1987)
2.93	(sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
3.27	(calculated-MCI $\chi$ , Bahnick & Doucette 1988)
3.02; 2.89	(Aldrich and Fluka humic acid, observed; predicted, Chin et al. 1989)

- 2.73–3.91 (aquifer materials, Stauffer et al. 1989)  
 5.00 (sediments average, Kayal & Connell 1990)  
 3.15, 2.76 (Menlo Park soil, Eustis sand, batch equilibrium-sorption isotherm, Podoll et al. 1989)  
 3.21, 3.16, 3.10, 3.00 (15, 25, 35, 50°C, Menlo Park soil 1.6% OC, flow sorption equilibrium, Podoll et al. 1989)  
 2.97, 2.67 (modified, unmodified EPA-6 sediments, batch equilibrium-sorption isotherm, Podoll et al. 1989)  
 3.11 (soil, RP-HPLC- $k'$  correlation, Szabo et al. 1990a)  
 3.29 (sandy surface soil, Wood et al. 1990)  
 2.97 (dissolved organic matter, Kan & Tomson 1990)  
 2.98; 2.965, 2.98 (sediment: concn ratio  $C_{\text{sed}}/C_{\text{w}}$ ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)  
 3.11 (calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
 3.16, 3.05, 3.06 (RP-HPLC- $k'$  correlation on different stationary phases, Szabo et al. 1995)  
 2.75 (HPLC-screening method; Müller & Kördel 1996)  
 4.06 (range 3.95–4.15); 2.08 (range 2.08–2.11) (4°C, low organic carbon sediment  $f_{\text{OC}} = 0.0002$ , batch equilibrium; column exptl., Piatt et al. 1996)  
 3.90 (range 3.81–4.00); 2.11 (range 2.11–2.13) (26°C, low organic carbon sediment  $f_{\text{OC}} = 0.0002$ , batch equilibrium; column exptl., Piatt et al. 1996)  
 3.74 (humic acid, HPLC- $k'$  correlation; Nielsen et al. 1997)  
 2.42–2.56 (5 soils, 20°C, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)  
 2.61, 2.63, 2.68, 2.77, 2.76, mean  $2.69 \pm 0.073$  (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)  
 2.91, 2.86, 2.88, 2.87, 2.89, 2.95, 3.07; mean  $2.88 \pm 0.22$  (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)  
 3.11 (3.00–3.19), 2.80 (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)  
 3.60; 3.10 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)  
 3.09–5.51; 2.60–5.0 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)  
 3.91; 4.12, 4.06, 4.94 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)  
 2.91, 3.02, 2.71 (soils: organic carbon  $\text{OC} \geq 0.1\%$ ,  $\text{OC} \geq 0.5\%$ ,  $0.1 \leq \text{OC} < 0.5\%$ , average, Delle Site 2001)  
 3.06 (average values for sediments  $\text{OC} \geq 0.5\%$ , Delle Site 2001)  
 4.43 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

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

Volatilization/Evaporation: rate of evaporation estimated to be  $1.675 \times 10^{-9} \text{ mol cm}^{-2} \text{ h}^{-1}$  at 20°C and air flow rate of  $50 \text{ L h}^{-1}$  (Gückel et al. 1973);  
 calculated  $t_{1/2} = 7.15 \text{ h}$  from 1 m depth of water (Mackay & Leinonen 1975; quoted, Haque et al. 1980);  
 $t_{1/2} = 16 \text{ h}$  for surface waters for a river 1-m deep, water velocity 0.5 m/s, wind velocity 1m/s (Southworth 1979; Herbes et al. 1980);  
 evaporation  $t_{1/2} = 50 \text{ h}$  in a river and  $t_{1/2} = 200 \text{ h}$  in a lake when considering current velocity and wind speed in combined with typical reaeration rates for natural bodies of water (Howard 1989);  
 $t_{1/2}(\text{exptl}) = 28 \text{ min}$  and  $t_{1/2}(\text{calc}) = 32 \text{ min}$  from solution (Mackay et al. 1983).

#### Photolysis:

$t_{1/2} = 71 \text{ h}$  calculated for direct photochemical transformation near-surface water and  $t_{1/2} = 550 \text{ d}$  in 5-m deep inland water body at 40°N at midday of midsummer (Zepp & Schlotzhauer 1979)  
 $k = 0.0392 \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988)  
 $k = 0.028 \text{ h}^{-1}$  in distilled water with  $t_{1/2} = 25 \text{ h}$  (Fukuda et al. 1988)  
 $k = 6.0 \times 10^{-4} \text{ min}^{-1}$  and  $t_{1/2} = 19.18 \text{ h}$ , photodegradation in methanol-water (3:7, v/v) solution with initial concentration of 50.0 ppm by high-pressure mercury lamp or sunlight (Wang et al. 1991);

$k(\text{exptl}) = 0.000511 \text{ min}^{-1}$  with  $t_{1/2}(\text{calc}) = 22.61 \text{ h}$  and the predicted  $k = 0.000303 \text{ min}^{-1}$  by QSPR, the pseudo-first-order direct photolysis rate constant of in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996)

$t_{1/2}(\text{calc}) = 15.42 \text{ h}$  direct photolysis half-life in atmospheric aerosol (QSPR, Chen et al. 2001).

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

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

$k_{\text{OH}} = (2.42 \pm 0.19) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with an estimated atmospheric lifetime  $\tau \sim 1\text{d}$ , and  $k_{\text{O}_3} < 2 \times 10^{-9} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$   $294 \pm 1 \text{ K}$  (relative rate method, Atkinson et al 1984)

$k_{\text{OH}} = (2.35 \pm 0.06) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 1 \text{ K}$  (relative rate method, Biermann et al. 1985)

$k_{\text{N}_2\text{O}_5} \sim (2 - 3) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with  $\text{N}_2\text{O}_5$  at  $298 \text{ K}$ , the calculated lifetime  $\tau \sim 10 \text{ d}$  due to night-time reaction with  $\text{N}_2\text{O}_5$  in atmosphere (relative rate method, Pitts et al. 1985)

$k_{\text{OH}}^* = 2.17 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \text{ K}$  (recommended, Atkinson 1985)

$k_{\text{OH}} = (2.59 \pm 0.24) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a lifetime of  $\sim 11 \text{ h}$ ,  $k_{\text{O}_3} < 3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $295 \pm 1 \text{ K}$  (relative rate method, Atkinson & Aschmann 1986)

$k_{\text{N}_2\text{O}_5} = (1.4 \pm 0.2) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $\text{N}_2\text{O}_5$  at  $298 \text{ K}$  (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}} = 2.17 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{O}_3} < 2 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{\text{N}_2\text{O}_5} = 1.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $\text{N}_2\text{O}_5$  at room temp. (Atkinson & Aschmann 1987, 1988)

$k_{\text{OH}} = (22.8 - 25.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $294\text{--}298 \text{ K}$  (review, Atkinson 1989)

$k_{\text{OH}}^* = 2.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \text{ K}$  (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 26.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}}^* = 23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \text{ K}$ , measured range  $306\text{--}366 \text{ K}$  with a calculated atmospheric lifetime of  $12 \text{ h}$  based on gas-phase OH reaction (Brubaker & Hites 1998)

$k_{\text{OH}} = (2.39 \pm 0.09) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2 \text{ K}$ , with a calculated tropospheric lifetime of  $5.8 \text{ h}$  using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis: not hydrolyzable (Mabey et al. 1982).

Biodegradation:

$k = 4 \times 10^{-6} \text{ g L}^{-1} \text{ d}^{-1}$  ultimate loss process (Lee & Ryan, 1976)

$k = (0.04 - 3.3) \times 10^{-6} \text{ g L}^{-1} \text{ d}^{-1}$  (Lee & Anderson 1977)

complete degradation in  $8 \text{ d}$  in gas-oil contaminated groundwater which was circulated through sand that had been inoculated with groundwater under aerobic conditions (Kappeler & Wuhrmann 1978; quoted, Howard 1989)

$k = 0.04 - 3 \text{ } \mu\text{g/L d}$  for microorganisms (Callahan et al. 1979)

$t_{1/2} = 1.9 \text{ d}$ , in deeper and slowly moving contaminated water (Herbes 1981; Wakeham et al. 1983; quoted, Howard 1989);

half-lives: of  $7, 24, 63$  and  $1700 \text{ d}$  in an oil polluted estuarine stream, clean estuarine stream, coastal waters, and in the Gulf stream, respectively (Lee 1977; quoted, Howard 1989)

$t_{1/2}(\text{aerobic}) = 12 \text{ h}$ , based on die-away test data for an oil polluted creek (Walker & Colwell 1976)

$t_{1/2} = 480 \text{ h}$ , for an estuarine river (Lee & Ryan 1976).

$t_{1/2}(\text{anaerobic}) = 25 \text{ d}$  at  $\text{pH } 8$  and  $t_{1/2} = 258 \text{ d}$  at  $\text{pH } 5$  (Hambrick et al. 1980);

$t_{1/2} = 1.9 \text{ d}$ , in deeper and slower moving contaminated water (Herbes 1981; Wakeham et al. 1983)

$k = 0.23 \text{ h}^{-1}$  (microbial degradation rate constant, Herbes et al. 1980, Hallett & Brecher 1984)

100% degradation within  $7 \text{ d}$  for an average of three static-flask screening test (Tabak et al. 1981)

$k = 3.2 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 9 \text{ h}$ ;  $k = 7.6 \times 10^{-2} \text{ h}^{-1}$  with  $t_{1/2} = 9 \text{ h}$  for mixed bacterial populations in water and sediment from the same stream (NRCC 1983)

$k = 0.14 \text{ h}^{-1}$  with  $t_{1/2} = 5 \text{ h}$ ;  $k < 4 \times 10^{-4} \text{ h}^{-1}$  with  $t_{1/2} > 72 \text{ d}$  for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)

degraded completely within  $1 \text{ wk}$  by microbes in non-autoclaved samples of  $0.04 \text{ mg/L}$  in groundwater from hazardous waste site (Lee et al. 1984)

$k = 0.024 \text{ d}^{-1}$  with  $t_{1/2} = 28 \text{ d}$  in groundwater with nutrients and acclimated microbes,  $k = 0.013 \text{ d}^{-1}$  with  $t_{1/2} = 53 \text{ d}$  in river water with acclimated microbes, and  $k = 0.018 \text{ d}^{-1}$  with  $t_{1/2} = 39 \text{ d}$  in river water with nutrients and acclimated microbes (Vaishnav & Babeu 1987)

$k = 0.337 \text{ d}^{-1}$  with  $t_{1/2} = 2.1 \text{ d}$  for Kidman sandy loam and  $k = 0.308 \text{ d}^{-1}$  with  $t_{1/2} = 2.2 \text{ d}$  for McLarin sandy loam all at  $-0.33 \text{ bar}$  soil moisture (Park et al. 1990)

$t_{1/2}(\text{aerobic}) = 12\text{--}480 \text{ h}$ , based on die-away test data and for estuarine river (Howard et al. 1991)

$t_{1/2}(\text{anaerobic}) = 500\text{--}6192 \text{ h}$ , based on anaerobic estuarine sediment die-away test data (Howard et al. 1991)  
removal rate of 2.4 and 0.43 mg (g of volatile suspended solid d) $^{-1}$ , degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation: estimated rate constant for bacteria,  $1 \times 10^{-7} \text{ ml cell}^{-1} \text{ h}^{-1}$  (Mabey et al. 1982).

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

$k_1 = 197 \text{ h}^{-1}$ ;  $k_2 = 1.667 \text{ h}^{-1}$  (*Daphnia pulex*, Southworth et al. 1978; quoted, Hawker & Connell 1986)

$\log k_2 = -0.70, -1.70 \text{ d}^{-1}$  (fish, calculated- $K_{ow}$ , Thomann 1989)

#### Half-Lives in the Environment:

Air: volatility of  $2.28 \times 10^4 \text{ s}$  (experimental),  $7.7 \times 10^3 \text{ s}$  (calculated) for depth of water body of 22.5 m ( $23^\circ\text{C}$ , Klöpffer et al. 1982);

estimated lifetime of  $\sim 1\text{d}$  due to reaction with photochemically produced hydroxyl radical, assuming an average daytime atmospheric OH radical concn of  $\sim 1 \times 10^6 \text{ molecule/cm}^3$  (Atkinson et al. 1984, 1987; quoted, Howard 1989);

calculated lifetime of  $\sim 11 \text{ h}$  due to reaction with OH radical (Atkinson & Aschmann 1986);

the atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radical and with  $\text{N}_2\text{O}_5$  can be calculated to range from  $\sim 4$  to  $13 \text{ h}$  and  $20\text{--}80 \text{ d}$ , respectively (Atkinson & Aschmann 1987);

$t_{1/2} = 2.96\text{--}29.6 \text{ h}$  based on photooxidation half-life in air (Howard et al. 1991);

calculated atmospheric lifetime of  $12 \text{ h}$  based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface Water:  $t_{1/2} = 16 \text{ h}$  (calculated for river water 1 m deep, water velocity 0.5 m/s, wind velocity 1 m/s from air-water partition coefficients (Southworth 1979; Hallett & Brecher 1984)

$t_{1/2} = 71 \text{ h}$  of photolysis in near surface water, but  $t_{1/2} = 550 \text{ d}$  for a depth of 5 m (calculated from surface water in midsummer at  $40^\circ\text{N}$  latitude, Zepp & Schlotzhauer 1979);

calculated  $t_{1/2} = 7.15 \text{ h}$ , based on evaporative loss for a water depth of 1 m at  $25^\circ\text{C}$  (Mackay & Leinonen 1975);

an overall  $t_{1/2} = 2.3 \text{ d}$  in Rhine river based on monitoring data (Zoeteman et al. 1980)

in coastal seawater mesocosm experiments:  $k = 0.058 \text{ d}^{-1}$  with  $t_{1/2} = 12 \text{ d}$  in winter at  $3\text{--}7^\circ\text{C}$  during the periods when volatilization dominates,  $k = 0.061 \text{ d}^{-1}$  with  $t_{1/2} = 11.3 \text{ h}$  with  $\text{HgCl}_2$  as poison and  $k = 0.896 \text{ d}^{-1}$  corresponding to  $t_{1/2} = 0.8 \text{ h}$  without poison (Wakeham et al. 1983);

$t_{1/2} = 12\text{--}480 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); photolysis  $t_{1/2} = 22.81 \text{ h}$  in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: estimated  $t_{1/2} = 0.6 \text{ yr}$  in the Netherlands (Zoeteman et al. 1981);

$t_{1/2} = 24\text{--}6193 \text{ h}$  based on estimated unacclimated aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:  $t_{1/2} = 4.9 \text{ h}$  in oil contaminated sediment and  $t_{1/2} > 88 \text{ d}$  in uncontaminated sediments (Herbes & Schwall 1978; quoted, Howard 1989);

desorption  $k = 0.031 \text{ d}^{-1}$  with  $t_{1/2} = 21.3 \text{ d}$  from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: an overall  $t_{1/2} = 3.6 \text{ months}$  in a solid waste site (Zoeteman et al. 1981);

$t_{1/2} = 0.12\text{--}125 \text{ d}$  (Sims & Overcash 1983);

$t_{1/2} = 12 \text{ d}$  for both 5 mg/kg and 50 mg/kg added (Bulman et al. 1987);

$t_{1/2} > 50 \text{ d}$  (Ryan et al. 1988);

$t_{1/2} > 80 \text{ d}$  (Howard 1989);

biodegradation  $k = 0.337 \text{ d}^{-1}$  with  $t_{1/2} = 2.1 \text{ d}$  for Kidman sandy loam soil and  $k = 0.308 \text{ d}^{-1}$  with  $t_{1/2} = 2.2 \text{ d}$  for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 398\text{--}1152 \text{ h}$ , based on soil-die-away test data (Howard et al. 1991);  $t_{1/2} = 0.02\text{--}46 \text{ wk}$ ,  $t_{1/2} < 2.1 \text{ yr}$  (quoted, Ludington soil, Wild et al. 1991).

Biota: elimination half-lives  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes,  $t_{1/2} = 2.0 \text{ d}$  from clam *Macoma balthica* (quoted, Meador et al. 1995).

TABLE 4.1.1.2.1

Reported aqueous solubilities of naphthalene at various temperatures and empirical temperature dependence equations

$$R \cdot \ln x = -\Delta H_{\text{fus}}/(T/K) + (0.000408) \cdot [(T/K) - 291.15]^2 - c + b \cdot (T/K) \quad (1)$$

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t_{1/2} + c \cdot t + d \quad (2)$$

$$R \cdot \ln x = -30.55/\theta + 28.7/(1/\theta - 1/T) + 0.31[\theta/T - 1 - \ln(\theta/T)] \quad (3)$$

$$\ln x = 1767.460/[R \cdot (T/K)] + (17.95209/R) \cdot \ln(T/K) + 1 \quad (4)$$

$$\log(S/\text{mol} \cdot \text{dm}^{-3}) = -31.24 - 143.5/(T/K) + 4.772 \cdot \ln(T/K) \quad (5)$$

1.

Hilpert 1916		Bohon & Claussen 1951		Wauchope & Getzen 1972			
shake flask-gravimetry		shake flask-UV		shake flask-UV			
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0	19	25	34.4	22.2	28.8	0	13.7
25	30	0	13.74	22.2	29.1	22.2	28.3
		0.4	13.74	24.5	30.8	24.5	30.7
		0.5	13.85	24.5	30.1	25.0	31.2
		0.9	14.59	24.5	30.7	29.9	37.3
		9.4	19.62	29.9	38.1	30.3	37.8
		10	19.42	29.9	38.2	34.5	44.3
		14.9	23.43	29.9	38.3	39.3	53.3
		15.9	24.56	30.3	38.1, 37.6	40.1	55.0
		19.3	28.05	34.5	44.6, 43.8	44.7	66.2
		25.6	36.6	39.3	52.6, 52.8	50.0	82.4
		30.1	42.97	40.1	54.8	50.2	83.1
		30.2	43.87	44.7	66.0	55.6	105
		35.2	54.45	44.7	65.5	64.5	156
		36.0	54.81	44.7	65.3	73.4	239
		42.8	73.49	50.2	78.6	75	258
				55.6	106		
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$		64.5	166	temp dependence eq. 1	
		2°C	4.14	64.5	151	ln x	mole fraction
		7°C	5.77	64.5	157	$\Delta H_{\text{fus}} =$	$36.36 \pm 0.17$
		12°C	7.24	73.4	240	$10^2 \cdot b$	$1.39 \pm 0.05$
		17°C	8.49	73.4	247	c	$13.4 \pm 0.2$
		22°C	10.17	73.4	244		
		27°C	12.80				
		32°C	14.23	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 36.36$			
		37°C	15.69				

(Continued)

TABLE 4.1.1.2.1 (Continued)

2.

Schwarz & Wasik 1977		Schwarz 1977		May 1980		May et al. 1983	
shake flask-fluorescence		shake flask-fluorescence		generator column-HPLC		generator column-HPLC/UV	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
from K <sub>WA</sub> measurements							
10	18.32	8.4	17.95	8.2	16.91	8.2	16.92
12	19.87	11.1	19.1	11.5	19.23	11.5	19.25
14	21.02	14	21.2	13.4	20.37	13.4	20.39
15	22.17	17.5	24.1	15.1	21.48	15.1	21.50
16	22.56	20.2	26.54	19.3	25.79	19.3	25.81
18	23.97	23.2	28.46	23.4	29.47	23.4	29.50
19	24.61	25	30.25	25.0	31.91	25.0	31.94
20	25.51	26.3	31.79	27.0	34.15	27.0	34.18
22	27.17	29.2	34.36				
24	28.84	31.8	36.28	temp dependence eq. 2		$\Delta_{\text{sol}}\text{H}/(\text{kJ mol}^{-1}) = 27.4$	
25	29.61			S	µg/kg	8–32°C	
26	30.63	$\Delta\text{H}_{\text{sol}}/(\text{kJ mol}^{-1}) = 22.1$		a	0.0013	data fitted to eq. 3	
28	34.10	for temp 8–32°C		b	–0.0097		
30	34.61			c	0.8886		
				d	8.21		
direct measurement							
12	18.58	$\Delta\text{H}_{\text{sol}}/(\text{kJ mol}^{-1}) = 26.36$					
18	24.35						
25	30.0						

3.

Bennet & Canady 1984		Shaw 1989		Perez-Tejeda et al. 1990	
shake flask-UV		recommended values		shake flask-UV	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
25	31.1	0	15	5	12.3
1.90	19.2	10	19	10	20.25
10.7	17.2	20	28	15	24.35
15.4	21.66	25	31	20	28.71
21.7	26.74	30	38	25	33.71
25.2	30.75	40	61	35	41.53
30.7	40.12	50	82	35	47.55
35.1	46.36	60	130	40	55.75
39.3	54.85	70	200		
44.9	68.97	75	260	data fitted to eq. 5	
data fitted to eq. 4					
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$					
25°C					



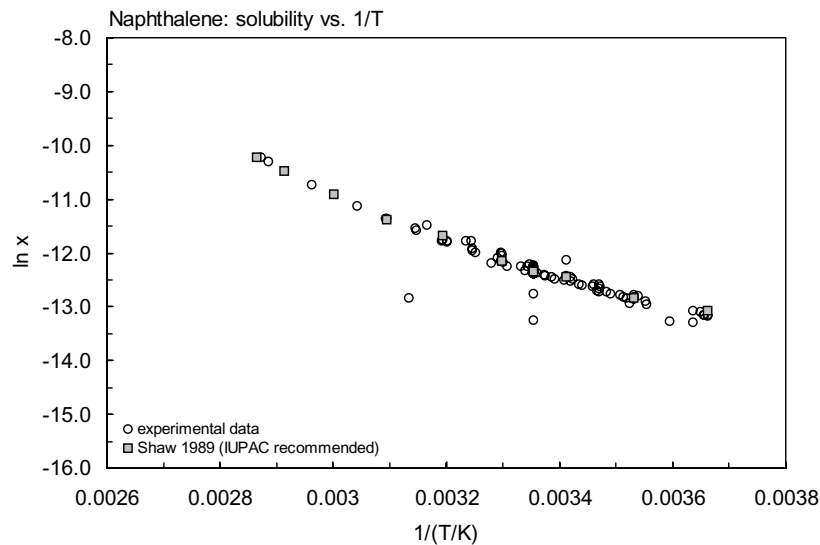


FIGURE 4.1.1.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for naphthalene.

TABLE 4.1.1.2.2  
Reported vapor pressures of naphthalene at various temperatures and coefficients for 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)

1.

Swan & Mack 1925		Stull 1947		Sears & Hopke 1949		Bradley & Cleasby 1953	
effusion		summary of literature data		manometry		effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	2.32	52.6	133.3	10	2.053	6.7	1.627
20	8.64	74.2	666.6	20	8.533	8.1	1.88
30	23.60	85.8	1333	30	21.87	12.3	2.96
		101.7	2666			12.7	3.13
eq. 4	P/mmHg	119.3	5333	eq. 2	P/mmHg	13.85	3.506
A	595.642	130.2	7999	A	1.115	15.65	4.266
B	29.820	145.5	13332	B	108.3	16.85	4.67
C	200.682	167.7	26664	C	27	17.35	5.09
		193.2	53329			18.7	5.106
		217.9	101325			20.7	7.12
		mp/°C	80.2			eq. 1	P/mmHg
						A	10.597
						B	3783

(Continued)

TABLE 4.1.1.2.2 (Continued)

2.

Camin & Rossini 1955		Miller 1963		Fowler et al. 1968		Zwolinski & Wilhoit 1971	
manometry		Knudsen effusion		Hg manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
126.325	6815	−43	0.00148	40.33	46.66	85.581	1333
130.836	8338	−33	0.00746	49.45	98.66	101.788	2666
134.548	9537	−23	0.0332	54.17	148.0	111.451	4000
138.677	10948	−13	0.1188	50.22	244.0	118.688	5333
143.930	13096			61.20	253.3	124.537	6666
155.766	19436	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.67$ at 25°C		65.05	338.6	129.476	7999
161.104	22878			70.18	500.0	137.581	10666
168.540	28550			70.98	521.3	144.146	13332
175.526	34818			75.61	725.3	156.749	19998
183.336	43159			76.7	789.3	166.262	26664
191.702	53748			80.34	931.9	173.966	33331
200.471	67072					180.561	39997
216.319	98125			eq. 2	P/mmHg	191.398	53329
217.237	99729			A	9.58102	200.237	66661
217.848	101112			B	2619.91	207.760	79993
218.638	102925			C	220.651	214.343	93326
						215.569	95992
bp/°C	217.955					216.768	98659
						217.942	101325
eq. 2	P/mmHg						
A	6.84577					eq. 2	P/mmHg
B	1606.529					A	7.01063
C	187.277					B	1733.71
						C	201.859
						bp/°C	217.942
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	72.68
						at bp	43.26

3.

Sinke 1974		Radchenko & K. 1974		Ambrose 1975		Macknick & Prausnitz 1979	
gas saturation		effusion		diaphragm gauge		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
−53.15	0.00028	9.0	2.357	263.61	0.23	7.15	1.76
−33.15	0.00837	10.7	3.113	267.98	0.40	12.8	3.133
−13.15	0.144	12.5	5.637	273.16	0.74	18.4	5.586
6.85	1.631	14.4	7.546	278.22	1.38	18.85	5.933
25	10.93	16.3	19.59	283.14	2.41	26.4	12.58
26.85	13.092	18.2	31.09	288.01	4.13	31.85	20.53
46.85	79.73	20.0	48.37	288.01	4.17	25	10.64
66.85	386.5	21.95	74.19	293.24	6.93		
80.28	999.8	23.91	112.6	293.25	6.95	eq. 1	P/mmHg
		25	12.26*	298.26	11.35	A	26.25
eq. 1	P/Pa			303.29	18.45	B	8575
A	13.83	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.72$ at 25°C		308.17	28.95		
B	3817			313.24	44.73		

TABLE 4.1.1.2.2 (Continued)

Sinke 1974		Radchenko & K. 1974		Ambrose 1975		Macknick & Prausnitz 1979	
gas saturation		effusion		diaphragm gauge		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
				318.21	68.82		
		eq. 1	P/mmHg	323.14	104.14		
		A	11.7041	328.24	158.41		
		B	3798.574	333.39	237.54		
		*calcd using eq. 1		333.34	238.73		
				333.34	238.47		
				338.10	340.58		
				343.06	488.58		
				$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.5$			
				at 25°C			
4.							
de Kruif 1980		de Kruif et al. 1981					
torsion-effusion		diaphragm gauge					
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
		solid		cont'd		liquid	
257.21	0.1	274.44	0.87	340.92	421.8		
262.44	0.2	276.40	1.10	348.82	717.5	355.23	1069
265.59	0.3	279.12	1.50	350.44	790.2	356.83	1155
267.88	0.4	280.62	1.78	352.44	914.5	359.78	1328
269.68	0.5	282.73	2.24	344.72	538.0	362.77	1526
271.17	0.6	285.37	3.07	345.76	586.6	355.38	1083
272.44	0.7	285.71	3.11	328.79	159.2	372.05	2305
273.56	0.8	287.98	3.98	324.57	118.5	377.33	2899
274.55	0.9	288.11	4.02	345.92	580.4	385.20	4006
275.44	1.0	290.46	5.16	324.87	121.9	381.92	3504
		290.88	5.35	347.53	650.0	372.45	2351
$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} =$		292.75	6.53	347.57	653.9	368.07	1929
298.15 K	72.6	320.34	83.91	344.72	547.1	363.74	1591
253–273 K	74.4	319.87	80.76	344.86	549.1	353.57	982
		275.50	0.99	352.00	901.3	357.10	1176
		282.12	2.10	319.58	78.38	361.10	1423
		277.86	1.30	319.59	77.9	367.72	1926
		325.41	126.7	325.96	132.1	380.51	3355
		288.51	4.22	341.26	419.9	388.20	4545
		293.83	7.29	349.02	724.1	348.80	3998
		297.40	10.42	346.18	597.6	374.67	2626
		306.67	25.27	352.90	941.6	368.46	1999
		310.71	36.37	338.91	359.7	387.32	4398
		302.92	17.84	346.85	629.9	357.44	1200
		318.58	72.36	350.69	820.2	362.57	1528
		282.13	2.10	349.15	751.1	353.51	995
		277.85	1.30	341.72	441.7	353.33	985
		288.50	4.21	348.6	717.3		

(Continued)

TABLE 4.1.1.2.2 (Continued)

de Kruif 1980		de Kruif et al. 1981					
torsion-effusion		diaphragm gauge					
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
		313.96	46.87	349.24	700.9		
		313.88	48.94	345.96	599.0		
		311.49	88.77	353.14	969.3		
		317.68	66.27				
		321.31	89.40	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} =$			
		324.05	112.0	298.15	72.5		
		339.29	361.8				

5. Colomina et al. 1982		Grayson & F. 1982		Sonnefeld et al. 1983		Van Ekeren et al. 1983	
effusion		gas saturation		gas saturation-HPLC		spinning-rotor gauge	
T/K	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
271.46	0.611	28.9	16.38	14.15	3.13	244.19	0.0163
275.08	0.94	42.7	58.33	14.15	3.24	245.31	0.0191
277.10	1.19	50	100.99	14.15	3.27	245.31	0.0192
279.93	1.63	60.2	264.32	19.49	6.0	246.59	0.0233
281.16	1.99	69.6	519.1	19.49	6.19	247.74	0.0268
282.69	2.23	79	970.5	25.05	10.1	247.74	0.0272
283.80	2.54	20	6.75	15.05	10.8	249.18	0.0373
284.63	2.80			25.05	10.4	250.45	0.04
		eq. 1a	P/mmHg	32.1	20.9	252.77	0.0554
$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.8$		A	31.80	32.05	21.0	255.86	0.0834
	at 25°C	B	8753	32.1	20.8		
						$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} =$	
eq. 1	P/Pa			eq. 1	P/Pa	248.51	72.92
A	14.01			A	14.299	298.15	72.92
B	3861.80			B	3960.03		

6. Sato et al. 1986		Sasse et al. 1988				Wania et al. 1994	
gas saturation-electrobalance		gas saturation				gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		solid		liquid			
24.85	10.7	−12.15	0.1653	80.16	968.85	−30.6	0.014
28.35	14.9	−12.1	0.1653	84.90	1240.4	−25.0	0.0217
30.95	19.2	−9.47	0.2266	84.93	1270.6	−20.1	0.0586
34.15	25.9	0.52	0.8199	87.16	1382.6	−14.9	0.108
41.65	52.8	10.17	2.413	84.23	1395.9	−10.0	0.2122
45.35	71.1	20.11	7.093	90.15	1590.5	−5.0	0.348
48.95	97.5	20.16	7.026			0	0.7634
49.45	101	29.98	18.265	For liquid			
51.85	124	30.03	18.80	eq. 2	P/mmHg	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 73.7$	
55.35	165	40.04	44.93	A	2.25180	(−30 to 0°C)	
57.75	200	40.04	45.46	B	76.496		
		50.04	106.8	C	−25.09	eq. 1	P/Pa

TABLE 4.1.1.2.2 (Continued)

Sato et al. 1986		Sasse et al. 1988				Wania et al. 1994	
gas saturation-electrobalance		gas saturation				gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
eq. 3	P/Pa	50.04	105.2			A	13.93
A	22.892960.05	60.05	238.2			B	3851
B	4025.3560.12	60.12	232.6				
C	-102.34370.11	70.11	491.0				
		70.16	491.02				
For solid							
		eq. 2	P/mmHg				
		A	10.05263				
		B	2907.918				
		C	236.459				

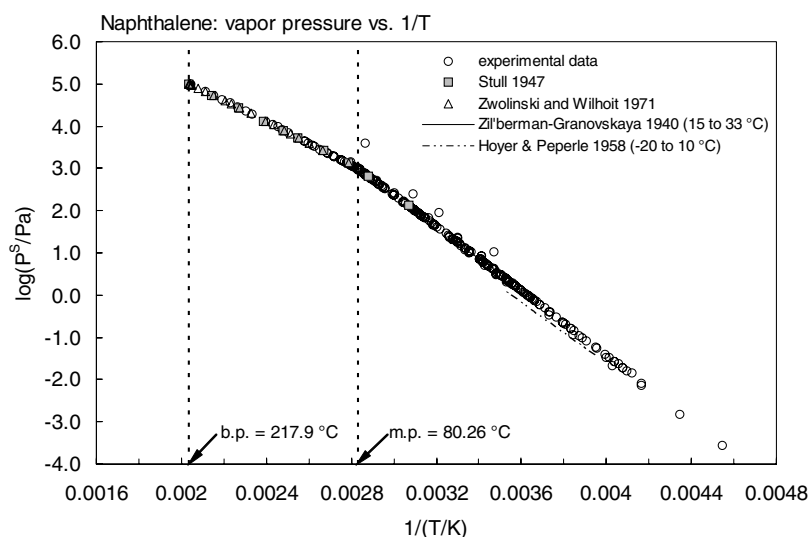


FIGURE 4.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for naphthalene.

TABLE 4.1.1.2.3

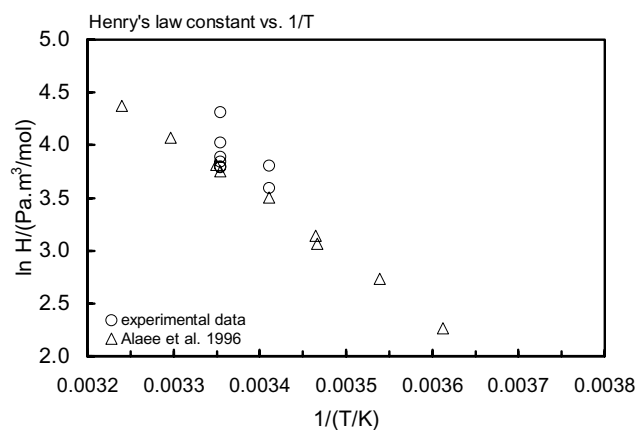
Reported Henry's law constants of naphthalene at various temperatures

Alaee et al. 1996	
gas stripping-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)
3.7	9.65
9.4	15.4
15.3	21.4
15.5	23.1
20	33.2
25	42.6
25.4	45.2
30.2	58.6

(Continued)

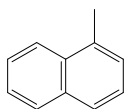
Alaee et al. 1996

gas stripping-GC



**FIGURE 4.1.1.2.3** Logarithm of Henry's law constant versus reciprocal temperature for naphthalene.

## 4.1.1.3 1-Methylnaphthalene



Common Name: 1-Methylnaphthalene

Synonym:  $\alpha$ -methylnaphthalene

Chemical Name: 1-methylnaphthalene

CAS Registry No: 90-12-0

Molecular Formula:  $C_{11}H_{10}$

Molecular Weight: 142.197

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

−30.43 (Lide 2003)

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

244.7 (Lide 2003)

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

1.02015, 1.01649 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.0125 (Dean 1985)

1.0202 (Lide 2003)

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

139.4 ( $20^{\circ}C$ , calculated-density)

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

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

60.06, 45.48 ( $25^{\circ}$ , bp, Dreisbach 1955)

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

4.853 (Dean 1985)

4.98, 6.95; 11.92 ( $-32.45$ ,  $34.25^{\circ}C$ , total phase change enthalpy, Chickos et al. 1999)

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

20.69, 28.82 ( $-32.45$ ,  $34.25^{\circ}C$ , Chickos et al. 1999)

49.3, 44.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

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

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

25.8 (shake flask-GC, Eganhouse & Calder 1976)

28.5 (shake flask-fluorescence, Mackay & Shiu 1977)

29.9\* (shake flask-fluorescence, measured range  $8.6$ – $31.7^{\circ}C$ , Schwarz & Wasik 1977)

29.5\* (shake flask-fluorescence, measured range  $10$ – $25^{\circ}C$ , Schwarz 1977)

31.7 (generator column-HPLC, Wasik et al. 1983)

27.02 (average lit. value, Pearlman et al. 1984)

30.2\* ( $20^{\circ}C$ , shake flask-GC, measured range  $20$ – $70^{\circ}C$ , Burris & MacIntyre 1986)

28.0 (recommended, IUPAC Solubility Data Series, Shaw 1989)

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):

7.165\* (manometer, extrapolated-Antoine eq., Camin & Rossini 1955)

$\log(P/mmHg) = 7.03592 - 1826.948/(195.002 + t/^{\circ}C)$ ; temp range  $142.1$ – $254.4^{\circ}C$  (Antoine eq., Hg manometer, Camin & Rossini 1955)

8.95 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.06899 - 1852.674/(197.716 + t/^{\circ}C)$ ; temp range  $130$ – $305^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

66.66\* ( $52.8^{\circ}C$ , Hg manometer, measured range  $52.8$ – $243.0^{\circ}C$ , Myers & Fenske 1955)

7.19\* (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

- $\log (P/\text{mmHg}) = 7.03592 - 1826.948/(195.002 + t/^{\circ}\text{C})$ ; temp range 107.68–278.32°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)  
 8.82\* (gas saturation-GC, Macknick & Prausnitz 1979)  
 8.84 (extrapolated-Clapeyron eq., Macknick & Prausnitz 1979)  
 $\log (P/\text{mmHg}) = 20.552 - 6933.2/(T/\text{K})$ ; temp range 5.70–38.6°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)  
 7221\* (151.15°C, differential pressure gauge, measured range 151.15–271.70°C, Wieczorek & Kobayashi 1981)  
 $\log (P/\text{atm}) = [1 - 517.727/(T/\text{K})] \times 10^{\{0.863323 - 5.26355 \times 10^{-4} \cdot (T/\text{K}) + 3.85750 \times 10^{-7} \cdot (T/\text{K})^2\}}$ ; temp range 278.85–593.38 K (Cox eq., Chao et al. 1983)  
 8.84 (interpolated Antoine eq., Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.15971 - 1825.586/(194.848 + t/^{\circ}\text{C})$ ; temp range: 142.1–245.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 7.43, 6.38 (GC-RT correlation with BP-1 column, Apolane column, Bidleman 1984)  
 7.816 (extrapolated Antoine eq., Dean 1985, 1992)  
 $\log (P/\text{mmHg}) = 7.03592 - 1826.946/(195.0 + t/^{\circ}\text{C})$ ; temp range 108–278°C (Antoine eq., Dean 1985, 1992)  
 0.895 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.03469 - 3006.467/(T/\text{K})$ ; temp range 278–313 K (Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.15928 - 1826.402/(-72.779 + T/\text{K})$ ; temp range 415–526 K (Antoine eq., Stephenson & Malanowski 1987)  
 8.93\* (pressure gauge, interpolated-Antoine eq. derived from exptl. data, temp range –14.44 to + 115°C, Sasse et al. 1988)  
 $\log (P_L/\text{mmHg}) = 7.27126 - 2006.862/(212.625 + t/^{\circ}\text{C})$ ; temp range –14.44 to 115.1°C, (Antoine eq., pressure gauge, Sasse et al. 1998)  
 7.43 ( $P_{\text{GC}}$  by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)  
 $\log (P/\text{mmHg}) = 29.8895 - 3.9535 \times 10^3/(T/\text{K}) - 7.2253 \cdot \log (T/\text{K}) + 1.1109 \times 10^{-11} \cdot (T/\text{K}) + 8.9552 \times 10^{-7} \cdot (T/\text{K})^2$ ; temp range 243–722 K (vapor pressure eq., Yaws 1994)  
 8.94, 8.93; 9.50, 8.12, 19.7; 7.42, 5.93 (quoted exptl. values; calculated; GC-RT correlation, Delle Site 1997)  
 $\log (P/\text{kPa}) = 6.39609 - 2006.662/[(T/\text{K}) - 60.525]$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)  
 6.55; 1.28 (supercooled liquid  $P_L$ ; calibrated GC-RT correlation, GC-RT correlation, Lei et al. 2002)  
 $\log (P_L/\text{Pa}) = -3258/(T/\text{K}) + 11.74$ ;  $\Delta H_{\text{vap.}} = -62.4 \text{ kJ} \cdot \text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)  
 8.85\* (24.05°C, transpiration method, measured range 294.1–324.2 K, Verevkin 2003)  
 $\ln (P/P^{\circ}) = 298.831/R - 83537.555/R \cdot (T/\text{K}) - (78.6/R) \cdot \ln[(T/\text{K})/298.15]$ ; where  $P^{\circ} = 101.325 \text{ kPa}$ , gas constant  $R = 8.31451 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  (vapor pressure eq. from transpiration measurements, temp range 294.1–324.2 K, Verevkin 2003)

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

- 26.3 (gas stripping, Mackay et al. 1979, 1982)  
 26.3 (gas stripping-GC, Mackay et al. 1982)  
 62.0 (wetted-wall column-GC, Fendinger & Glotfelty 1990)  
 36.5 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 24.3 (gas stripping-GC, Shiu & Mackay 1997)  
 52.1 (gas stripping-GC, Altschuh et al. 1999)  
 47.8\* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)  
 $\ln K_{\text{AW}} = -5821.5/(T/\text{K}) + 15.636$ ;  $\Delta H = 48.4 \text{ kJ mol}^{-1}$ ; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

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

- 3.87 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)  
 3.87 (Hansch & Leo 1979)  
 3.87 (recommended, Sangster 1989, 1994)  
 3.87 (recommended, Hansch et al. 1995)



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

Bioconcentration Factor,  $\log BCF$ :

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

- 3.33, 3.06 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)  
 3.36 (sediment from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)  
 2.96–3.83 (aquifer materials, Stauffer et al. 1989)

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

Volatilization:

Photolysis: calculated  $t_{1/2} = 22$  h for direct sunlight photolysis of 50% conversion at 40°N latitude of midday in midsummer in near surface water,  $t_{1/2} = 180$  d in 5-m deep inland water and  $t_{1/2} = 190$  d in inland water with a suspended sediment concentration of 20 mg/L partitioning (Zepp & Schlotzhauer 1979);  
 $t_{1/2} = 180$  d under summer sunlight in surface water (Mill & Mabey 1985);  
 direct photolysis  $t_{1/2} = 11.14$  h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).

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 original reference:

$k_{OH} = (5.30 \pm 0.48) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{O_3} < 1.3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{N_2O_5} = (3.3 \pm 0.7) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with  $N_2O_5$  at  $298 \pm 2$  K (relative rate method, Atkinson & Aschmann 1987, 1988)

$k_{OH} = 5.30 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 59.77 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1996)

$k_{OH} = 5.30 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ ,  $(4.09 \pm 0.20) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  at  $(298 \pm 2) \text{ K}$  with a calculated tropospheric lifetime to be 2.9 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule} \cdot \text{cm}^{-3}$  (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis:

Biodegradation:  $k = 0.415 \text{ d}^{-1}$  with  $t_{1/2} = 1.7$  d for Kidman sandy loam soil and  $t_{1/2} = 0.321 \text{ d}^{-1}$  with  $t_{1/2} = 2.2$  d for McLaurin sandy loam soil, all at  $-3.3$  bar soil moisture (Park et al. 1990).

Biotransformation:

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

Half-Lives in the Environment:

Air: atmospheric lifetimes of alkyl-substituted naphthalenes due to reaction with OH radical and with  $N_2O_5$  calculated to range from ~4 to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);

direct photolysis  $t_{1/2} = 11.14$  h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001); a calculated tropospheric lifetime to be 2.9 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule} \cdot \text{cm}^{-3}$  for the reaction with OH radical (Phouongphouang & Arey 2002).

Water: computed near-surface  $t_{1/2} = 22$  h and for direct photochemical transformation at latitude 40°N, midday, midsummer, and  $t_{1/2} = 80$  d with no sediment-water partitioning and  $t_{1/2} = 190$  d with sediment-water partitioning for direct photolysis in 5 m deep inland water body integrated over full summer d at latitude 40°N (Zepp & Schlotzhauer 1979);

$t_{1/2} = 180$  d under summer sunlight (Mill & Mabey 1985).

Soil: biodegradation  $k = 0.415 \text{ d}^{-1}$  with  $t_{1/2} = 1.7$  d for Kidman sandy loam soil,  $k = 0.321 \text{ d}^{-1}$  with  $t_{1/2} = 2.2$  d for McLaurin sandy loam soil (Park et al. 1990).

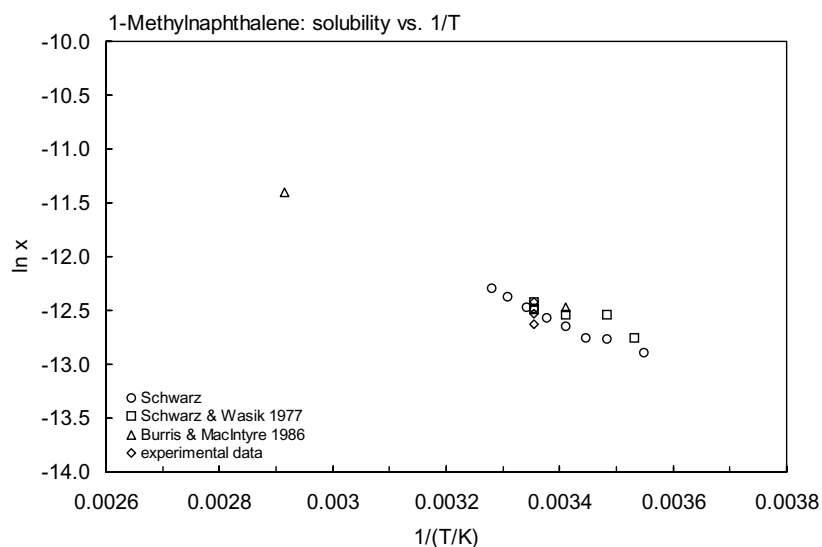
Sediment:

Biota: elimination  $t_{1/2} = 2$  d from Oyster for naphthalenes (quoted, Meador et al. 1995).

**TABLE 4.1.1.3.1**  
**Reported aqueous solubilities of 1-methylnaphthalene at various temperatures**

Schwarz 1977		Schwarz & Wasik 1977		Burris & MacIntyre 1986	
shake flask-fluorescence		shake flask-fluorescence		shake flask-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
8.6	19.91	10	22.75	20	30.2
14.5	22.61	14	28.44	70	87.9
17.1	22.89	20	28.44		
20.0	25.31	25	29.86		
23.0	27.59				
25.0	30.0				
26.1	30.43				
29.2	33.28				
31.7	36.26				

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 19.1$



**FIGURE 4.1.1.3.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-methylnaphthalene.

TABLE 4.1.1.3.2

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

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & \ln P/P^{\circ} = A - B/(T/K) - C \cdot \ln [(T/K)/298.15] & 4(a) \end{array}$$

1.

Camin & Rossini 1955		Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979	
ebulliometry		Hg manometer		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
142.140	5524	52.8	66.66	107.68	1333	5.70	1.760
153.600	8314	63.5	133.3	123.57	2666	11.40	2.920
157.539	9510	75.8	266.6	133.66	4000	18.10	5.248
161.689	10942	83.0	400.0	141.21	5333	22.15	7.133
167.212	13088	88.9	533.3	147.319	6666	28.85	12.59
179.971	19442	93.3	666.6	152.474	7999	32.35	15.73
185.505	22881	97.1	799.9	160.932	10666	34.90	18.93
193.280	28542	103.8	1067	167.781	13332	38.60	23.46
200.536	34832	108.8	1333	180.927	19998		
208.677	43162	117.6	2000	190.846	26664	eq. 1a	P/mmHg
217.375	53762	124.4	2666	198.908	33331	A	20.552
226.498	67057	134.4	4000	205.750	39997	B	6933.2
246.243	84026	142.2	5333	217.043	53329		
243.177	98081	148.3	6666	226.250	66661		
243.949	99655	153.7	7999	234.084	79993		
244.555	101030	161.9	10666	240.938	93326		
245.326	102757	168.5	13332	242.215	95992		
		182.0	19998	243.463	98659		
eq. 2	P/mmHg	191.6	26664	244.078	99992		
A	7.03592	206.0	39997	244.685	101325		
B	1826.948	217.0	53329				
C	195.002	225.5	66661	eq. 2	P/mmHg		
		233.3	79993	A	7.03592		
$\Delta H_v/(kJ\ mol^{-1}) = 63.82$		240.0	93326	B	1826.948		
at 25°C		243.0	101325	C	195.002		
				bp/°C	244.685		
				$\Delta H_v/(kJ\ mol^{-1}) = 46.0$			
				at bp			

(Continued)

TABLE 4.1.1.3.2 (Continued)

2.

Wieczorek & Kobayashi 81		Sasse et al. 1988		Verevkin 2003	
differential pressure gauge		electronic manometer		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
151.15	7221	−14.44	0.189	20.95	6.86
158.75	9929	−9.64	0.317	24.05	8.85
166.42	12812	10.14	23386	27.05	11.17
175.40	16969	20.18	6.093	30.15	14.29
182.48	21024	30.15	13.73	33.15	17.51
189.45	25738	40.04	28.40	35.15	20.29
196.03	30891	49.90	56.53	36.15	22.51
202.35	36636	59.89	107	38.05	25.25
210.18	44906	69.98	194	39.05	26.72
217.70	54250	79.94	35.42	42.15	32.68
225.93	66313	89.99	579	45.15	41.63
233.82	79716	100.06	950	47.15	53.96
240.26	92116	110.04	1507	51.05	67.87
243.27	98620	115.10	1888		
244.60	101629			eq. 4a	P/kPa
254.66	126232	eq. 2	P/mmHg	P <sup>o</sup>	101.325 kPa
263.69	151814	A	7.27126	A	298.831/R
271.70	177915	B	2006.862	B	83537.555/R
		C	212.625	C	78.6/R
data fitted to				R = 8.314 J K <sup>−1</sup> mol <sup>−1</sup>	
Chebyshev polynomial		$\Delta H_v/(kJ\ mol^{-1}) = 60.58$		$\Delta H_v/(kJ\ mol^{-1}) = 60.7$	
temp range 424–593 K		at 25°C		at 25°C	

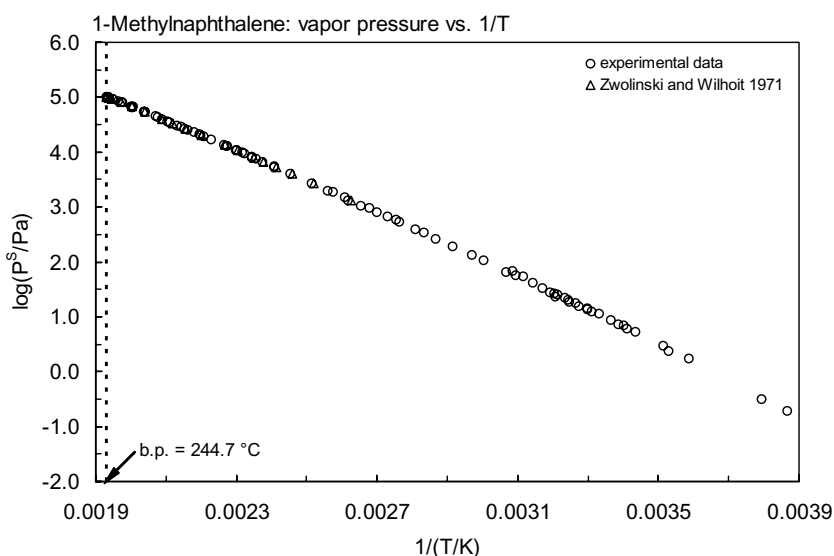
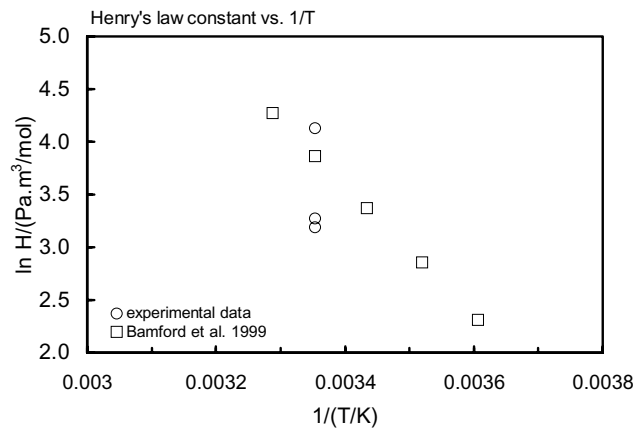


FIGURE 4.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 1-methylnaphthalene.

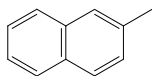
**TABLE 4.1.1.3.3**  
**Reported Henry’s law constants of 1-methylnaphthalene at various temperatures and temperature dependence equations**

Bamford et al. 1999		
gas stripping-GC/MS		
t/°C	H/(Pa m³/mol)	H/(Pa m³/mol)
		average
4.1	9.41, 10.7	10.1
11.0	16.6, 18.2	17.4
18.0	27.8, 30.8	29.2
25.0	44.8, 51.0	47.8
31.0	65.7, 78.2	71.7
ln K <sub>AW</sub> = A – B/(T/K)		
A	15.636	
B	5821.5	
enthalpy, entropy change:		
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 48.4 \pm 1.4$		
$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 130$		
at 25°C		



**FIGURE 4.1.1.3.3** Logarithm of Henry’s law constant versus reciprocal temperature for 1-methylnaphthalene.

## 4.1.1.4 2-Methylnaphthalene



Common Name: 2-Methylnaphthalene

Synonym:  $\beta$ -methylnaphthalene

Chemical Name: 2-methylnaphthalene

CAS Registry No: 91-57-6

Molecular Formula:  $C_{11}H_{10}$

Molecular Weight: 142.197

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

34.6 (Weast 1972–73; Lide 2003)

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

241.1 (Weast 1977; Lide 2003)

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

1.0058 (Weast 1982–83; Lide 2003)

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

141.4 ( $20^{\circ}C$ , calculated-density)

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

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

59.40, 45.20 ( $25^{\circ}$ , bp, Dreisbach 1955)

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

11.924 (Parks & Huffman 1931)

5.61, 12.13; 17.74 (15.35,  $34.25^{\circ}C$ ; total phase change enthalpy, Chickos et al. 1999)

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

39.25 (Tsonopoulos & Prausnitz 1971)

19.43, 39.43 (15.35,  $34.25^{\circ}C$ , Chickos et al. 1999)

58.87, 44.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ , F: 0.805 (mp at  $34.6^{\circ}C$ ))

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

24.6 (shake flask-GC, Eganhouse & Calder 1976)

25.4 (shake flask-fluorescence, Mackay & Shiu 1977)

20.0 (Vozňáková et al. 1978)

25.6 (average lit. value, Pearlman et al. 1984)

27.3 (generator column-HPLC, Vadas et al. 1991)

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):

9.07\* (Hg manometer, extrapolated-Antoine eq., Camin & Rossini 1955)

$\log (P/mmHg) = 7.06850 - 1840.268/(198.395 + t/^{\circ}C)$ ; temp range  $139.1$ – $242^{\circ}C$  (Antoine eq., Hg manometer, Camin & Rossini 1955)

10.67 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 7.06850 - 1840.268/(198.395 + t/^{\circ}C)$ , temp range  $130$ – $300^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

9.07\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 7.06850 - 1840.268/(198.395 + t/^{\circ}C)$ ; temp range  $104.85$ – $274.3^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

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

5.60 ( $20^{\circ}C$ , Vozňáková et al. 1978)

8629\* ( $151.26^{\circ}C$ , differential pressure gauge, measured range  $151.26$ – $279.81^{\circ}C$ , Wiczorek & Kobayashi 1981)

$\log (P/atm) = [1 - 514.242/(T/K)] \times 10^4 \{0.879050 - 5.85793 \times 10^{-4} \cdot (T/K) + 4.19235 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range  $378.0$ – $629.32 K$  (Cox eq., Chao et al. 1983)

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

$\log (P/\text{kPa}) = 6.19638 - 1842.831/(198.692 + t/^{\circ}\text{C})$ ; temp range 139.2–241.76°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6.31 (GC-RT correlation, supercooled liquid, Bidleman 1984)

9.033 (extrapolated, Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.0685 - 1840.268/(198.4 + t/^{\circ}\text{C})$ ; temp range 105–274°C (Antoine eq., Dean 1985, 1992)

9.33 (extrapolated from Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.21475 - 1858.19/(-72.479 + T/\text{K})$ ; temp range 423–515 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 56.2052 - 5.2563 \times 10^3/(T/\text{K}) - 16.195 \cdot \log (T/\text{K}) + 8.1583 \times 10^{-11} \cdot (T/\text{K}) + 3.0253 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 308–761 K (vapor pressure eq., Yaws 1994)

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

32.23 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

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

20.265\* (26°C EPICS-GC, Hansen et al. 1993)

46.0 (gas stripping-HPLC/fluor., De Maagd et al. 1998)

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

51.3\* (gas stripping-GC; Bamford et al. 1999)

$\ln K_{AW} = -5099.83/(T/\text{K}) + 13.23$ ;  $\Delta H = 42.4 \text{ kJ mol}^{-1}$ ; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

18620 (20°C, selected value based on Hansen et al. 1993 data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 2.245 - 399/(T/\text{K})$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

3.864 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

3.86 (Hansch & Leo 1979)

4.11 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)

3.70 (HPLC- $k'$  correlation, Hanai et al. 1981)

4.01 (HPLC-RT correlation, Eadsforth 1986)

4.09 (HPLC-RT correlation, Wang et al. 1986)

4.00 (recommended, Sangster 1989)

3.86 (recommended, Hansch et al. 1995)

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

2.61 (quoted from Davies & Dobbs 1984, Sabljic 1987)

2.65 (calculated-MCI  $\chi$ , Sabljic 1987)

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

3.93 (natural sediments, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)

3.40 (sediment 4.02% from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)

3.719; 3.72, 3.71 (sediment: concn ratio  $C_{\text{sed}}/C_{\text{w}}$ ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)

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

Volatilization:

Photolysis:  $t_{1/2}$  (calc) = 54 h for direct sunlight photolysis at 40°N latitude of midday in midsummer in near surface water,  $t_{1/2}$  = 410 d in inland water and  $t_{1/2}$  = 440 d in inland water with sediment partitioning (Zepp & Schlotzhauer 1979);

$t_{1/2}$  = 410 d under summer sunlight in surface water (Mill & Mabey 1985);

$k = 0.042 \text{ h}^{-1}$  with  $t_{1/2}$  = 6.4 h in distilled water (Fukuda et al. 1988);

direct photolysis  $t_{1/2}$  = 9.23 h predicted - QSPR, in atmospheric aerosol (Chen et al. 2001).

Hydrolysis:

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

$k_{\text{OH}} = (5.23 \pm 0.42) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated atmospheric lifetime of ~5 h, and

$k_{\text{O}_3} < 4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $295 \pm 1 \text{ K}$  (relative rate, Atkinson & Aschmann 1986)

$k_{\text{N}_2\text{O}_5} = (4.2 \pm 0.9) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with  $\text{N}_2\text{O}_5$  at  $298 \pm 2 \text{ K}$  (relative rate method, Atkinson & Aschmann 1987)

$k_{\text{OH}} = 5.23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k_{\text{O}_3} < 0.4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{N}_2\text{O}_5} = 4.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $\text{N}_2\text{O}_5$  at room temp. (Atkinson & Aschmann 1987, 1988)

$k_{\text{OH}} = 52.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \text{ K}$  (Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 57.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}} = (4.86 \pm 0.25) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2 \text{ K}$  with a calculated tropospheric lifetime to be 3.4 h using a global tropospheric 12-h daytime average OH radical concn of  $2.0 \times 10^6 \text{ molecule/cm}^3$  (relative rate method, Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

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

#### Half-Lives in the Environment:

Air: calculated atmospheric lifetime of ~4 h due to reaction with OH radical (Atkinson & Aschmann 1986)

atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radicals and with  $\text{N}_2\text{O}_5$  can be calculated to range from ~4 to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);

direct photolysis  $t_{1/2} = 9.23 \text{ h}$  (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001);

a calculated tropospheric lifetime to be 3.4 h using a global tropospheric 12-h daytime average OH radical concn of  $2.0 \times 10^6 \text{ molecule/cm}^3$  for the reaction with OH radical (Phousong-phouang & Arey 2002).

Surface water: computed near-surface  $t_{1/2} = 54 \text{ h}$  and for direct photochemical transformation at latitude  $40^\circ\text{N}$ , midday, midsummer;  $t_{1/2} = 410 \text{ d}$  with no sediment-water partitioning and  $t_{1/2} = 440 \text{ d}$  with sediment-water partitioning by direct photolysis in a 5-m deep Inland Water Body (Zepp & Schlotzhauer 1979);

$t_{1/2} = 410 \text{ d}$  under summer sunlight (Mill & Mabey 1985);

rate constants and half-lives:  $k = 0.064 \text{ d}^{-1}$ ,  $t_{1/2} = 11 \text{ d}$  in spring at  $8\text{--}16^\circ\text{C}$ ,  $k = 0.687 \text{ d}^{-1}$ ,  $t_{1/2} = 1.0 \text{ d}$  in summer at  $20\text{--}22^\circ\text{C}$ ,  $k = 0.054 \text{ d}^{-1}$ ,  $t_{1/2} = 13 \text{ d}$  in winter at  $3\text{--}7^\circ\text{C}$  for the periods when volatilization appears to dominate, and  $k = 0.046 \text{ d}^{-1}$ ,  $t_{1/2} = 15.1 \text{ d}$  with  $\text{HgCl}_2$  as poison, and  $k = 0.954 \text{ d}^{-1}$ ,  $t_{1/2} = 0.7 \text{ d}$  without poison in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes (quoted, Meador et al. 1995).

**TABLE 4.1.1.4.1**

**Reported vapor pressures of 2-methylnaphthalene 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)		

Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Wieczorek & Kobayashi 1981	
ebulliometry		selected values		differential pressure gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
139.193	5536	104.85	1333	151.26	8629
145.431	6951	120.68	2666	158.72	10992
150.655	8339	130.73	4000	164.34	13183



TABLE 4.1.1.4.1 (Continued)

Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Wieczorek & Kobayashi 1981	
ebulliometry		selected values		differential pressure gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
154.676	9539	138.25	5333	169.89	15615
158.689	10942	144.329	6666	175.93	18756
164.155	13100	149.459	7999	181.84	22550
176.722	19433	157.872	10666	189.18	27850
182.322	22882	164.486	13332	196.20	33812
190.033	28551	177.752	19998	202.04	39538
197.234	34820	187.610	26664	209.49	48007
205.329	43163	195.619	33331	217.00	57974
213.963	53782	202.414	39997	225.34	70794
223.026	67089	213.626	53329	232.47	83506
239.613	98125	222.764	66661	239.90	96992
240.336	99734	230.537	79993	246.90	114865
240.957	101114	237.336	93326	254.69	134992
241.760	102929	238.602	95992	263.24	160539
		239.840	98659	271.29	188158
eq. 2	P/mmHg	240.449	99992	279.81	221176
A	7.06850	241.052	101325		
B	1840.268				
C	198.395	eq. 2	P/mmHg	exptl data fitted to Chebyshev polynomial temp range 424–639 K	
bp/°C	241.052	A	7.06850		
		B	1840.268		
		C	198.395		
		bp/°C	241.052		

$\Delta H_v/(\text{kJ mol}^{-1}) = 46.0$   
at bp

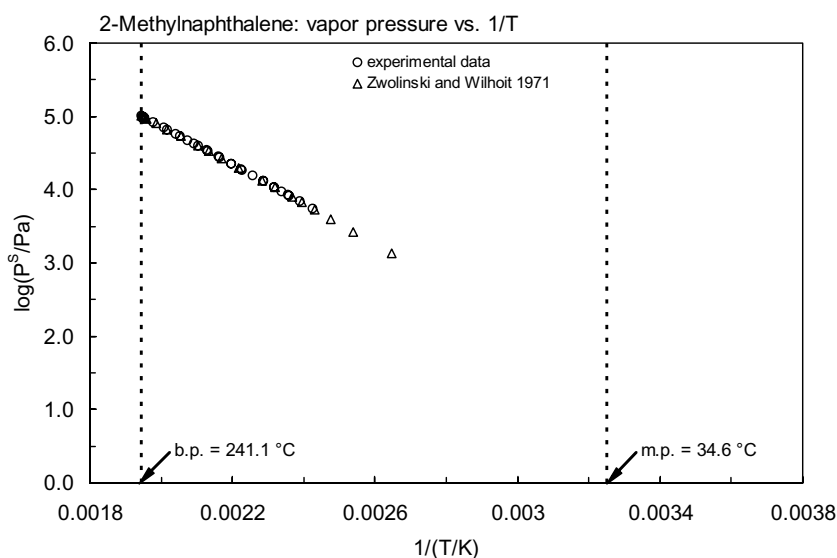


FIGURE 4.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylnaphthalene.

TABLE 4.1.1.4.2

Reported Henry's law constants of 2-methylnaphthalene at various temperatures and temperature dependence equations

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

Hansen et al. 1993		Bamford et al. 1999		
EPICS-GC		gas stripping-GC/MS		
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)
26.0	20.265	4.1	10.5, 16.2	average 13.0
35.8	22.900	11.0	18.2, 24.4	21.0
46.0	26.243	18.0	28.8, 38.3	33.2
		25.0	42.1, 62.5	51.3
eq. 4	H/(Pa m <sup>3</sup> /mol)	31.0	56.2, 95.5	73.3
A	7.0 ± 0.14			
B	1234 ± 44	eq. 1	K <sub>AW</sub>	
		A	13.2307	
		B	5100	
		enthalpy, entropy change:		
		$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 42.4 \pm 4.2$		
		$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{mol}^{-1}) = 110$		
		at 25°C		

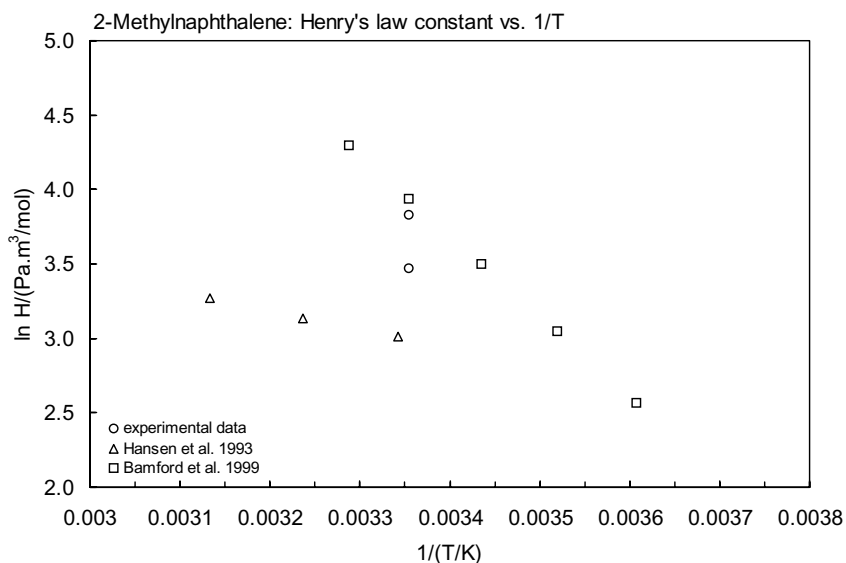
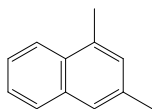


FIGURE 4.1.1.4.2 Logarithm of Henry's law constant versus reciprocal temperature for 2-methylnaphthalene.

## 4.1.1.5 1,3-Dimethylnaphthalene



Common Name: 1,3-Dimethylnaphthalene

Synonym:

Chemical Name: 1,3-dimethylnaphthalene

CAS Registry No: 575-41-7

Molecular Formula:  $C_{12}H_{12}$

Molecular Weight: 156.223

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

−6.0 (Weast 1982–83, Dean 1985; Lide 2003)

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

263 (Dreisbach 1955; Weast 1982–83; Dean 1985; Lide 2003)

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

1.0063, 1.0026 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.0144 (Weast 1982–83; Dean 1985; Lide 2003)

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

154.0 ( $20^{\circ}C$ , calculated-density)

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

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

69.58, 48.69 ( $25^{\circ}C$ , bp, Dreisbach 1955)

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

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

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

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

8.00 (shake flask-fluorescence, Mackay & Shiu 1977)

7.81 (average lit. value, Pearlman et al. 1984)

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

1.947 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0469 - 1845.6/(180.0 + t/^{\circ}C)$ ; temp range  $150$ – $313^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [1 - 540.353/(T/K)] \times 10^{[1.72680 - 7.87991 \times 10^{-4} \cdot (T/K) + 42.8535 \times 10^{-7} \cdot (T/K)^2]}$ ; temp range  $400.0$ – $541.0 K$  (Cox eq., Chao et al. 1983)

6.950 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.6347 - 2295.4/(232.4 + t/^{\circ}C)$ ; temp range  $20$ – $148^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.2698 - 2076.0/(210 + t/^{\circ}C)$ ; temp range  $148$ – $310^{\circ}C$  (Antoine eq., Dean 1985, 1992)

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

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

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

4.421 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.42 (Hansch & Leo 1979)

4.42 (recommended, Sangster 1993)

4.42 (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 original reference:

$k_{OH} = (7.49 \pm 0.39) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $(298 \pm 2) \text{ K}$  with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  for the reaction with OH radical (Phouongphouang & Arey 2002).

Surface water:

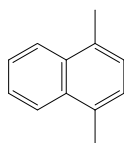
Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes (quoted, Meador et al. 1995).

## 4.1.1.6 1,4-Dimethylnaphthalene



Common Name: 1,4-Dimethylnaphthalene

Synonym:

Chemical Name: 1,4-dimethylnaphthalene

CAS Registry No: 571-58-4

Molecular Formula:  $C_{12}H_{12}$

Molecular Weight: 156.223

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

7.60 (Lide 2003)

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

268 (Dreisbach 1955, Weast 1982–83; Lide 2003)

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

1.0166, 1.0129 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.0166 (Weast 1982–83)

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

153.7 ( $20^{\circ}C$ , calculated-density)

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

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

70.315, 48.62 ( $25^{\circ}C$ , bp, Dreisbach 1955)

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

10.6 (Chickos et al. 1999)

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

37.87, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

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

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

11.4 (shake flask-fluorescence, Mackay & Shiu 1977)

11.40 (average lit. value, Pearlman et al. 1984)

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

1.55 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0527 - 1869.0/(180.0 + t/^{\circ}C)$ ; temp range  $155\text{--}310^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [1 - 544.363/(T/K)] \times 10^{\{1.57594 - 8.55425 \times 10^{-4} \cdot (T/K) + 51.4189 \times 10^{-7} \cdot (T/K)^2\}}$ ; temp range  $397.0\text{--}544 K$  (Cox eq., Chao et al. 1983)

2.27 (calculated-TSA, Amidon & Anik 1981; selected, Ma et al. 1990)

4.50 (interpolated, Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.6347 - 2345.8/(232.6 + t/^{\circ}C)$ ; temp range  $20\text{--}148^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.2698 - 2076.0/(210 + t/^{\circ}C)$ ; temp range  $148\text{--}310^{\circ}C$  (Antoine eq., Dean 1985, 1992)

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

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

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

4.372 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.37 (Hansch & Leo 1979)

4.37 (recommended, Sangster 1989, 1993)

4.37 (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 original reference:

$k_{OH} = (5.79 \pm 0.36) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $(298 \pm 2)K$  with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  (relative rate method, Phousongphouang & Arey 2002)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

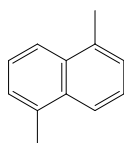
Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes (quoted, Meador et al. 1995).

## 4.1.1.7 1,5-Dimethylnaphthalene



Common Name: 1,5-Dimethylnaphthalene

Synonym:

Chemical Name: 1,5-dimethylnaphthalene

CAS Registry No: 571-61-9

Molecular Formula:  $C_{12}H_{12}$

Molecular Weight: 156.223

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

82 (Dreisbach 1955; Weast 1982–83; Lide 2003)

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

265 (Dreisbach 1955; Weast 1982–83; Lide 2003)

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

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

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

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ , F: 0.276 (mp at  $82^{\circ}C$ ))

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

2.74 (shake flask-GC, Eganhouse & Calder 1976)

3.38 (shake flask-fluorescence, Mackay & Shiu 1977)

3.12 (average lit. value, Pearlman et al. 1984)

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

$\log (P/mmHg) = 7.0493 - 1855.0/(180.0 + t/^{\circ}C)$ ; temp range  $150\text{--}313^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1.93; 0.513 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -3346/(T/K) + 11.51$ ;  $\Delta H_{vap} = -64.1\ kJ\cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

35.5 (gas stripping-fluorescence, Mackay et al. 1982)

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

36.3 (gas stripping, Shiu & Mackay 1997)

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

4.38 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.38 (Hansch & Leo 1979)

4.38 (recommended, Sangster 1989, 1993)

4.38 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

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

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

Volatilization:

Photolysis:

Hydrolysis:

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

$k_{\text{OH}} = (6.01 \pm 0.35) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $(298 \pm 2) \text{ K}$  with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  (relative rate method, Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: a calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

Groundwater:

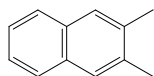
Sediment:

Soil:

Biota: elimination  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes (quoted, Meador et al. 1995).



## 4.1.1.8 2,3-Dimethylnaphthalene



Common Name: 2,3-Dimethylnaphthalene

Synonym: guaiene

Chemical Name: 2,3-dimethylnaphthalene

CAS Registry No: 581-40-8

Molecular Formula:  $C_{12}H_{12}$

Molecular Weight: 156.223

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

105 (Dreisbach 1955; Weast 1972–73; Lide 2003)

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

268 (Dreisbach 1955; Weast 1982–83; Lide 2003)

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

1.003 (Weast 1982–83; Lide 2003)

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

155.8 ( $20^{\circ}C$ , calculated-density)

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

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

70.315, 48.97 ( $25^{\circ}C$ , bp, Dreisbach 1955)

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

25.10 (Ruelle & Kesselring 1997)

15.9 (Chickos et al. 1999)

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

42.06, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ , F: 0.164 (mp at  $105^{\circ}C$ ))

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

1.99 (shake flask-GC, Eganhouse & Calder 1976)

3.0 (shake flask-fluorescence, Mackay & Shiu 1977)

2.50 (average lit. value, Pearlman et al. 1984)

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

1.55 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0527 - 1869.0/(180.0 + t/^{\circ}C)$ ; temp range  $155$ – $315^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1.86 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 631.969/(T/K)] \times 10^{1.09999 - 10.2378 \times 10^{-4} \cdot (T/K) + 11.3931 \times 10^{-7} \cdot (T/K)^2}$ ; temp range  $333.15$ – $408.15 K$  (Cox eq., Chao et al. 1983)

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

$\log(P/kPa) = 5.27335 - 1383.083/(141.333 + t/^{\circ}C)$ ; temp range  $105$ – $135^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.543 (interpolated, Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.40396 - 2111.9/(201.1 + t/^{\circ}C)$ ; temp range  $20$ – $155^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.0527 - 1869/(180 + t/^{\circ}C)$ ; temp range  $155$ – $315^{\circ}C$  (Antoine eq., Dean 1985, 1992)

0.437 (Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.635 - 4172.6/(T/K)$ ; temp range  $278$ – $301 K$  (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.97875 - 2959.733/(-59.936 + T/K)$ ; temp range  $333$ – $373 K$  (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.18084 - 1544.764/(-116.821 + T/K)$ ; temp range  $378$ – $408 K$  (Antoine eq.-III, Stephenson & Malanowski 1987)

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

- 38.92 (calculated-P/C, Eastcott et al. 1988)
- 92.16, 64.9 (quoted, calculated-bond contribution method, Meylan & Howard 1991)
- 59.9 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

- 4.396 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)
- 4.40 (Hansch & Leo 1979)
- 4.40 (recommended, Sangster 1993)
- 4.40 (recommended, Hansch et al. 1995)

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

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

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

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

Volatilization:

Photolysis:

Hydrolysis:

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

$k_{\text{OH}} = (7.68 \pm 0.48) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , with a calculated atmospheric lifetime of  $\sim 4 \text{ h}$ , and

$k_{\text{O}_3} < 4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $295 \pm 1 \text{ K}$  (relative rate method, Atkinson & Aschmann 1986)

$k_{\text{N}_2\text{O}_5} = (5.7 \pm 1.9) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $\text{N}_2\text{O}_5$  at  $298 \pm 2 \text{ K}$  (relative rate method, Atkinson & Aschmann 1987)

$k_{\text{O}_3} < 0.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}} = 7.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{N}_2\text{O}_5} = 5.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $\text{N}_2\text{O}_5$  at room temp. (Atkinson & Aschmann 1987, 1988)

$k_{\text{OH}} = (76.8 \pm 4.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $295 \pm 1 \text{ K}$  (Atkinson 1989)

$k_{\text{OH}} = 77 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \text{ K}$  (Atkinson 1990)

$k_{\text{OH}} = 100.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}} = (6.15 \pm 0.47) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $(298 \pm 2) \text{ K}$  using a relative rate method with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  (Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated atmospheric lifetime of  $\sim 4 \text{ h}$  due to reaction with OH radical (Atkinson & Aschmann 1986); the atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radicals and with  $\text{N}_2\text{O}_5$  can be calculated to range from  $\sim 4$  to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);

calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

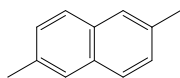
Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes (quoted, Meador et al. 1995).

## 4.1.1.9 2,6-Dimethylnaphthalene



Common Name: 2,6-Dimethylnaphthalene

Synonym:

Chemical Name: 2,6-dimethylnaphthalene

CAS Registry No: 581-42-0

Molecular Formula:  $C_{12}H_{12}$

Molecular Weight: 156.223

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

112 (Lide 2003)

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

262 (Dreisbach 1955; Dean 1985; Lide 2003)

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

1.003, 0.999 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.142 (Dean 1985)

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

155.8 (calculated-density)

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

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

69.45, 48.70 ( $25^{\circ}C$ , bp, Dreisbach 1955)

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

24.27 (Tsonopoulos & Prausnitz 1971)

25.06 (calorimetry, Osborn & Douslin 1975; quoted, Ruelle & Kesselring 1997; Chickos et al. 1999)

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

63.18 (Tsonopoulos & Prausnitz 1971)

65.39, 45.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ , F: 0.140 (mp at  $112^{\circ}C$ ))

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

1.30 (shake flask-GC, Eganhouse & Calder 1976)

2.0 (shake flask-fluorescence, Mackay & Shiu 1977)

1.72 (average lit. value, Pearlman et al. 1984)

0.997 (generator column-HPLC, Vadas et al. 1991)

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

20.41 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0460 - 1841.0/(180.0 + t/^{\circ}C)$ ; temp range  $150-310^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

0.75 (calculated-TSA, Amidon & Anik 1981)

1.38 (extrapolated- Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 687.081/(T/K)] \times 10^4 \{1.14901 - 11.9220 \times 10^{-4} \cdot (T/K) + 17.3468 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range  $328.15-418.15 K$  (Cox eq., Chao et al. 1983)

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

$\log(P/kPa) = 5.19014 - 1325.209/(139.781 + t/^{\circ}C)$ ; temp range  $111-145^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2.036 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.3968 - 2080.3/(200.8 + t/^{\circ}C)$ ; temp range  $20-150^{\circ}C$  (Antoine eq., Dean 1992)

$\log(P/mmHg) = 7.0460 - 1841/(180 + t/^{\circ}C)$ ; temp range  $150-310^{\circ}C$  (Antoine eq., Dean 1985, 1992)

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

$\log(P_g/kPa) = 11.290 - 3047.828/(T/K)$ ; temp range  $333-368 K$  (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 8.45107 - 2512.509/(-89.765 + T/\text{K})$ ; temp range 384–418 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.18084 - 1320.21/(-133.876 + T/\text{K})$ ; temp range 384–418 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -6.9795 - 2.9488 \times 10^3/(T/\text{K}) + 7.4483 \cdot \log (T/\text{K}) - 1.15821 \times 10^{-2} \cdot (T/\text{K}) + 4.3391 \times 10^{-6} (T/\text{K})^2$ ; temp range 383–777 K (vapor pressure eq., Yaws 1994)

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

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

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

4.313 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.31 (Hansch & Leo 1979)

4.38 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)

4.31 (recommended, Sangster 1989, 1993)

4.31 (recommended, Hansch et al. 1995)

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

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

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

Volatilization:

Photolysis: rate constant in distilled water  $k = 0.045 \text{ h}^{-1}$  with  $t_{1/2} = 15.5 \text{ h}$  (Fukuda 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 original reference:

$k_{OH} = (6.65 \pm 0.35) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $(298 \pm 2) \text{ K}$  with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  (relative rate method, Phouongphouang & Arey 2002)

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: a calculated tropospheric lifetime to be 1.9–2.4 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  for the reaction with OH radical (Phouongphouang & Arey 2002).

Surface water:

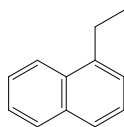
Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes (quoted, Meador et al. 1995)

## 4.1.1.10 1-Ethynaphthalene



Common Name: 1-Ethynaphthalene

Synonym:  $\alpha$ -ethynaphthalene

Chemical Name: 1-ethynaphthalene

CAS Registry No: 1127-76-0

Molecular Formula:  $C_{12}H_{12}$

Molecular Weight: 156.223

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

−13.9 (Lide 2003)

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

258.6 (Lide 2003)

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

1.00816, 1.00446 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

1.0082 (Weast 1982–83; Lide 2003)

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

155.0 ( $20^{\circ}C$ , calculated-density)

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

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

67.42, 46.92 ( $25^{\circ}C$ , bp, Dreisbach 1955)

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

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

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

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

10.7 (shake flask-fluorescence, Mackay & Shiu 1977)

10.0\* (shake flask-fluorescence, Schwarz & Wasik 1977)

10.0\* (shake flask-fluorescence, Schwarz 1977)

11.58 (generator column-HPLC, Wasik et al. 1981)

10.31 (average lit. value, 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):

133.3\* ( $70.0^{\circ}C$ , summary of literature data, temp range  $70.0$ – $258.1^{\circ}C$ , Stull 1947)

3.0 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.9599 - 1791.4/(180.5 + t/^{\circ}C)$ ; temp range  $145$ – $310^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

2.51\* (extrapolated from liquid state, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.03159 - 1841.320/(185.28 + t/^{\circ}C)$ ; temp range  $120$ – $292^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/atm) = [1 - 531.480/(T/K)] \times 10^{0.923623 - 6.97505 \times 10^{-4} \cdot (T/K) + 5.07450 \times 10^{-7} \cdot (T/K)^2}$ ; temp range  $393.15$ – $565.45$  K (Cox eq., Chao et al. 1983)

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

$\log(P_L/kPa) = 6.15645 - 1841.32/(-87.87 + T/K)$ ; temp range  $393$ – $565$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.5650 - 3.7597 \times 10^3/(T/K) + 2.6035 \cdot \log(T/K) - 1.1581 \times 10^{-2} \cdot (T/K) + 5.1365 \times 10^{-6} \cdot (T/K)^2$ ; temp range  $259$ – $776$  K (vapor pressure eq., Yaws 1994)

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

- 14.8 (calculated-P/C, Eastcott et al. 1988)
- 36.7 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 69.4 (gas stripping-GC, Altschuh et al. 1999)

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

- 4.39 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)
- 4.38 (calculated-fragment const., Yalkowsky et al. 1983)
- 4.42 (calculated-solvatochromic parameters and  $V_{\text{I}}$ , Kamlet et al. 1988)
- 4.40 (recommended, Sangster 1989, 1994)
- 4.44 (calculated-molar volume, Wang et al. 1992)
- 4.8016 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 4.39 (recommended, Hansch et al. 1995)

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

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

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

- 3.77 (sediment, HPLC- $k'$  correlation, Vowles & Mantoura 1987)
- 3.89 (HPLC-capacity factor correlation, Hodson & Williams 1988)
- 3.78 (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,  $k_{\text{OH}}$  for reaction with OH radical,  $k_{\text{NO}_3}$  with  $\text{NO}_3$  radical and  $k_{\text{O}_3}$  with  $\text{O}_3$ , or as indicated \*data at other temperatures see original reference:

$k_{\text{OH}} = (3.64 \pm 0.41) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $(298 \pm 2)\text{K}$  with a calculated tropospheric lifetime to be 3.8 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: a calculated tropospheric lifetime to be 3.8 h using a global tropospheric 12-h daytime average OH radical concentration of  $2.0 \times 10^6 \text{ molecule cm}^{-3}$  for the reaction with OH radical (Phouongphouang & Arey 2002).

Surface water:

Groundwater:

Sediment:

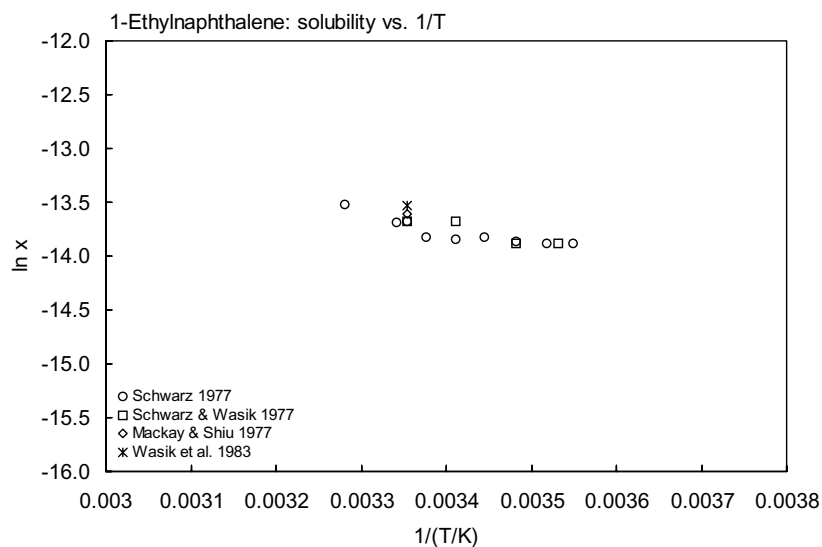
Soil:

Biota: elimination  $t_{1/2} = 2 \text{ d}$  from Oyster for naphthalenes (quoted, Meador et al. 1995).

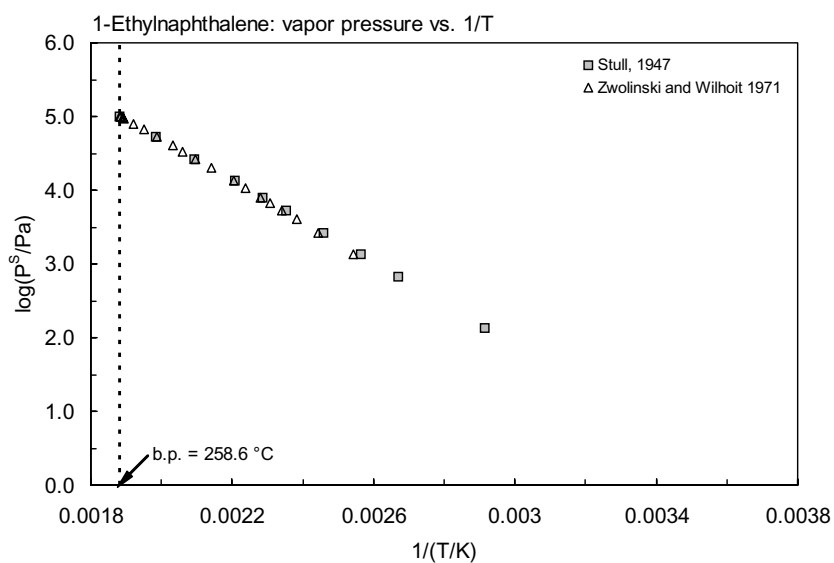
TABLE 4.1.1.10.1

Reported aqueous solubilities and vapor pressures of 1-ethylnaphthalene at various temperatures

Aqueous solubility				Vapor pressure			
Schwarz 1977		Schwarz & Wasik 1977		Stull 1947		Zwolinski & Wilhoit 1971	
shake flask-fluorescence		shake flask-fluorescence		summary of literature data		selected values	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	P/Pa
8.6	8.124	10	8.1	70.0	133.3	120.0	1333
11.1	8.124	14	8.1	101.4	666.6	136.04	2666
14.0	8.28	20	10	116.8	1333	146.22	4000
17.1	8.593	25	10	133.8	2666	153.85	5333
20.0	8.436			152.0	5333	160.01	6666
23.0	8.593			164.1	7999	165.22	7999
25.0	10.0			180.0	13332	173.76	10666
26.1	9.842			204.6	26664	180.67	13332
31.7	11.72			230.8	53329	193.94	19998
				258.1	101325	203.96	26664
						212.10	33331
				mp/°C	-27	219.01	39997
						230.41	53329
						239.71	66661
						247.62	79993
						254.54	93326
						255.83	95992
						257.09	98659
						258.94	101325
						log P = A - B/(C + t/°C)	
						P/mmHg	
						A	7.03159
						B	1841.320
						C	185.28
						bp/°C	258.33
						$\Delta H_v$ /(kJ mol <sup>-1</sup> ) =	
						at 25°C	—
						at bp	48.1



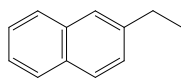
**FIGURE 4.1.1.10.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-ethylnaphthalene.



**FIGURE 4.1.1.10.2** Logarithm of vapor pressure versus reciprocal temperature for 1-ethylnaphthalene.



## 4.1.1.11 2-Ethyl-naphthalene



Common Name: 2-Ethyl-naphthalene

Synonym:  $\beta$ -ethyl-naphthalene

Chemical Name: 2-ethyl-naphthalene

CAS Registry No: 939-27-5

Molecular Formula:  $C_{12}H_{12}$

Molecular Weight: 156.223

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

−7.4 (Lide 2003)

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

258 (Lide 2003)

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

0.9922 (Weast 1982–83; Lide 2003)

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

157.4 ( $20^{\circ}C$ , calculated from density)

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

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

66.99, 47.33 ( $25^{\circ}$ , bp, Dreisbach 1955)

64.7 (Lei et al. 2002)

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

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

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

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

7.97 (shake flask-GC, Eganhouse & Calder 1976)

7.97 (average lit. 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):

3.76 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 8.0819 - 1886.0/(191.0 + t/^{\circ}C)$ ; temp range 145–300 $^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

3.24\* (extrapolated from liq. state, Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981)

$\log(P/mmHg) = 7.07566 - 1880.73/(191.41 + t/^{\circ}C)$ ; temp range 119.14–291.9 $^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

4.21\* (extrapolated exptl. data, Macknick & Prausnitz 1979; quoted, Mackay & Shiu 1981)

$\log(P/mmHg) = 21.485 - 7435.9/(T/K)$ ; temp range 13.05–45.1 $^{\circ}C$  (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)

$\log(P/atm) = [1 - 531.189/(T/K)] \times 10^{\{0.871612 - 5.23140 \times 10^{-4} \cdot (T/K) + 3.70623 \times 10^{-7} \cdot (T/K)^2\}}$ ; temp range 286.2–565.05 K (Cox eq., Chao et al. 1983)

4.21 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.46683 - 3232.791/(T/K)$ ; temp range 286–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.20056 - 1880.73/(-82.74 + T/K)$ ; temp range 393–565 K (Antoine eq.-II, Stephenson & Malanowski 1987)

3.71\* (pressure gauge in vacuum cell, interpolated-Antoine eq. derived from exptl. data, temp range, −4.65–125 $^{\circ}C$ , Sasse et al. 1988)

$\log(P_L/mmHg) = 6.83511 - 1799.779/(189.505 + t/^{\circ}C)$ ; temp range −4.65 to 125.09 $^{\circ}C$  (Antoine eq., pressure gauge, Sasse et al. 1988)

$\log(P/kPa) = 7.46683 - 3232.79/(T/K)$ ; temp range 5–50 $^{\circ}C$  (regression eq. from literature data, Shiu & Ma 2000)

2.56; 0.633 (supercooled liquid  $P_L$ ; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -3381/(T/K) + 11.75$ ;  $\Delta H_{vap} = -64.7\ kJ \cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

- 82.2 (calculated-P/C, Mackay & Shiu 1981)  
 63.2 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 54.5 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

- 4.377 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)  
 4.43 (HPLC-k' correlation, Vowles & Mantoura 1987)  
 4.38 (recommended, Sangster 1989, 1994)  
 4.38 (recommended, Hansch et al. 1995)  
 4.00 (HPLC-k' correlation, Ritter et al. 1995)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K<sub>OC</sub>:

- 3.76 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)  
 3.76 (calculated-MCI <sup>1</sup>χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Volatilization:

Photolysis: k = 0.038 h<sup>-1</sup> in distilled water with t<sub>1/2</sub> = 18.4 h (Fukuda et al. 1988).

Hydrolysis:

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

k<sub>OH</sub> = (4.02 ± 0.55) × 10<sup>-11</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at (298 ± 2) K with a calculated tropospheric lifetime to be 3.5 h using a global tropospheric 12-h daytime average OH radical concentration of 2.0 × 10<sup>6</sup> molecule cm<sup>-3</sup> (relative rate method, Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: t<sub>1/2</sub> = 18.4 h in distilled water (Fukuda et al. 1988).

Groundwater:

Sediment:

Soil:

Biota: elimination t<sub>1/2</sub> = 2 d from Oyster for naphthalenes (quoted, Meador et al. 1995).

**TABLE 4.1.1.11.1**

**Reported vapor pressures of 2-ethylnaphthalene at various temperatures and the coefficients for the vapor pressure equations**

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<b>Zwolinski &amp; Wilhoit 1971</b>	<b>Macknick &amp; Prausnitz 1979</b>	<b>Sasse et al. 1988</b>	
<b>selected values</b>	<b>gas saturation</b>	<b>electronic manometer</b>	
<b>t/°C</b>	<b>P/Pa</b>	<b>t/°C</b>	<b>P/Pa</b>
119.14	1333	13.05	1.533
135.28	2666	17.90	2.213

TABLE 4.1.1.11.1 (Continued)

Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979		Sasse et al. 1988	
selected values		gas saturation		electronic manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
145.52	4000	22.90	3.40	10.17	0.880
153.19	5333	29.50	6.213	20.08	2.426
159.38	6666	34.85	9.799	20.16	2.40
164.61	7999	39.40	13.16	30.11	6.05
173.19	10666	45.10	20.0	40.01	13.33
180.13	13332			49.93	27.33
193.45	19998	eq. 1a	P/mmHg	59.92	54.26
203.49	26664	A	21.485	69.96	103.6
211.65	33331	B	7435.9	79.98	187.9
218.57	39997			90.01	326.8
230.00	53329			100.08	551.8
239.31	66661			110.08	898.1
247.22	79993			120.02	1420
254.15	93326			125.09	1771
255.44	94659				
255.83	95992			eq. 2	P/mmHg
256.70	98659			A	6.83541
257.32	99992			B	1799.779
257.93	101325			C	189.505
eq. 2	P/mmHg				
A	7.07566				
B	1880.73				
C	191.41				
bp/°C	257.93				
$\Delta H_v/(\text{kJ mol}^{-1}) = 48.1$					
at bp					

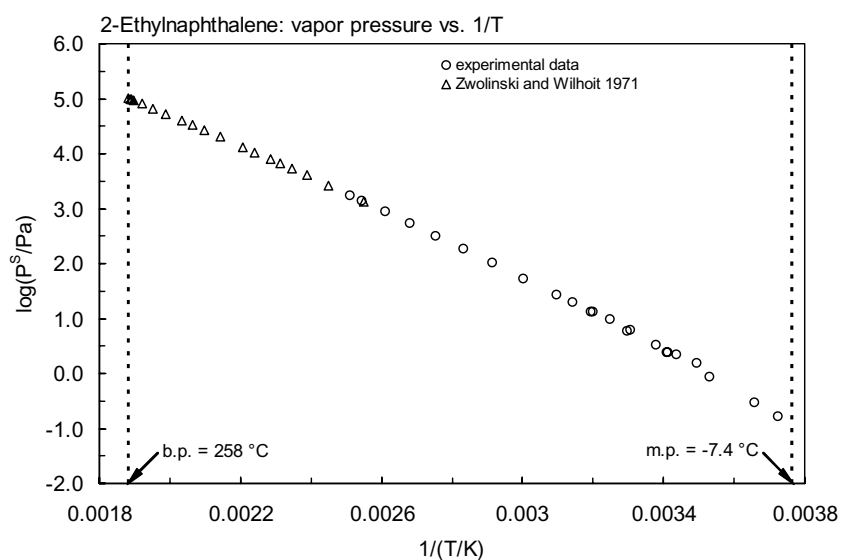
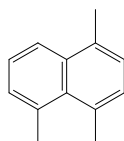


FIGURE 4.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for 2-ethylnaphthalene.

## 4.1.1.12 1,4,5-Trimethylnaphthalene



Common Name: 1,4,5-Trimethylnaphthalene

Synonym:

Chemical Name: 1,4,5-trimethylnaphthalene

CAS Registry No: 2131-41-1

Molecular Formula:  $C_{13}H_{14}$

Molecular Weight: 170.250

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

63 (Lide 2003)

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

285 (Zwolinski & Wilhoit 1971)

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

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

169.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ , F: 0.424 (mp at  $63^{\circ}C$ ))

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

2.10 (shake flask-fluorescence, Mackay & Shiu 1977)

2.04 (average lit. value, Pearlman et al. 1984)

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

0.681 (supercooled liquid  $P_L$ , Chao et al. 1983)

$\log(P_L/atm) = [1 - 558.187/(T/K)] \times 10^4 \{0.998467 - 7.03095 \times 10^{-4} \cdot (T/K) + 1.71801 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range 415.15–558.15 K (Cox eq., Chao et al. 1983)

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

23.50 (calculated-P/C, Eastcott et al. 1988)

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

4.90 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)

4.79 (calculated-solubility and mp, Mackay et al. 1980)

4.94 (calculated-solvatochromic parameters and intrinsic molar volume  $V_I$ , Kamlet et al. 1988)

$5.10 \pm 0.50$  (recommended, Sangster 1989)

4.91 (calculated-molar volume, Wang et al. 1992)

5.6829 (calculated-UNIFAC group contribution, Chen et al. 1993)

4.79 (recommended, Sangster 1993)

4.90 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

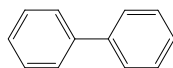
Sorption Partition Coefficient,  $\log K_{OC}$ :

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

Half-Lives in the Environment:

Biota: elimination  $t_{1/2} = 2$  d from Oyster for naphthalenes (quoted, Meador et al. 1995).

## 4.1.1.13 Biphenyl



Common Name: Biphenyl

Synonym: diphenyl, phenylbenzene

Chemical Name: biphenyl

CAS Registry No: 92-52-4

Molecular Formula:  $C_{12}H_{10}$

Molecular Weight: 154.207

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

68.93 (Lide 2003)

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

256.1 (Lide 2003)

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

0.866 (Weast 1982–1983)

1.04 (Lide 2003)

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

148.3 ( $20^{\circ}C$ , calculated-density)

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

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

18.58 (Parks & Huffman 1931)

18.66 (exptl., Chickos et al. 1999)

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

51.05 (Miller et al. 1984)

54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.371 (mp at  $68.93^{\circ}C$ )

0.35 (Mackay et al. 1980, 1983; Shiu & Mackay 1986; Shiu et al. 1987)

0.381 (calculated,  $\Delta S_{fus} = 54\ J/mol\ K$ , Passivirta et al. 1999)

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):

5.94 (shake flask-UV, Andrews & Keefer 1949)

7.48\* (shake flask-UV, measured range  $0.4$ – $42.8^{\circ}C$ , Bohon & Claussen 1951)

3.87 (shake flask-UV, Sahyun 1966)

7.08\* (shake flask-UV, measured range  $0$ – $64.5^{\circ}C$ , Wauchope & Getzen 1972)

$R \cdot \ln x = -4520/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 298.15]^2 - 20.8 + 0.0273 \cdot (T/K)$ , temp range  $24.6$ – $73.4^{\circ}C$   
(shake flask-UV measurements, Wauchope & Getzen 1972)

7.45 (shake flask-GC, Eganhouse & Calder 1976)

7.0 (shake flask-fluorescence, Mackay & Shiu 1977)

8.50 (shake flask-nephelometry, Hollifield 1979)

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

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

6.71 (generator column-GC/ECD, Miller et al. 1984, 1985; quoted, Hawker 1989b)

7.09 (recommended, Pearlman et al. 1984)

7.05 (vapor saturation-UV, Akiyoshi et al. 1987)

6.5 ( $29^{\circ}C$ , shake flask-GC/FID; Stucki & Alexander 1987)

7.20, 7.55 (generator column-HPLC/UV, Billington et al. 1988)

10.67 (calculated average of HPLC-RI, Brodsky & Ballschmiter 1988)

7.2\* (recommended, IUPAC Solubility Data Series, Shaw 1989)

$\log [S_L/(mol/L)] = 1.872 - 973.4/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$\ln x = -1.5792 - 3669.26/(T/K)$ , temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

5.37, 5.32 (generator column-GC/ECD, different flow rates, Oleszek-Kudlak et al. 2004)

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

- 7933\* (162.5°C, isoteniscope-manometer, measured range 162.5–255.2°C, Chipman & Peltier 1929)  
 104\* (69.20°C, temp range 69.20–271.2°C, Cunningham 1930; quoted, Boublik et al. 1984)  
 133.3\* (70.6°C, summary of literature data, temp range 70.6–254.0°C, Stull 1947)  
 1.30 (effusion method, Bright 1951)  
 $\log(P/\text{mmHg}) = 10.38 - 3799/(T/K)$ ; temp range 4.0–34.5°C (Antoine eq., effusion, Bright 1951)  
 0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)  
 1.273\* (effusion method, Bradley & Cleasby 1953; selected, Bidleman 1984; Neely 1983; Erickson 1986)  
 $\log(P/\text{cmHg}) = 11.282 - 4263/(T/K)$ ; temp range 15.05–40.55°C (Antoine eq., Bradley & Cleasby 1953)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 12910.0/(T/K)] + 8.218583$ ; temp range 70.6–254.9°C (Antoine eq., Weast 1972–73)  
 7.60 (selected  $P_L$ , Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1982; Bopp 1983)  
 1.41\* (effusion method, interpolated-Antoine eq., measured range 24.9–50.33°C, Radchenko & Kitiagorodskii 1974; selected, Bidleman 1984)  
 $\log(P/\text{mmHg}) = 12.6789 - 4367.436/(T/K)$ ; temp range 24.9–50.33°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)  
 16.0\* (53.05°C, gas saturation-GC, measured range 53.05–81.05°C, Sharma & Palmer 1974)  
 2040\* (123.0°C, pressure transducer, measured range 123.0–327.55°C, Nasir et al. 1980)  
 1.40 (HPLC-RT correlation, Swann et al. 1983)  
 $\log(P/\text{atm}) = [1 - 528.437/(T/K)] \times 10^4 \{0.821410 - 2.73337 \times 10^{-4} \cdot (T/K) + 1.02285 \times 10^{-7} \cdot (T/K)^2\}$ ; temp range: 342.35–673.15 K (Cox eq., Chao et al. 1983)  
 5.608 ( $P_L$  supercooled liquid converted from literature  $P_S$  with  $\Delta S_{\text{fus}}$ , Bidleman 1984)  
 3.35, 3.41 ( $P_{GC}$  by GC-RT correlation with octadecane as reference standard, different columns, BP-1 column, Apolane-87 column, Bidleman 1984)  
 $\log(P/\text{kPa}) = 6.36895 - 1997.558/(202.608 + t/^\circ\text{C})$ ; temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 1.19 ± 0.03; 1.03, 1.29, 0.579, 0.969 (gas saturation-GC; quoted lit. values Burkhard et al. 1984, 1985b)  
 1.15\* (24.7°C, gas saturation-GC/FID, measured range 5.2–24.7°C, Burkhard et al. 1984)  
 $\log(P/\text{Pa}) = 14.840 - 4402.1/(T/K)$ ; temp range 5.2–24.7°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)  
 0.423, 0.703, 0.594 (calculated-MW, GC-RI correlation, calculated-MCI  $\chi$ , Burkhard et al. 1985a)  
 2.03 (supercooled liquid  $P_L$ , GC-RI correlation, Burkhard et al. 1985b)  
 $\log(P/\text{mmHg}) = 7.24541 - 1998.725/(202.733 + t/^\circ\text{C})$ ; temp range 69–271°C (Antoine eq., Dean 1985, 1992)  
 5.61; 6.62 (supercooled liquid  $P_L$ , quoted lit.; GC-RT correlation, Foreman & Bidleman 1985)  
 2.43; 6.90 (selected  $P_S$ ; supercooled liq.  $P_L$ , Shiu & Mackay 1986; Shiu et al. 1987; Sklarew & Girvin 1987)  
 1.443; 1.23 ( $P_S$ , interpolated - Antoine equations; Stephenson & Malanowski 1987)  
 $\log(P_S/\text{kPa}) = 11.71929 - 4143.054/(T/K)$ ; temp range 297–324 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_S/\text{kPa}) = 28.5175 - 21141.5/(374.85 + T/K)$ ; temp range 283–342 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.37526 - 1794.8/(-74.85 + T/K)$ ; temp range 390–563 K (Antoine eq.-III, Stephenson & Malanowski 1987)  
 3.35 ( $P_{GC}$  by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)  
 $\log(P/\text{mmHg}) = 53.0479 - 5.3509 \times 10^3/(T/K) - 14.955 \cdot \log(T/K) + 2.1039 \times 10^{-9} \cdot (T/K) + 2.4345 \times 10^{-6} \cdot (T/K)^2$ ; temp range 342–789 K (vapor pressure eq., Yaws 1994)  
 0.422–2.54; 2.03–7.04 (quoted range of lit.  $P_S$  values; lit.  $P_L$  values, Delle Site 1997)  
 5.31; 2.02 (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_S$  with fugacity ratio  $F$ , Passivirta et al. 1999)  
 $\log(P_S/\text{Pa}) = 11.05 - 3201/(T/K)$  (solid, Passivirta et al. 1999)  
 $\log(P_L/\text{Pa}) = 8.20 - 2228/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $\log(P/\text{kPa}) = 14.840 - 4402.1/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)  
 3.63; 0.822 (supercooled liquid  $P_L$ , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)  
 $\log(P_L/\text{Pa}) = -3265/(T/K) + 11.51$ ;  $\Delta H_{\text{vap}} = -62.5 \text{ kJ} \cdot \text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at  $25^\circ\text{C}$  or as indicated and reported temperature dependence equations):

- 41.34 (gas stripping-GC, Mackay et al. 1979)
- 30.4 (gas stripping-GC, Mackay et al. 1980)
- 11.55 (gas stripping-GC, Warner et al. 1987)
- 19.57 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
- 86.5 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 31.20 (gas stripping-GC, Shiu & Mackay 1997)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 6.33 - 1255/(T/K)$  (Passivirta et al. 1999)

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

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

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^\circ\text{C}$  or as indicated:

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

Bioconcentration Factor,  $\log BCF$ :

- 2.64 (trout, calculated- $k_1/k_2$ , Neely et al. 1974)
- 3.12 (rainbow trout, Veith et al. 1979; Veith & Kosian 1983)
- 2.53 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 2.73, 2.45, 3.41 (algae, fish, activated sludge, Freitag et al. 1985; selected, Halfon & Reggiani 1986)

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

- 3.15 (soil, Kenaga 1980)  
 3.0, 3.27 (Aldrich humic acid, reversed phase separation, Landrum et al. 1984)  
 3.57, 3.77 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/L DOC: Landrum et al. 1984)  
 5.58, 4.04 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)  
 5.68, 5.34, 5.23, 3.57 (humic materials in natural water: Huron River 6.7% DOC spring, Grand River 10.7% DOC spring, Lake Michigan 4.7% DOC spring, Lake Erie 9.6% DOC spring, RP-HPLC separation method, Landrum et al. 1984)  
 3.52, 2.94 (Apison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium, Southworth & Keller 1986)  
 3.40 (calculated, soil, Chou & Griffin 1987)  
 3.04, 3.32, 3.26, 3.04, 3.08 (5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)  
 4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)  
 3.03, 3.12 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ , average values, Delle Site 2001)

Sorption Partition Coefficient, log  $K_p$ :

- 2.146 (lake sediment, calculated- $K_{OW}$ ,  $f_{OC}$ , Formica et al. 1988)

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

- Volatilization/Evaporation:  $t_{1/2} = 7.52$  d evaporation from water depth of 1 m (Mackay & Leinonen 1975), rate of volatilization  $k = 0.92$  g  $m^{-2}$   $h^{-1}$  (Metcalf et al. 1988)  
 Photolysis:  $k = 5.1 \times 10^{-4}$   $h^{-1}$  to  $7.4 \times 10^{-3}$   $h^{-1}$  with  $H_2O_2$  under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988);  
 photodegradation  $k = 5.1 \times 10^{-4}$   $min^{-1}$  and  $t_{1/2} = 22.61$  h in methanol-water (3:7, v/v) with initial concentration of 16.2 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991).  
 Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with  $NO_3$  radical and  $k_{O_3}$  with  $O_3$  or as indicated, \*data at other temperatures see reference:  
 $k_{OH} = (8.06 \pm 0.77) \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  with an estimated lifetime of ~3 d, and  $k_{O_3} < 2.0 \times 10^{-19}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  at  $294 \pm 1$  K (relative rate method, Atkinson et al. 1984)  
 $k_{OH} = (8.5 \pm 0.8) \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  at 295 K (relative rate method, Atkinson & Aschmann 1985)  
 $k_{OH} = (7 \pm 2) \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  at 298 K (recommended, Atkinson 1985)  
 $k_{OH}(calc) = 7.9 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$ ,  $k_{OH}(obs.) = (5.8 - 8.2) \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)  
 $k_{OH}(calc) = 7.1 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$ ,  $k_{OH}(obs.) = 7.0 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  (SAR structure-activity relationship, Atkinson 1987b)  
 $k_{O_3} < 2 \times 10^{-19}$   $cm^3$  molecule $^{-1}$   $s^{-1}$ ;  $k_{OH} = 7.0 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$ ;  $k_{N_2O_5} < 2.0 \times 10^{-19}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  for reaction with  $N_2O_5$  at room temp. (Atkinson & Aschmann 1988)  
 $k_{OH}^* = 7.2 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  at 298 K (recommended, Atkinson 1989)  
 $k_{OH}(calc) = 6.44 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  (molecular orbital calculations, Klamt 1993)  
 $k_{OH}(exptl) = 7.2 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$ ,  $k_{OH}(calc) = 6.7 \times 10^{-12}$   $cm^3$  molecule $^{-1}$   $s^{-1}$  with a calculated tropospheric lifetime of 2.0 d (Kwok et al. 1995)

## Hydrolysis:

- Biodegradation: 100% degraded by activated sludge in 47 h cycle (Monsanto Co. 1972);  
 $k = 109$   $yr^{-1}$  in the water column and  $k = 1090$   $yr^{-1}$  in the sediment, microbial degradation pseudo first-order rate constant (Wong & Kaiser 1975; selected, Neely 1981);  
 $k = 9.3-9.8$   $nmol$   $L^{-1}$   $d^{-1}$  with an initial biphenyl concentration of 4.4-4.7  $\mu mol/L$ , and  $k = 3.2$   $nmol$   $L^{-1}$   $d^{-1}$  with initial concentration of 2.9  $\mu mol/L$ , rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)  
 $t_{1/2} = 1.5$  d, estimated by using water die-away test (Bailey et al. 1983)  
 $t_{1/2}(aq. aerobic) = 36-168$  h, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)  
 $t_{1/2}(aq. anaerobic) = 144-672$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)



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

#### Biotransformation

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

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

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

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

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

#### Half-Lives in the Environment:

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

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

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

$t_{1/2} = 7.8\text{--}110 \text{ h}$ , based on photooxidation half-life in air (Howard et al. 1991);

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

Surface water:  $t_{1/2} \sim 1.5 \text{ d}$  in river water (Bailey et al. 1983);

$t_{1/2} = 36\text{--}168 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

photolysis  $t_{1/2} = 19.18 \text{ min}$  in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:  $t_{1/2} = 72\text{--}336 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil:  $t_{1/2} = 36\text{--}168 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota: estimated  $t_{1/2} = 29 \text{ h}$  from fish in simulated ecosystem (Neely 1980).

**TABLE 4.1.1.13.1**

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

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
			experimental		smoothed		
0.40	2.83	24.6	7.13	0	2.64	0	2.72
2.4	2.97	24.6	7.29	24.6	6.96	10	4.1
5.2	3.38	24.6	7.35	25	7.08	20	6.3
7.6	3.64	29.9	8.77	29.9	8.73	25	7.2
10	4.06	29.9	8.64	30.3	8.88	30	9.1
12.6	4.58	29.9	8.95	38.4	12.7	40	14.4
14.9	5.11	30.3	8.55	40.1	13.8	50	22
15.9	5.27	30.3	8.54	47.5	19.5	69	37
25	7.48	30.3	8.48	50	22.0		
25.6	7.78	38.4	13.2	50.1	22.1		
30.1	9.64	38.4	13.3	50.2	22.2		
30.4	9.58	38.4	13.5	54.7	27.7		
33.3	11.0	40.1	13.1	59.2	34.8		
34.9	11.9	40.1	13.4	60.5	37.2		
36	12.5	40.1	13.4	64.5	45.9		
42.8	17.2	47.5	18.8				

(Continued)

TABLE 4.1.1.13.1 (Continued)

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
for supercooled liquid:		47.5	19.0	temp dependence eq. 1			
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$		47.5	18.7	$\ln x$	mole fraction		
at 275 K	7.03	50.1	20.6	$\Delta H_{\text{fus}}$	$18.9 \pm 0.50$		
280 K	10.13	50.1	21.6	$10^2 \cdot b$	$2.73 \pm 0.12$		
285 K	11.25	50.1	21.8	c	$20.8 \pm 0.4$		
290 K	12.55	50.2	20.7				
295 K	13.43	50.2	21.8				
300 K	15.02	54.7	28.3				
305 K	18.58	54.7	28.8				
310 K	21.42	59.2	36.4				
315 K	21.09	59.2	36.3				
		59.2	36.0				
		60.5	40.4				
		64.5	43.7, 44.7				
		64.5	46.5				
		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.91$					

Empirical temperature dependence equations:

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

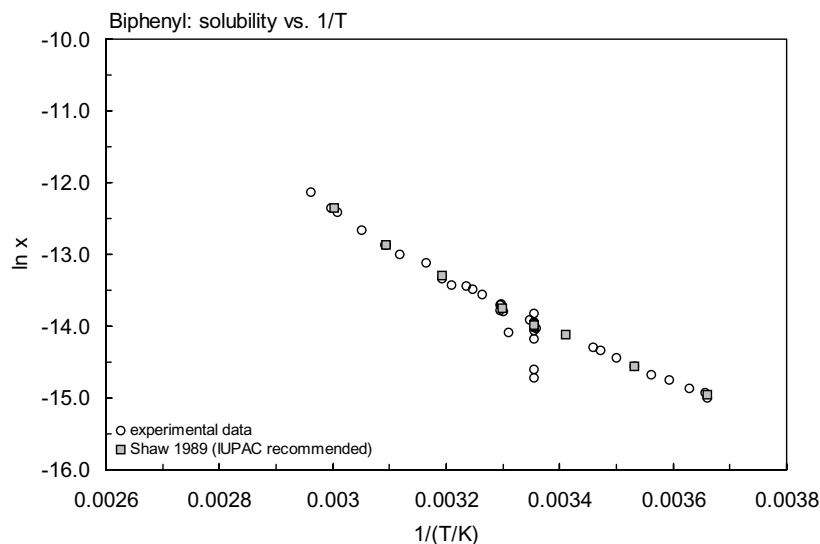


FIGURE 4.1.1.13.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for biphenyl.

TABLE 4.1.1.13.2

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

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K)^2 & (5) & & \end{aligned}$$

1.

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

2.

Radchenko & K. 1974		Nasir et al. 1980		Burkhard et al. 1984		Cunningham 1930	
Knudsen effusion		pressure transducer		gas saturation-GC		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.9	1.433	123.0	2040	5.2	0.106	69.20	104
31.75	2.976	143.81	4773	14.9	0.361	93.3	413
33.7	3.734	164.69	9962	24.7	1.15	148.7	4833
35.5	4.538	181.28	16447	eq. 1	P/Pa	160.0	7239
37.6	5.726	200.87	28599			171.1	10548
39.57	6.913	223.66	51518			182.2	15031
41.52	8.26	245.65	86254			193.3	21098

(Continued)

TABLE 4.1.1.13.2 (Continued)

2.

Radchenko & K. 1974		Nasir et al. 1980		Burkhard et al. 1984		Cunningham 1930	
Knudsen effusion		pressure transducer		gas saturation-GC		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.48	10.26	257.91	111343			204.4	28958
45.45	12.35	274.09	154493			215.6	39093
47.4	15.49	296.14	235345			226.7	51986
50.0	19.46	315.19	329300			237.8	68051
		327.55	400175			248.9	88252
eq. 1	P/mmHg					255.3	101353
A	12.6789	data fitted to Chebyshev polynomial				260.0	112384
B	4367.436					271.2	142032
for temp range 24.9–50°C							
Sharma & Palmer 1974						eq. 2	P/kPa
gas saturation-GC						A	6.36895
t/°C	P/Pa					B	1997.558
53.05	16.0					C	202.608
61.05	34.66					bp/°C	255.208
71.95	92.0						
81.05	220.0						

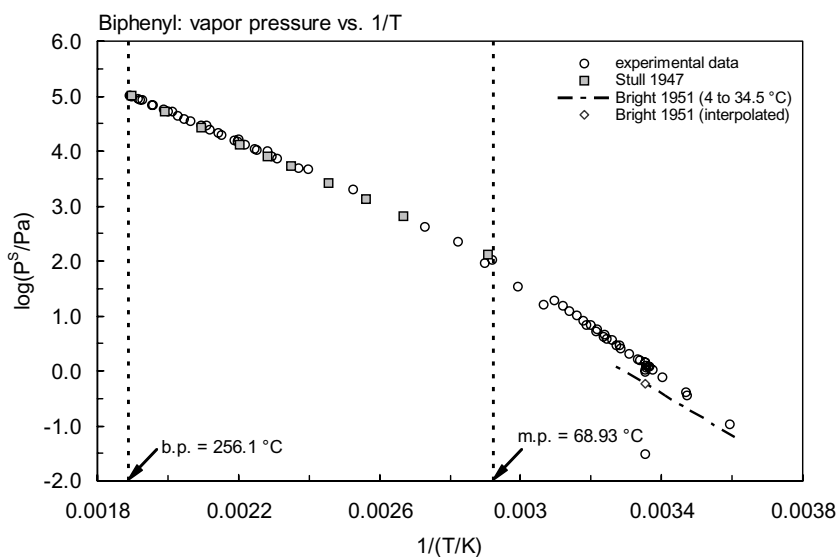
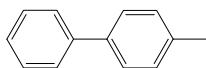


FIGURE 4.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for biphenyl.

**4.1.1.14 4-Methylbiphenyl**

Common Name: 4-Methylbiphenyl

Synonym: 4-phenyltoluene

Chemical Name: 4-methylbiphenyl

CAS Registry No: 644-08-6

Molecular Formula:  $C_{13}H_{12}$

Molecular Weight: 168.234

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

49.5 (Lide 2003)

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

267.5 (2003)

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

1.015 ( $27^{\circ}C$ , Weast 1982–83; Lide 2003)

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

165.7 ( $27^{\circ}C$ , calculated-density)

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

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.575 (mp at  $49.5^{\circ}C$ )

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

1.834, 4.05, 7.03 ( $4.9$ ,  $25$ ,  $40^{\circ}C$ , generator column-HPLC/GC, Doucette & Andren 1988a)

$S/(mol/L) = 9.18 \times 10^{-6} \exp(0.038 \cdot t/^{\circ}C)$  (generator column-GC/ECD, temp range  $4.9$ – $40^{\circ}C$ , Doucette & Andren 1988a); or

$\log x = -1436/(T/K) - 1.541$ ; temp. range  $4.9$ – $40^{\circ}C$  (generator column-GC/ECD, Doucette & Andren 1988a)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

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

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

4.63 (generator column-HPLC/GC, calculated-group contribution, TSA, Doucette & Andren 1987)

4.63 (recommended, Sangster 1989, 1994)

4.63 (recommended, Hansch et al. 1995)

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

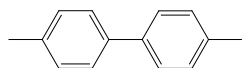
Bioconcentration Factor,  $\log BCF$ :

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

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

Half-Lives in the Environment:

## 4.1.1.15 4,4'-Dimethylbiphenyl



Common Name: 4,4'-Dimethylbiphenyl

Synonym: 4,4'-dimethyl-1,1'-biphenyl

Chemical Name: 4,4'-dimethylbiphenyl

CAS Registry No: 613-33-2

Molecular Formula:  $C_{14}H_{14}$

Molecular Weight: 182.261

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

125 (Weast 1982–83; Ruelle & Kesselring 1997; Lide 2003)

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

295 (Weast 1982–83; Lide 2003)

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

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

194.0 (Ruelle & Kesselring 1997)

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

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S = 56$  J/mol K), F: 0.104 (mp at  $125^{\circ}C$ )

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

0.0687, 0.175, 0.441 (4.9, 25,  $40^{\circ}C$ , generator column-GC, Doucette & Andren 1988a)

$S/(mol/L) = 2.90 \times 10^{-7} \exp(0.052 \cdot t/^{\circ}C)$  (generator column-GC/ECD, temp range  $4$ – $40^{\circ}C$ , Doucette & Andren 1988a)

$\log x = -1913/(T/K) - 1.288$ ; temp. range  $4.9$ – $40^{\circ}C$  (generator column-GC/ECD, Doucette & Andren 1988a)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

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

0.931 (calculated-P/C)

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

5.09 (generator column-GC/ECD, Doucette & Andren 1987)

5.09 (recommended, Sangster 1989, 1994)

5.09 (recommended, Hansch et al. 1995)

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

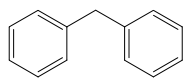
Bioconcentration Factor,  $\log BCF$ :

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

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

Half-Lives in the Environment:

## 4.1.1.16 Diphenylmethane



Common Name: Diphenylmethane

Synonym: diphenyl methane, 1,1'-methylenebis-benzene

Chemical Name: diphenylmethane

CAS Registry No: 101-81-5

Molecular Formula:  $C_{13}H_{12}$

Molecular Weight: 168.234

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

25.4 (Lide 2003)

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

265 (Lide 2003)

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

1.00592, 1.00192 ( $20^{\circ}C$ ,  $25^{\circ}C$ . Dreisbach 1955)

1.001 ( $26^{\circ}C$  Lide 2003)

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

168.1 ( $27^{\circ}C$ , from density, Stephenson & Malanowski 1987)

167.2 ( $20^{\circ}C$ , calculated-density)

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

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

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

64.02 (Bright 1951)

66.845, 45.34 ( $25^{\circ}C$ , bp, Dreisbach 1955)

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

18.28 (Dreisbach 1955)

18.58 (Parks & Huffman 1931; Chickos et al. 1999)

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

61.92 (Stephenson & Malanowski 1987)

62.34, 62.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K, F: 0.991 (mp at  $25.4^{\circ}C$ ))

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

14.10 (shake flask/UV, Andrews and Keefer 1949)

16.40 (Deno & Berkheimer 1960)

3.76 (Lu et al. 1978)

3.00 (shake flask-nephelometry, Hollifield 1979)

16.19 (lit. mean, 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):

133.3\* ( $76.0^{\circ}C$ , summary of literature data, temp range  $76.0$ – $264.5^{\circ}C$ , Stull 1947)

1.09 (effusion method, interpolated from reported Antoine eq., Bright 1951)

$\log(P/mmHg) = 9.12 - 3341/(T/K)$ ; temp range  $5.1$ – $26.5^{\circ}C$  (Antoine eq., effusion, Bright 1951)

2.266 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.16125 - 1944.42/(190.0 + t/^{\circ}C)$ ; temp range  $150$ – $310^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

3904\* ( $151.49^{\circ}C$ , static-differential pressure gauge, measured range  $151.49$ – $336.32^{\circ}C$ , Wiecezorek & Kobayashi 1980)

0.0452 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.94201 - 1668.355/(186.212 + t/^{\circ}C)$ ; temp range  $217.5$ – $282.2^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- 13100\* (457.95 K, vapor-liquid equilibrium, measured range 457.95–581.85 K, Klara et al. 1987)  
 0.052 (extrapolated-Antoine eq., Dean 1985, 1992)  
 $\log(P/\text{mmHg}) = 6.291 - 1261/(105 + t/^{\circ}\text{C})$ ; temp range 217–282°C (Antoine eq., Dean 1985, 1992)  
 0.0885 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 5.8765 - 1707.9/(-101.15 + T/\text{K})$ ; temp range 295–383 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log(P_L/\text{kPa}) = 6.28615 - 1944.42/(-83.15 + T/\text{K})$ ; temp range 423–583 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log(P/\text{mmHg}) = 50.8894 - 5.2749 \times 10^3/(T/\text{K}) - 14.246 \cdot \log(T/\text{K}) - 4.2994 \times 10^{-10} \cdot (T/\text{K}) + 2.4197 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
 temp range 298–768 K (vapor pressure eq., Yaws 1994)  
 1.456\* (22.25°C, transpiration-GC, measured range –0.95 to 22.25°C, Verevkin 1999)

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

0.931 (calculated-P/C, Mackay et al. 1992)

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

- 4.14 (Hansch & Leo 1979)  
 4.22 (HPLC-RT correlation, Burkhard et al. 1985)  
 4.33 (HPLC-RT correlation, Eadsforth 1986)  
 4.14 (recommended, Sangster 1989, 1994)  
 4.14 (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,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 4.1.1.16.1**

**Reported vapor pressures of diphenylmethane 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		Bright 1951		Wieczorek & Kobayashi 1980		Verevkin 1999	
summary of literature data		effusion method		static-differential pressure gauge		transpiration-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
76.0	133.3	Data presented in graph		151.49	3904	–0.95	0.07946
107.4	666.6			151.77	3929	5.15	0.1584
122.8	1333			158.06	4942	10.15	0.3261
138.8	2666	eq. 1	P/mmHg	164.06	6182	15.05	0.6196
157.8	5333	A	9.12	170.31	7799	18.65	0.9556
170.2	7999	B	3341	176.25	9487	22.25	1.456
186.3	13332	temp range 5.1–26.5°C		182.32	11487	eq. 1a	P/Pa
210.7	26664			189.57	14279		
237.5	53329			196.01	17435		
264.5	101325	ΔH <sub>subl</sub> /(kJ mol <sup>–1</sup> ) = 64.015		202.69	21342	B	10639



TABLE 4.1.1.16.1 (Continued)

Stull 1947		Bright 1951		Wieczorek & Kobayashi 1980		Verevkin 1999	
summary of literature data		effusion method		static-differential pressure gauge		transpiration-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
mp/°C	26.5			209.7	26436	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 88.48$	
				217.16	32381	at 284.3 K	
				225.99	41037	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 87.63$	
				232.67	58832	at 298.15 K	
				247.79	70500		
				255.23	83501	30.25	3.099
				263.79	100021	35.05	4.653
				264.36	100938	40.05	7.019
				272.29	119269	44.95	10.19
				280.24	137819	55.05	21.63
		581.85	250200	288.0	1377.37	60.05	30.55
				295.97	162025	65.15	47.05
		eq. 3	P/kPa	303.88	186511	70.15	67.41
		A	15.1413	311.45	218741	eq. 1a	P/Pa
		B	5078.0	320.63	253090	A	27.43
		C	53.89	336.32	298026	B	7981.2
fitted to Chebyshev Polynomial						$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 66.36$	
						at 323.3 K	
						$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 67.83$	
						at 298.15 K	

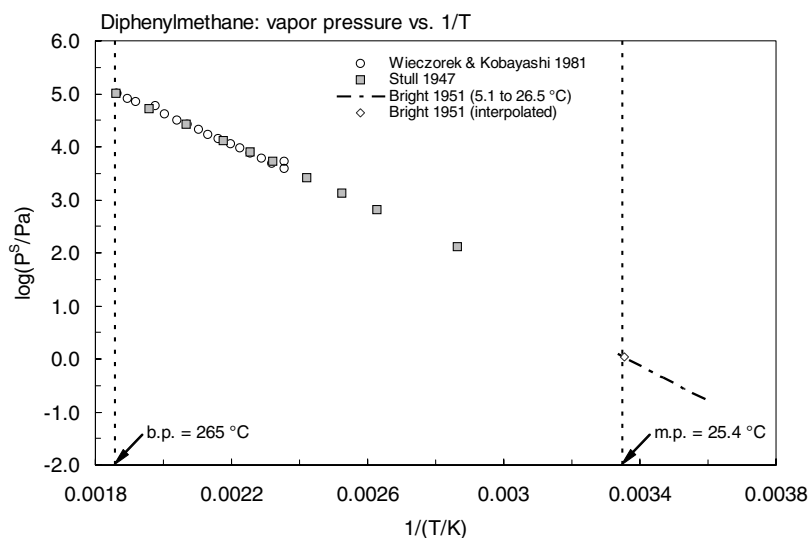
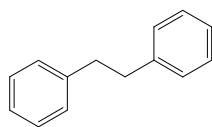


FIGURE 4.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for diphenylmethane.

## 4.1.1.17 Bibenzyl



Common Name: Bibenzyl

Synonym: 1,2-Diphenylethane, dibenzyl, 1,1'-(1,2-ethanediyl) bis-benzene

Chemical Name: 1,2-diphenylethane

CAS Registry No: 103-29-7

Molecular Formula:  $C_{14}H_{14}$

Molecular Weight: 182.261

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

52.5 (Lide 2003)

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

284 (Lide 2003)

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

0.9780 ( $25^{\circ}C$  Lide 2003)

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

190.2 ( $60^{\circ}C$ , calculated-density, Stephenson & Malanowski 1987)

186.4 ( $25^{\circ}C$ , calculated-density)

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

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

23.43 (Parks & Huffman 1931)

30.54 (Stephenson & Malanowski 1987)

22.73 (Chickos et al. 1999)

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

94.14 (Stephenson & Malanowski 1987)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S = 56\ J/mol\ K$ , F: 0.537 (mp at  $52.5^{\circ}C$ ))

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

4.37 (shake flask-UV, Andrews & Keefer 1950b)

4.37 (quoted, Pearlman et al. 1984)

1.89; 0.44 (generator column-HPLC/UV; HPLC-RT correlation, Swann et al. 1983)

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\* ( $86.8^{\circ}C$ , summary of literature data, temp range  $86.8$ – $284.0^{\circ}C$ , Stull 1947)

0.198 (effusion method, interpolated from reported Antoine eq., Bright 1951)

$\log(P/mmHg) = 9.86 - 3783/(T/K)$ ; temp range  $17.1$ – $44.2^{\circ}C$  (Antoine eq., effusion, Bright 1951)

17.1\* ( $60^{\circ}C$ , inclined piston, measured range  $60$ – $140^{\circ}C$ , Osborn & Scott 1980)

$\log(P/atm) = [1 - 547.288/(T/K)] \times 10^{\{0.914704 - 6.08831 \times 10^{-4} \cdot (T/K) + 5.11258 \times 10^{-7} \cdot (T/K)^2\}}$ ; temp range  $333.15$ – $413.15\ K$ , (Cox eq., Chao et al. 1983)

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

$\log(P_s/kPa) = 11.319 - 4386/(T/K)$ , temp range  $286$ – $308\ K$ , (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.93271 - 2636.21/(-22.009 + T/K)$ ; temp range  $369$ – $557\ K$  (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 48.5573 - 5.2841 \times 10^3/(T/K) - 13.41 \cdot \log(T/K) - 1.0073 \times 10^{-9} \cdot (T/K) + 2.1338 \times 10^{-6} \cdot (T/K)^2$ ; temp range  $324$ – $780\ K$  (vapor pressure eq., Yaws 1994)

0.734; 0.249 (supercooled liquid  $P_L$ , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -3522/(T/K) + 11.67$ ;  $\Delta H_{vap} = -67.4\ kJ \cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

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

- 4.79, 4.82 (Hansch & Leo 1979)
- 4.76 (quoted, HPLC- $k'$  correlation, Hammers et al. 1982)
- 3.67 (HPLC-RT correlation, Swann et al. 1983)
- 4.60 (HPLC-RT correlation, Webster et al. 1985)
- 4.71 (HPLC-RT correlation, Eadsworth 1986)
- $4.70 \pm 0.20$  (recommended, Sangster 1989)
- 4.79 (recommended, Sangster 1993)
- 4.79 (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,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 4.1.1.17.1**

**Reported vapor pressures of bibenzyl 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		Bright 1951		Osborn & Scott 1980	
summary of literature data		effusion method		inclined piston	
$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa
86.8	133.3	Data presented in graph		60	17.1
119.8	666.6			65	24.1
136.0	1333			70	34.0
153.7	2666			75	47.7
173.7	5333	eq. 1	P/mmHg	80	65.9
186.0	7999	A	9.56	85	89.7
202.8	13332	B	3783	90	121.2
227.8	26664	temp range 17.1–44.2°C		95	161.9
255.0	53329	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 72.38$		100	213.6
284.0	101325			105	280.1
				110	364.2
mp/°C	51.5			115	469.8
				120	602.4
				125	761.8
				130	961.1
				135	1202.7
				140	1498
data fitted to a 4-constant vapor pressure eq.					

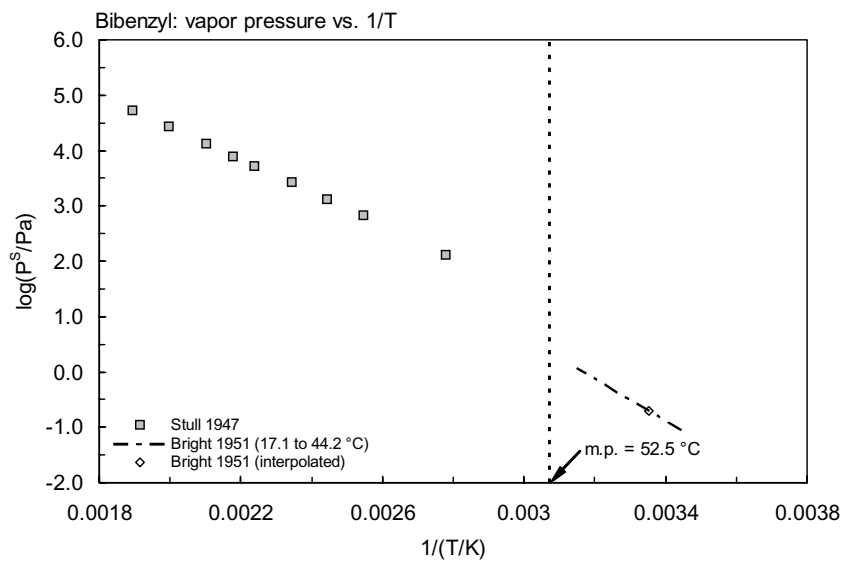
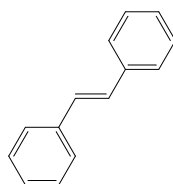


FIGURE 4.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for bibenzyl.

4.1.1.18 *trans*-Stilbene

Common Name: *trans*-1,2-Diphenylethene

Synonym: *trans*-stilbene, *trans*-diphenylethylene, E-stilbene

Chemical Name: *trans*-1,2-diphenylethene

CAS Registry No: 103-30-0

Molecular Formula: C<sub>14</sub>H<sub>12</sub>

Molecular Weight: 180.245

Melting Point (°C):

124.2 (Lide 2003)

Boiling Point (°C):

307 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.9707 (Weast 1982–83; Lide 2003)

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

185.0 (Ruelle & Kesselring 1997)

185.7 (20°C, calculated-density)

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

Enthalpy of Sublimation, ΔH<sub>subl</sub> (kJ/mol):

100.7 (Van Ekeren et al. 1983)

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

30.125 (Stephenson & Malanowski 1987)

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

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

76.73 (Stephenson & Malanowski 1987)

68.81, 69.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.106 (mp at 124.2°C)

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

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

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\* (113.2°C, summary of literature data, temp range 113.2–306.5°C, Stull 1947)

0.00764\* (manometer-spinning rotor friction gauge, torsion mass loss effusion, measured range 297.45–364.5 K, Van Ekeren et al. 1983)

0.0274 (34.65°C, effusion-quartz crystal microbalance, Offringa et al. 1983)

0.00647 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P<sub>s</sub>/kPa) = 12.25604 – 5201.358/(T/K); temp range 298–343 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log (P<sub>L</sub>/kPa) = 6.97928 – 2610.05/(–54.759 + T/K); temp range 419–580 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

log (P/mmHg) = 68.6303 – 6.3776 × 10<sup>3</sup>/(T/K) – 21.015 · log (T/K) + 5.7813 × 10<sup>–3</sup> · (T/K) + 1.8334 × 10<sup>–12</sup> · (T/K)<sup>2</sup>; temp range 397–820 K (vapor pressure eq., Yaws 1994)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

4.81 (Hansch & Leo 1979)

- 4.81 (recommended, Sangster 1989)  
 4.81 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor,  $\log BCF$ :

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

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

Half-Lives in the Environment:

**TABLE 4.1.1.18.1**

**Reported vapor pressures of *trans*-stilbene at various temperatures and the coefficients for the vapor pressure equations**

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

Stull 1947		Van Ekeren et al. 1983					
Summary of literature data		Spinning rotor fraction gauge		Torsion mass loss effusion		Static method	
t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa
113.2	133.3	24.3	0.00704	44.97	0.100	69.17	1.43
145.8	666.6	24.3	0.00699	50.78	0.200	69.45	1.44
161.0	1333	24.3	0.00715	54.27	0.300	71.25	1.83
179.8	2666	24.43	0.0693	56.80	0.400	71.52	1.80
199.0	5333	27.24	0.0102	60.43	0.600	72.2	1.94
211.5	7999	27.24	0.0104	64.14	0.900	73.70	2.25
227.4	13332	27.24	0.0105	65.11	1.00	74.18	2.39
251.7	26664	30.65	0.0151	69.45	1.44	75.73	2.81
287.3	53329	30.65	0.015	71.25	1.83	75.83	2.80
306.5	101325	32.03	0.0196	71.25	1.80	75.86	2.83
mp/ $^{\circ}C$	124	32.03	0.0195	72.2	1.94	77.15	3.10
		34.96	0.0287	73.7	2.25	78.27	3.55
		34.96	0.0288	74.18	2.39	8.06	4.34
		34.96	0.0289	75.73	2.81	80.39	4.39
		37.33	0.0386	75.86	2.83	81.79	5.07
		37.33	0.0387	76.88	3.10	83.36	5.84
		40.61	0.0584	78.27	3.55	85.04	6.86
		40.61	0.0585	80.79	4.39	86.35	7.71
		43.32	0.0792	81.79	5.07	86.38	7.74
		25	0.00765	83.36	5.84	86.51	7.90
				85.04	6.86	87.35	8.47
				86.35	7.71	89.74	10.57
				86.51	7.90	90.43	11.22
				87.35	8.47	91.35	12.20
				89.74	10.57		
				90.43	11.22		
				91.35	12.20		
				$\Delta H_{fus} = 100.17 \text{ kJ/mol}$			
				at 331.64 K			

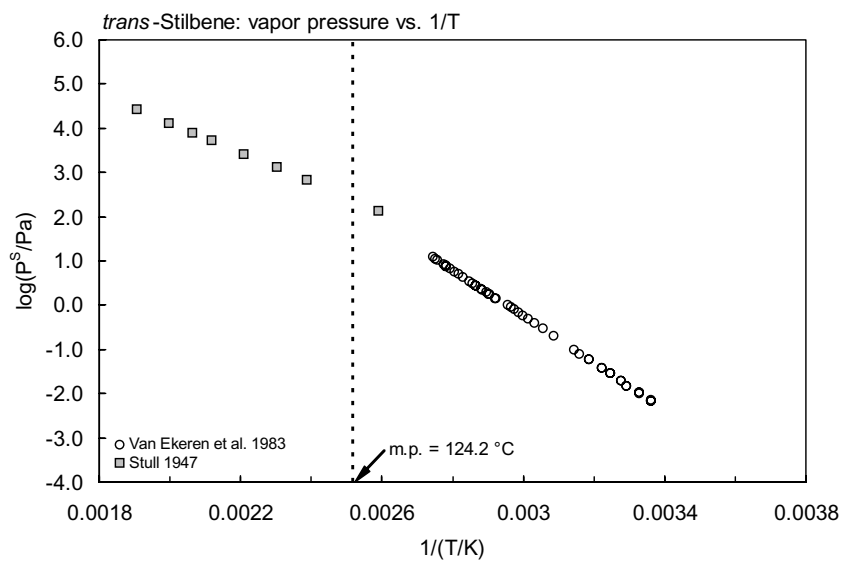
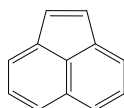


FIGURE 4.1.18.1 Logarithm of vapor pressure versus reciprocal temperature for *trans*-stilbene.

## 4.1.1.19 Acenaphthylene



Common Name: Acenaphthylene

Synonym:

Chemical Name: acenaphthylene

CAS Registry No: 208-96-8

Molecular Formula:  $C_{12}H_8$

Molecular Weight: 152.192

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

91.8 (Lide 2003)

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

280 (Lide 2003)

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

0.899 (Dean 1985)

0.8987 ( $17^{\circ}C$ , Lide 2003)

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

141.2 (Ruelle & Kesselring 1997)

167.1 ( $17^{\circ}C$ , calculated-density)

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

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

10.96 (Ruelle & Kesselring 1997)

1.4, 6.95, 10.96; 12.36 ( $-156.55$ ,  $88.45$ ,  $88.85^{\circ}C$ ; total phase change enthalpy, Chickos et al. 1999)

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

30.3 (Passivirta et al. 1999)

42.4, 37.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.221 (mp at  $91.8^{\circ}C$ )

0.458 (calculated,  $\Delta S_{fus} = 30.3\ J/mol\ K$ , Passivirta et al. 1999)

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

3.93 (misquoted from Mackay & Shiu 1977)

16.1 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

$\log [S_L/(mol/L)] = 1.315 - 573.5/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

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

0.893\* (gas saturation-HPLC/fluoro/UV, Sonnefeld et al. 1983)

$\log (P/Pa) = 12.768 - 3821.55/(T/K)$ ; temp range  $10-50^{\circ}C$  (Antoine eq., Sonnefeld et al. 1983)

0.893 (generator column-HPLC, Wasik et al. 1983)

1.105 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 9.500 - 3714/(T/K)$ ; temp range  $286-318\ K$  (Antoine eq., Stephenson & Malanowski 1987)

0.90 (selected, Mackay et al. 1992, 1996; quoted, Shiu & Mackay 1997)

0.90; 1.97 (quoted solid  $P_s$  from Mackay et al. 1992; converted to supercooled liquid  $P_L$  with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 11.11 - 3201/(T/K)$  (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.53 - 2751/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

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

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

11.40 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

12.7\* (gas stripping-GC, measured range  $4.1-31^{\circ}C$ , Bamford et al. 1999)



$\ln K_{AW} = -6278.6/(T/K) + 15.757$ ;  $\Delta H = 52.2 \text{ kJ mol}^{-1}$ ; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

$\log [H/(\text{Pa m}^3/\text{mol})] = 8.22 - 2178/(T/K)$  (Passivirta et al. 1999)

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

- 4.07 (calculated as per Leo et al. 1971)
- 3.94 (Yalkowsky & Valvani 1979)
- 3.72 (calculated-fragment const., Mabey et al. 1982)
- 4.08 (selected, Mills et al. 1982)
- 4.06 (calculated-molar refraction MR, Yoshida et al. 1983)
- 3.90 (calculated-MCI  $\chi$  as per Rekker & De Kort 1979, Ruepert et al. 1985)
- 3.55 (HPLC-RT correlation, Chin et al. 1986)
- 4.07–4.10; 4.08 (quoted lit. range; lit. mean, Meadors et al. 1995)
- 4.00; 3.67 (quoted lit.; calculated, Passivirta et al. 1999)

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

Bioconcentration Factor,  $\log BCF$ :

- 3.0 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al. 1982)
- 2.58 (Isnard & Lambert 1988)

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

- 3.83, 3.75 (soil, RP-HPLC correlation on CIHAC, on PIHAC, Szabo et al. 1990b)
- 4.91–5.21; 3.60–3.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 4.96; 5.05, 5.14, 5.45 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

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

Volatilization:

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

$t_{1/2} = 0.7 \text{ h}$  on silica gel,  $t_{1/2} = 2.2 \text{ h}$  on alumina and  $t_{1/2} = 44 \text{ h}$  on fly ash for different atmospheric particulate substrates determined in the rotary photoreactor (appr. 25  $\mu\text{g/g}$  on substrate) (Behymer & Hites 1985); direct photolysis  $t_{1/2} = 9.08 \text{ h}$  (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).

Photodegradation  $k = 3 \times 10^{-5} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 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 see reference:

$k = 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 5 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (calculated, Mabey et al. 1982)

$k_{O_3} \sim 5.50 \times 10^{-16} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ ,  $k_{OH} = (11.0 \pm 0.1) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$  and  $k_{NO_3} = (54 \pm 0.8) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$  at  $296 \pm 2 \text{ K}$  (relative rate methods, Atkinson & Aschmann 1988)

$k_{OH} = 11.0 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$  at  $296 \text{ K}$  (Atkinson 1989)

$k_{OH} = 12.4 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$  at  $296 \pm 2 \text{ K}$  with a atmospheric lifetime of 1.1 h assuming an average ambient 12-h daytime OH radical concn of  $2 \times 10^6 \text{ molecule/cm}^3$ ;  $k_{O_3} = 1.60 \times 10^{-16} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$  at  $296 \text{ K}$  with lifetime of 2.5 h assuming ambient  $O_3$  concn of  $7 \times 10^{11} \text{ molecule/cm}^3$  (relative rate method, Reisen & Arey 2002)

Hydrolysis: not hydrolyzable (Mabey et al. 1982; Howard et al. 1991).

Biodegradation: > 98% degradation within 7 d, based on domestic sewer for an average of three static-flask screening test (Tabak et al. 1981);

aerobic  $t_{1/2} = 1020\text{--}1440 \text{ h}$ , based on soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

anaerobic  $t_{1/2} = 4080\text{--}5760 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

## Half-Lives in the Environment:

Air:  $t_{1/2} = 0.191\text{--}1.27$  h, based on photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Atmospheric lifetime of 1.1 h and 2.5 h due to reaction with OH and O<sub>3</sub> at 296 K, respectively (Reisens & Arey 2002)

Surface water:  $t_{1/2} = 1020\text{--}1440$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Kincannon & Lin 1985; quoted, Howard et al. 1991).

Groundwater:  $t_{1/2} = 2040\text{--}2880$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 1020\text{--}1440$  h, based on soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);  
 $t_{1/2} > 50$  d (Ryan et al. 1988).

Biota: elimination  $t_{1/2} = 1$  d from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.19.1

Reported vapor pressures and Henry's law constants of acenaphthylene at various temperatures and the coefficients for the vapor pressure equations

Vapor pressure		Henry's law constant		
Sonnefeld et al. 1983		Bamford et al. 1999		
gas saturation-HPLC		gas stripping-GC/MS		
t/°C	P/Pa	t/°C	H/(Pa m³/mol)	H/(Pa m³/mol)
				average
11.20	0.206	4.1	1.98, 2.87	2.38
11.20	0.205	11.0	3.76, 4.86	4.27
11.20	0.216	18.0	6.67, 8.33	7.46
20.56	0.590	25.0	10.9, 14.6	12.7
20.56	0.585	31.0	16.2, 23.7	19.6
20.56	0.588			
30.40	1.50	ln K <sub>AW</sub> = A – B/(T/K)		
30.40	1.54	A	15.7566	
30.40	1.52	B	6278.6	
39.05	3.30			
39.05	3.41	enthalpy, entropy change:		
39.05	3.27	ΔH/(kJ·mol <sup>-1</sup> ) = 52.2 ± 3.3		
39.05	3.34	ΔS/(J·K <sup>-1</sup> mol <sup>-1</sup> ) = 131		
25.0	0.89	at 25°C		
log P/Pa = A – B/(T/K)				
A	12.768			
B	3821.55			

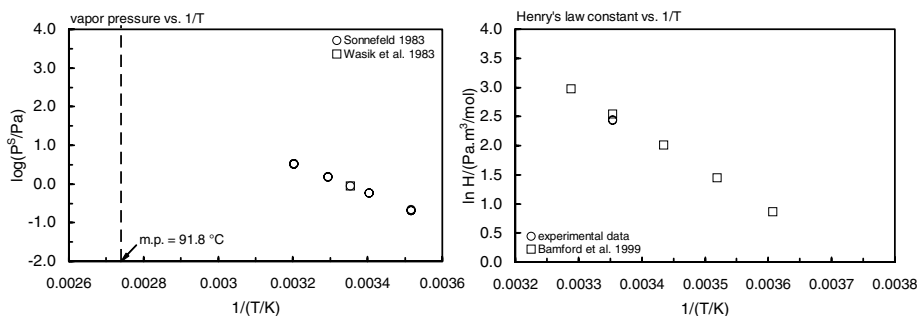
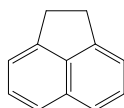


FIGURE 4.1.1.19.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for acenaphthylene.

## 4.1.1.20 Acenaphthene



Common Name: Acenaphthene

Synonym: 1,8-hydroacenaphthylene, ethylenenaphthalene, periethylenenaphthalene, 1,2-dihydro-acenaphthalene

Chemical Name: 1,8-hydroacenaphthylene

CAS Registry No: 83-32-9

Molecular Formula:  $C_{12}H_{10}$

Molecular Weight: 154.207

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

93.4 (Lide 2003)

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

279 (Weast 1982–82; Lide 2003)

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

1.069 ( $95^{\circ}C$ , Dean 1985)

1.222 (Lide 2003)

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

126.2 ( $20^{\circ}C$ , calculated-density)

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

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

84.68 (Radchenko & Kitiagorodskii 1974)

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

21.88 (differential calorimetry, Wauchope & Getzen 1972)

21.46 (calorimetry, Osborn & Douslin 1975; Chickos et al. 1999)

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

60.25 (Wauchope & Getzen 1972)

59.83 (Casellato et al. 1973)

56.90 (Ubbelohde 1978)

58.55, 41.09 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{\text{fus}} = 56\ J/mol\ K$ ), F: 0.213 (mp at  $93.4^{\circ}C$ )

0.197 (calculated, Passivirta et al. 1999)

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):

6.14 (Deno & Berkheimer 1960)

3.88\* (shake flask-UV, measured range  $0-74.7^{\circ}C$ , Wauchope & Getzen 1972)

$R \cdot \ln x = -5230/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 17.1 + 0.0186 \cdot (T/K)$ ; temp range  $22.2-73.4^{\circ}C$  (shake flask-UV measurements, Wauchope & Getzen 1972)

3.59 (shake flask-UV, Vesala 1974)

3.47 (shake flask-GC, Eganhouse & Calder 1976)

3.93 (shake flask-fluorescence, Mackay & Shiu 1977)

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

2.42 (shake flask-GC, Rossi & Thomas 1981)

4.47 (average lit. value, Pearlman et al. 1984)

4.16 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

3.8\* (recommended, IUPAC Solubility Data Series, Shaw 1989)

3.88 (shake flask-HPLC, Haines & Sandler 1995)

$\log [S_L/(mol/L)] = 2.505 - 1127/(T/K)$  (supercooled liquid  $S_L$ , Passivirta et al. 1999)

$\ln x = 0.684974 - 4541.77/(T/K)$ ; temp range  $5-50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

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

- 2560\* (147.2°C, static isoteniscope method, measured range 147.2–287.8°C, Mortimer & Murphy 1923)  
 $\log(P/\text{mmHg}) = 8.033 - 2835/(T/K)$ ; temp range 147.2–287.8°C (Antoine eq. static isoteniscope method, Mortimer & Murphy 1923)
- 666.6\* (114.8°C, summary of literature data, temp range 114.8–277.5°C, Stull 1947)
- 0.207 (Hoyer & Peperle 1958)  
 $\log(P/\text{mmHg}) = 11.50 - 4264/(T/K)$ ; temp range –15 to 30°C (Knudsen effusion method, Hoyer & Peperle 1958)
- 4.02 (extrapolated-Antoine eq., Weast 1972–73)  
 $\log(P/\text{mmHg}) = [-0.2185 \times 13078.5/(T/K)] + 8.069478$ ; temp range 114.8–277.5°C (Antoine eq., Weast 1972–73)
- 3.07 (extrapolated-Antoine eq., liquid state  $P_L$ , Boublik et al. 1973)
- 8.622\* (54.1°C, effusion method, measured range 54.1–83.45°C, Radchenko & Kitiagorodskii 1974)  
 $\log(P/\text{mmHg}) = 12.2930 - 4422.921/(T/K)$ ; temp range 54.10–83.15°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)
- 0.373\* (manometry-extrapolated, measured range 65–140°C, Osborn & Douslin 1975)
- 0.287\* (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)  
 $\log(P/\text{Pa}) = 14.669 - 4535.39/(T/K)$ ; temp range 10–50°C (Antoine eq., gas saturation, Sonnefeld et al. 1983)
- 0.287 (gas saturation/generator column-HPLC, Wasik et al. 1983)
- 3.03, 1.48 (extrapolated-Antoine eq., Boublik et al. 1984)  
 $\log(P_L/\text{kPa}) = 6.84571 - 2527.716/(244.912 + t/^\circ\text{C})$ ; temp range 147.2–287.8°C (Antoine eq. from reported exptl. data of Mortimer & Murphy 1923, Boublik et al. 1984)
- $\log(P_L/\text{kPa}) = 6.38504 - 2102.491/(203.124 + t/^\circ\text{C})$ ; temp range 95–140°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1966, Boublik et al. 1984)
- 3.07 (extrapolated from liquid state  $P_L$ , Dean 1985)  
 $\log(P/\text{mmHg}) = 7.72819 - 2534.234/(245.576 + t/^\circ\text{C})$ ; temp range 147–187°C (Antoine eq., Dean 1985, 1992)
- $\log(P/\text{mmHg}) = 8.033 - 2834.99/(T/K)$ ; temp range 147–288°C (Antoine eq., Dean 1985, 1992)
- 0.237, 0.319 (19.95°C, 26.85°C, gas saturation-GC, Sato al. 1986)
- 0.427\* (gas saturation, interpolated-Antoine eq., temp range 20–169°C, Sato al. 1986)  
 $\ln(P/\text{Pa}) = 22.9288 - 5183.86/(T/K - 80.153)$ ; temp range: 293.1–342 K (Antoine eq., gas saturation, Sato et al. 1986)
- 0.311 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P_S/\text{kPa}) = 10.883 - 4290.5/(T/K)$ ; temp range 290–311 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_S/\text{kPa}) = 9.4944 - 3248.008/(-48.055 + T/K)$ ; temp range 338–366 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.3519 - 2082.356/(-71.578 + T/K)$ ; temp range 368–413 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 7.30401 - 2975/(10.674 + T/K)$ ; temp range 388–552 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- 0.336, 0.211, 0.383; 0.287; 0.375; 0.377, 0.122, 0.306, 0.862 (quoted lit. values: effusion method; gas saturation-HPLC; calculated, Delle Site 1997)
- 0.30; 1.52 (quoted solid  $P_S$  from Mackay et al. 1992; converted to supercooled liquid  $P_L$  with fugacity ratio  $F$ , Passivirta et al. 1999)  
 $\log(P_S/\text{Pa}) = 11.20 - 3492/(T/K)$  (solid, Passivirta et al. 1999)  
 $\log(P_L/\text{Pa}) = 8.13 - 2367/(T/K)$  (supercooled liquid, Passivirta et al. 1999)
- $\log(P/\text{kPa}) = 10.883 - 4290.5/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 1.52; 0.428 (supercooled liquid  $P_L$ , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)  
 $\log(P_L/\text{Pa}) = -3337/(T/K) + 11.37$ ;  $\Delta H_v = -63.9 \text{ kJ}\cdot\text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

- 14.79 (gas stripping-GC, Mackay et al. 1979)
- 15.7 (gas stripping-GC, Mackay & Shiu 1981; Mackay et al. 1982)
- 24.42 (gas stripping-GC, Warner et al. 1987)

- 6.45 (wetted-wall column-GC, Fendinger & Glotfelty 1990)  
 9.17 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)  
 16.20 (gas stripping-fluorescence, Shiu & Mackay 1997)  
 18.5\* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)  
 $\ln K_{AW} = -6242.48/(T/K) + 16.0$ ,  $\Delta H = 51.9 \text{ kJ mol}^{-1}$ ; measured range 4.1–31°C, (gas stripping-GC, Bamford et al. 1999)  
 $\log [H/(\text{Pa m}^3/\text{mol})] = 5.63 - 1240/(T/K)$  (Passivirta et al. 1999)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C or as indicated:

- 3.92 (shake flask-LSC, Veith et al. 1979, 1980)  
 3.92; 4.49 (shake flask-GC; RP-HPLC-RT correlation; Veith et al. 1980)  
 3.92 (23°C, shake flask, Banerjee et al. 1980)  
 3.92 (recommended, Sangster 1989, 1993)  
 3.92 (recommended, Hansch et al. 1995)

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

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

Bioconcentration Factor,  $\log BCF$ :

- 2.59 (bluegill sunfish, Veith et al. 1979, 1980)  
 2.59 (bluegill sunfish, Barrows et al. 1980)  
 2.59 (bluegill sunfish, Davies & Dobbs, 1984)

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

- 5.38 (sediments average, Kayal & Connell 1990)  
 3.79 (RP-HPLC correlation on CIHAC, Szabo 1990b)  
 3.59 (RP-HPLC correlation on PIHAC, Szabo 1990b; quoted, Pussemier et al. 1990)  
 3.58; 3.79 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 3.40–5.33; 3.80–5.40 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)  
 4.79; 4.89, 4.31, 4.20 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

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

Volatilization:

Photolysis: half-lives on different atmospheric substrates determined in the rotary photoreactor (appr. 25 µg/g on substrate):  $t_{1/2} = 2.0 \text{ h}$  on silica gel,  $t_{1/2} = 2.2 \text{ h}$  on alumina and  $t_{1/2} = 44 \text{ h}$  on fly ash (Behymer & Hites 1985);  
 $k = 0.23 \text{ h}^{-1}$  in distilled water with  $t_{1/2} = 3 \text{ h}$  (Fukuda et al. 1988);  
 direct photolysis  $t_{1/2} = 7.67 \text{ h}$  (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).

Hydrolysis: not hydrolyzable (Mabey et al. 1982).

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:

- $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$  for singlet  $O_2$ ,  $k = 8000 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical at 25°C (Mabey et al. 1982)  
 $k_{OH}(\text{exptl}) = 1.03 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{calc}) = 1.49 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al. 1988)  
 $k_{O_3} < 5.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH} = (1.03 \pm 0.13) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $k_{NO_3} = (4.6 \pm 2.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 2 \text{ K}$  (relative rate methods, Atkinson & Aschmann 1988)  
 $k_{OH} = (103 - 58.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296–300 K (Atkinson 1989)  
 $k_{OH}(\text{calc}) = 84.03 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1996)  
 $k_{OH}^* = 58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 325–365 K with a calculated atmospheric lifetime of 4.9 h based on gas-phase OH reaction (Brubaker & Hites 1998)  
 $k_{OH} = 8.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 2 \text{ K}$  with a atmospheric lifetime of 1.8 h assuming an average ambient 12-h daytime OH radical concn of  $2 \times 10^6 \text{ molecule/cm}^3$  (Reisen & Arey 2002)

Biodegradation: significant degradation within 7 d for a domestic sewer test (Tabak et al. 1981);

aerobic  $t_{1/2} = 295\text{--}2448 \text{ h}$ , based on aerobic soil column test data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

anaerobic  $t_{1/2} = 1180\text{--}9792$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:  $3 \times 10^{-9}$  mL cell<sup>-1</sup> h<sup>-1</sup>, estimated bacterial transformation rate constant (Mabey et al. 1982).

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

Sorption ( $k_1$ )-Desorption ( $k_2$ ) Rate constants: desorption rate constant of 0.018 d<sup>-1</sup> with  $t_{1/2} = 38.5$  d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 0.879\text{--}8.79$  h, based on estimated photooxidation half-life in air (Howard et al. 1991);  
calculated atmospheric lifetime of 4.9 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water:  $t_{1/2} = 3\text{--}300$  h, based on photolysis half-life in water (Howard et al. 1991).

Groundwater:  $t_{1/2} = 590\text{--}4896$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption  $t_{1/2} = 38.5$  d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil:  $t_{1/2} = 295\text{--}2448$  h, based on aerobic soil column test data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

$t_{1/2} > 50$  d (Ryan et al. 1988).

Biota:  $t_{1/2} < 1.0$  d in the tissue of bluegill sunfish (Veith et al. 1980).

**TABLE 4.1.1.20.1**  
**Reported aqueous solubilities of acenaphthene at various temperatures**

Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV				IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
	experimental		smoothed data		
22.2	3.57	0	1.45	0	1.5
30.0	4.76	22.2	3.46	20	3.2
30.0	4.60	25.0	3.88	25	3.8
30.0	4.72	30.0	4.80	30	4.8
34.5	6.00	34.5	5.83	40	7.4
34.5	5.68	39.3	7.20	50	9.2
34.5	5.75	44.7	9.20	60	19
39.3	6.80	50	11.9	70	32
39.3	7.10	50.1	11.9	75	43
39.3	7.00	55.6	15.6		
44.7	9.40	64.5	24.3		
44.7	9.40	65.2	25.2		
44.7	9.30	69.8	32.1		
50.1	12.5	71.9	35.9		
50.1	12.4	73.4	39.0		
50.1	12.4	74.7	41.8		
55.6	15.8	75.0	42.5		
55.6	16.3				
55.6	15.9				
64.5	25.9	temp dependence eq. 1			
64.5	27.8	ln x	mole fraction		
65.2	23.7	$\Delta H_{fus}$	$21.88 \pm 0.21$		
65.2	23.4	$10^2 \cdot b$	$1.86 \pm 0.11$		
65.2	22.8	c	$20.8 \pm 0.4$		
69.8	30.1				
69.8	34.3				

TABLE 4.1.1.20.1 (Continued)

Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV				IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
69.8	33.6				
71.9	35.2				
73.4	39.1				
79.4	40.1				
74.7	40.8				
74.7	39.3				

$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 21.88$

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

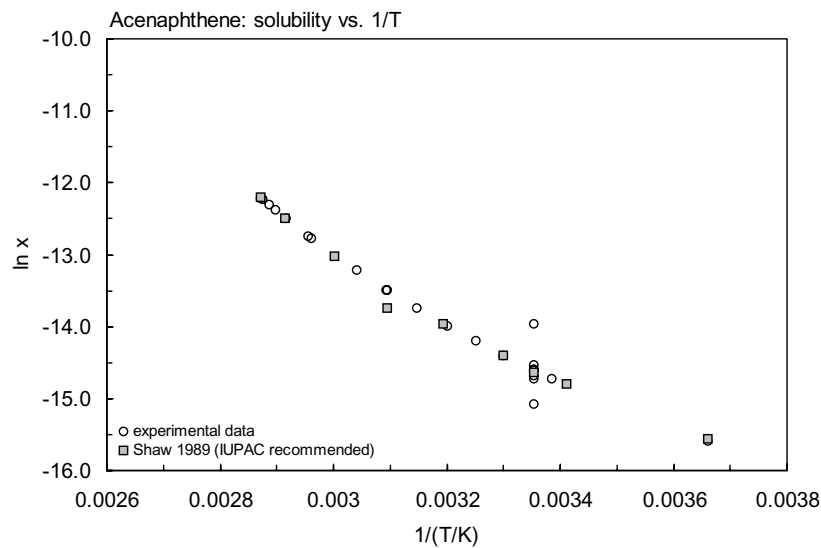


FIGURE 4.1.1.20.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for acenaphthene.

TABLE 4.1.1.20.2

Reported vapor pressures of acenaphthene 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.

Mortimer & Murphy 1923		Stull 1947		Hoyer & Peperle 1958		Radchenko & K. 1974	
static isoteniscope method		summary of literature data		effusion		effusion method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
147.2	2560	114.8	666.6	data presented as		54.1	8.622
182.4	8479	131.2	1333	eq. 1	P/mmHg	57.85	10.576
182.4	8479	148.7	2666	A	11.50	58.95	13.180
210.2	19732	168.2	5333	B	4264	61.3	16.545
210.4	19865	181.2	7999	temp range -15–35°C		64.55	20.438
227.2	31277	197.5	13332	$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 83.26$		67.25	26.757
233.2	36264	222.1	26664			69.5	31.304
246.2	49943	250.0	53329			71.8	37.77
246.6	50383	277.5	101325			73.65	47.22
247.0	51049					76.0	57.23
252.4	57929	mp/°C	55			78.05	67.66
252.5	57955					80.5	82.045
264.4	76047					83.45	130.30
264.4	76460						
275.3	97779					eq. 1	P/mmHg
275.4	97779					A	12.2930
275.4	97779					B	4222.924
286.8	124030						
287.0	124296						
287.8	125723						
eq. 1	P/mmHg						
A	8.033						
B	2835						
temp range 147–288°C							

## 2.

Osborn & Douslin 1975		Sonnefeld et al. 1983		Sato et al. 1986	
inclined-piston manometry		gas saturation-HPLC		gas saturation-electrobalance	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
solid					
65.0	25.865	10.87	0.048	19.95	0.237
70.0	30.797	10.87	0.0504	26.85	0.519
75.0	46.796	10.87	0.0515	30.85	0.792
80.0	70.526	20.45	0.167	35.75	1.30
85.0	104.92	20.45	0.161	37.95	1.60
90.0	153.45	20.45	10.66	43.35	3.21
92.0	185.05	30.15	0.539	45.35	4.21
92.5	195.05	30.15	0.512	48.35	5.76



TABLE 4.1.1.20.2 (Continued)

Osborn & Douslin 1975		Sonnefeld et al. 1983		Sato et al. 1986	
inclined-piston manometry		gas saturation-HPLC		gas saturation-electrobalance	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
liquid		32.15	0.580	51.85	7.68
95.0	214.91	38.9	1.35	58.05	9.72
100.0	281.04	38.9	1.32	60.25	12.0
105.0	364.23	38.9	1.32	63.65	15.6
110.0	468.35	25	0.287	68.85	23.5
115.0	597.94				
120.0	755.39	eq. 1	P/Pa	eq. 3	P/Pa
125.0	948.97	A	14.385	A	22.9288
130.0	1184	B	4616.07	B	5183.86
135.0	1469			C	-80.153
140.0	1809				

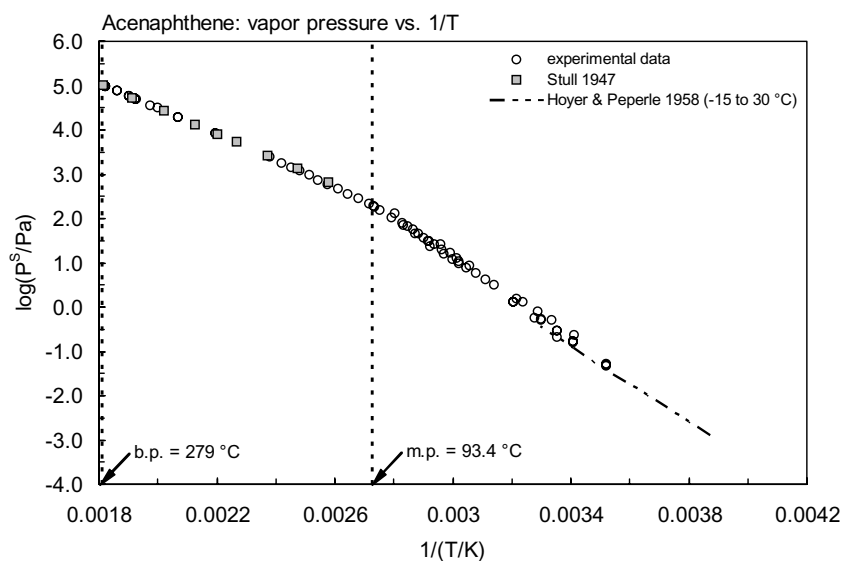


FIGURE 4.1.1.20.2 Logarithm of vapor pressure versus reciprocal temperature for acenaphthene.

TABLE 4.1.1.20.3

Reported Henry's law constants of acenaphthene at various temperatures

Bamford et al. 1999		
gas stripping–GC/MS		
t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)
		average
4.1	3.27, 3.79	3.52
11.0	5.98, 6.62	6.29
18.0	10.5, 11.4	10.9
25.0	17.5, 19.6	18.5
31.0	26.5, 30.8	28.6

$\ln K_{AW} = A - B/(T/K)$   
 $K_{AW}$   
A 15.997  
B 6242.5  
enthalpy, entropy change:  
 $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 51.9 \pm 1.3$   
 $\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 133$   
at 25°C

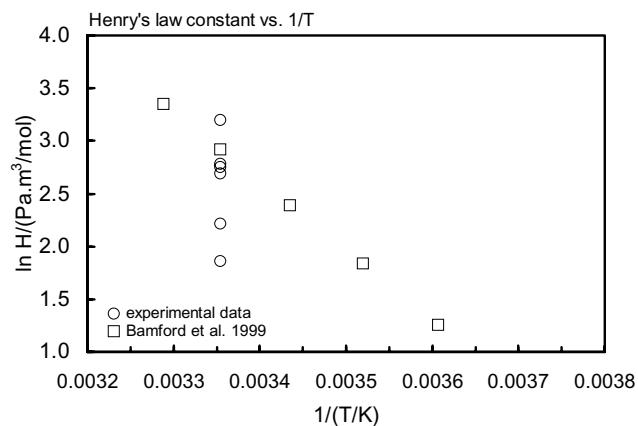
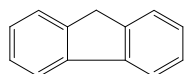


FIGURE 4.1.1.20.3 Logarithm of Henry's law constant versus reciprocal temperature for acenaphthene.

## 4.1.1.21 Fluorene



Common Name: Fluorene

Synonym: 2,3-benzindene, diphenylenemethane, 9H-fluorene

Chemical Name: diphenylenemethane

CAS Registry No: 86-73-7

Molecular Formula:  $C_{13}H_{10}$

Molecular Weight: 166.218

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

114.77 (Lide 2003)

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

295 (Dean 1985; Lide 2003)

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

1.203 ( $0^{\circ}C$ , Lide 2003)

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

138.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

19.54 (Wauchope & Getzen 1972)

19.58 (Osborn & Douslin 1975; Ruelle & Kesselring 1997; Chickos et al. 1999)

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

50.63 (Wauchope & Getzen 1972)

48.53 (Casellato et al. 1973)

50.48, 51.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

50.5 (Passivirta et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.132 (mp at  $114.77^{\circ}C$ )

0.161 (calculated,  $\Delta S_{fus} = 50.5\ J/mol\ K$ , Passivirta et al. 1999)

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):

1.90 (Pierotti et al. 1959)

1.66 (shake flask, binding to bovine serum albumin, Sahyun 1966)

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

$R \cdot \ln x = -4670/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 24.2 + 0.0309 \cdot (T/K)$ ; temp range  $24.6$ – $73.4^{\circ}C$  (shake flask-UV measurements, Wauchope & Getzen 1972)

1.98 (shake flask-fluorescence, Mackay & Shiu 1977)

1.68\* (generator column-HPLC, measured range  $6.6$ – $31^{\circ}C$ , May et al. 1978)

$S/(\mu g/kg) = 324.0 + 5.413 \cdot (t/^{\circ}C) + 0.8059 \cdot (t/^{\circ}C)^2 + 0.0025 \cdot (t/^{\circ}C)^3$ ; temp range  $4$ – $29^{\circ}C$  (generator column-HPLC/UV, May et al. 1978)

1.62\* ( $24^{\circ}C$ , generator column-HPLC, measured range  $279.75$ – $304.25\ K$ , May et al. 1983)

1.68 (generator column-HPLC, Wasik et al. 1983)

1.83 (average lit. value, Pearlman et al. 1984)

1.90 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

1.96 (generator column-HPLC/UV, Billington et al. 1988)

1.9\* (recommended, IUPAC Solubility Data Series, Shaw 1989)

2.23 (generator column-HPLC, Vadas et al. 1991)

$\log [S_L/(mol/L)] = 1.664 - 1024/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$\ln x = 0.82861 - 4824/(T/K)$ ; temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

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

- 2400\* (161.0°C, static isoteniscope method, measured range 161.0–300.4°C, Mortimer & Murphy 1923)  
 $\log (P/\text{mmHg}) = 8.059 - 2957/(T/K)$ ; temp range 161–300.4°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)
- 666.6\* (129.3°C, summary of literature data, temp range 129.3–295.0°C, Stull 1947)
- 0.087\* (effusion method, measured range 33.3–49.55°C, Bradley & Cleasby 1953)  
 $\log (P/\text{cmHg}) = 10.325 - 4324/(T/K)$ ; temp range 33.3–49.55°C (Antoine eq., Bradley & Cleasby 1953)
- 1.66 (extrapolated-Antoine eq., liquid state  $P_L$ , Weast 1972-73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 13682.8/(T/K)] + 8.18894$ ; temp range 129.3–295°C (Antoine eq., Weast 1972-73)
- 1.13 (extrapolated-Antoine eq., liquid state  $P_L$ , Boublik et al. 1973)
- 1.133 (extrapolated-Antoine eq., supercooled liquid  $P_L$ , Dean 1985)
- 0.127\* (static method-manometry, measured range 75.8–114°C, Osborn & Douslin 1975)
- 0.0946 (Irwin 1982)
- 0.080\* (gas saturation-HPLC/UV, measured range 10–50°C, Sonnefeld et al. 1983)  
 $\log (P/\text{Pa}) = 14.385 - 4616.07/(T/K)$ ; temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)
- 0.080 (generator column-HPLC, Wasik et al. 1983)
- 0.473, 0.380 ( $P_{GC}$  by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)  
 $\log (P/\text{kPa}) = 2.88490 - 2635.371/(243.022 + t/^\circ\text{C})$ ; temp range 161–300.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 0.403 (Yamasaki et al. 1984)  
 $\log (P/\text{mmHg}) = 7.7619 - 2637.1/(243.2 + t/^\circ\text{C})$ ; temp range 161–300°C (Antoine eq., Dean 1985, 1992)
- 0.0875\* (gas saturation, interpolated-Antoine eq. derived from exptl. data, temp range 34–72°C, Sato et al. 1986)  
 $\ln (P/\text{Pa}) = 17.0935 - 2815.52/(T/K - 153.984)$ ; temp range 307.7–347.5 K (Antoine eq., gas saturation, Sato et al. 1986)
- 0.088 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_s/\text{kPa}) = 10.449 - 4324/(T/K)$ ; temp range 306–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_s/\text{kPa}) = 10.04542 - 4122.908/(T/K)$ ; temp range 348–388 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 8.31368 - 4133.08/(86.582 + T/K)$ ; temp range 402–568 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- 0.0850\*, 0.566 (pressure gauge in vacuum cell: solid  $P_s$ , supercooled liquid  $P_L$ , extrapolated for 25°C from reported Antoine eq., measured temp range 30.03–154.81°C, Sasse et al. 1988)  
 $\log (P_s/\text{mmHg}) = 11.64431 - 4268.644/(262.656 + t/^\circ\text{C})$ ; temp range: 30.03–100.08°C (Antoine eq., pressure gauge, Sasse et al. 1988)  
 $\log (P_L/\text{mmHg}) = 7.74839 - 2641.73/(230.963 + t/^\circ\text{C})$ ; temp range 110.06–154.83°C (Antoine eq., pressure gauge, Sasse et al. 1988)
- 0.474 ( $P_{GC}$  by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
- 0.793, 0.652 (supercooled  $P_L$  converted from literature  $P_s$  with different  $\Delta S_{fus}$  values, Hinckley et al. 1990)  
 $\log (P/\text{mmHg}) = 53.9382 - 5.322 \times 10^3/(T/K) - 16.059 \cdot \log (T/K) + 4.5696 \times 10^{-3} \cdot (T/K) + 8.1430 \times 10^{-13} \cdot (T/K)^2$ ; temp range 388–870 K (vapor pressure eq., Yaws 1994)
- 0.407 (supercooled liquid  $P_L$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
- 0.0575, 0.0885; 0.080; 0.0851 (quoted exptl.: effusion method; gas saturation; manometry, Delle Site 1997)
- 0.0792, 0.243; 0.00594, 0.00477 (quoted lit.; calculated; GC-RT correlation, Delle Site 1997)
- 0.72; 0.116 (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_s$  with fugacity ratio  $F$ , Passivirta et al. 1999)  
 $\log (P_s/\text{Pa}) = 11.27 - 3638/(T/K)$  (solid, Passivirta et al. 1999)  
 $\log (P_L/\text{Pa}) = 8.63 - 2614/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $\log (P/\text{Pa}) = 14.385 - 4616.07/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.526; 0.194 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)  
 $\log (P_L/\text{Pa}) = -3492/(T/K) + 11.43$ ;  $\Delta H_{vap} = -66.9 \text{ kJ} \cdot \text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)

0.086\* (25.05°C, transpiration method, measured range 288.7–359.2 K, Verevkin 2004)

$\ln (P/\text{Pa}) = 298.47/R - 95086.65/[R(T/K)] - (30.2/R) \cdot \ln [(T/K)/298.15]$ ; temp range 288.7–359.2 K (transpiration method, Verevkin 2004)

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

7.75 (batch stripping, Mackay & Shiu 1981)

10.13 (batch stripping, Mackay et al. 1982)

11.85 (batch stripping, Warner et al. 1987)

6.45 (wetted-wall column, Fendinger & Glotfelty 1990)

9.75 (gas stripping-fluorescence, Shiu & Mackay 1997)

6.50 (gas stripping-HPLC/fluorescence, De Maagd et al. 1998)

9.81\* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)

$\ln K_{\text{AW}} = -5869.62/(T/K) + 14.193$ ;  $\Delta H = 48.8 \text{ kJ mol}^{-1}$ ; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

$\log (H/(\text{Pa m}^3/\text{mol})) = 6.97 - 1590/(T/K)$  (Passivirta et al. 1999)

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

4.18 (Hansch & Leo 1979)

4.12 (Chou & Jurs 1979)

4.18 (HPLC- $k'$  correlation, Rekker & De Kort 1979)

3.91 (HPLC- $k'$  correlation, Hanai et al. 1981)

4.18 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)

4.18 (shake flask-UV, Yalkowsky et al. 1983b)

4.23 (HPLC-RT correlation, Rapaport et al. 1984)

4.18 (shake flask-GC, Haky & Leja 1986)

4.10 (RP-HPLC-RT correlation, Chin et al. 1986)

4.23 (HPLC-RT correlation, Wang et al. 1986)

4.13 (TLC-RT correlation, De Voogt et al. 1990)

4.18 (recommended, Sangster 1993)

4.18 (recommended, Hansch et al. 1995)

$4.32 \pm 0.19$ ,  $3.68 \pm 0.62$  (HPLC- $k'$  correlation: ODS column; Diol column, Helweg et al. 1997)

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

6.68 (calculated, Finizio et al. 1997)

6.79\*; 6.59 (generator column-GC; calculated- $C_{\text{O}}/C_{\text{A}}$ , measured range 0–40°C, Harner & Bidleman 1998)

$\log K_{\text{OA}} = -7.74 + 4332/(T/K)$ ; temp range 0–40°C (generator column-GC, Harner & Bidleman 1998)

6.83, 6.79 (calculated- $S_{\text{oct}}$  and vapor pressure  $P$ , quoted lit., Abraham et al. 2001)

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

3.67 (microorganisms-water, calculated- $K_{\text{OW}}$ , Mabey et al. 1982)

2.70 (*Daphnia magna*, Newsted & Giesy 1987)

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

3.95; 3.87 (Aldrich and Fluka humic acids, observed; predicted, Chin et al. 1989)

5.47 (sediments average, Kayal & Connell 1990)

3.76 (RP-HPLC correlation, Pussemier et al. 1990)

4.15, 4.21 (RP-HPLC correlation on CIHAC, on PIHAC, Szabo 1990b)

4.68 (humic acid, HPLC- $k'$  correlation, Nielsen et al. 1997)

3.24–5.75; 4.10–5.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

4.81; 4.93, 4.24, 4.63 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

- 3.95 (Askov soil, a Danish Agricultural soil, Sverdrup et al. 2002)  
 3.93–6.19 (sediment/water, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluor., ten Hulscher et al. 2003)

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

##### Volatilization:

Photolysis: half-lives on different atmospheric particulate substrates determined in rotary photoreactor (approx. 25  $\mu\text{g/g}$  on substrate):  $t_{1/2} = 110$  h on silica gel,  $t_{1/2} = 62$  h on alumina and  $t_{1/2} = 37$  h on fly ash (Behymer & Hites 1985);

photolysis rate  $k < 2 \times 10^{-5} \text{ s}^{-1}$  with  $t_{1/2} > 1.6$  d (Kwok et al. 1997);

direct photolysis  $t_{1/2} = 7.69$  h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001)

Photodegradation  $k = 9.0 \times 10^{-7} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002).

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

$k(\text{calc}) < 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 3 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)

$k_{\text{OH}}(\text{calc}) = 13.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 300 K (SAR structure-activity relationship, Arey et al. 1989, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 9.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculation, Klamt 1996)

$k_{\text{OH}}(\text{exptl}) = (16 \pm 5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{calc}) = 9.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated lifetime  $\tau = 9$  h;  $k_{\text{NO}_3}(\text{exptl}) = (3.5 \pm 1.2) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated lifetime  $\tau = 1.3$  d; and  $k_{\text{O}_3}(\text{exptl}) < 2 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated lifetime  $\tau > 82$  d at  $297 \pm 2$  K (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)

$k_{\text{OH}}^* = 23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 306–366 K with a calculated atmospheric lifetime of 22 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: significant degradation with gradual adaptation within 7 d for an average of three static-flask screening test (Tabak et al. 1981);

nonautoclaved groundwater samples of approx. 0.06 mg/L are degraded at rates of about 30% per week by microbes (Lee et al. 1984);

$t_{1/2}(\text{aq. aerobic}) = 768\text{--}1440$  h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 3072\text{--}5760$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

$k_1 = 12.3 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.051 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 6.81\text{--}68.1$  h, based on reported rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);

photolysis  $t_{1/2} > 1.6$  d; calculated tropospheric lifetimes of 9 h, 1.3 d and  $> 82$  d due to reactions with OH radical,  $\text{NO}_3$  radical and  $\text{O}_3$ , respectively, at room temp. (Kwok et al. 1997);

calculated atmospheric lifetime of 22 h based on gas-phase reactions with OH radical (Brubaker & Hites 1998).

Surface water:  $t_{1/2} = 768\text{--}1440$  h, based on aerobic soil die-away test data (Howard et al. 1991).

Groundwater:  $t_{1/2} = 1536\text{--}2880$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

##### Sediment:

Soil:  $t_{1/2} = 768\text{--}1440$  h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} > 50$  d (Ryan et al. 1988).

Biota: elimination  $t_{1/2} = 7$  d from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.21.1

Reported aqueous solubilities of fluorene at various temperatures

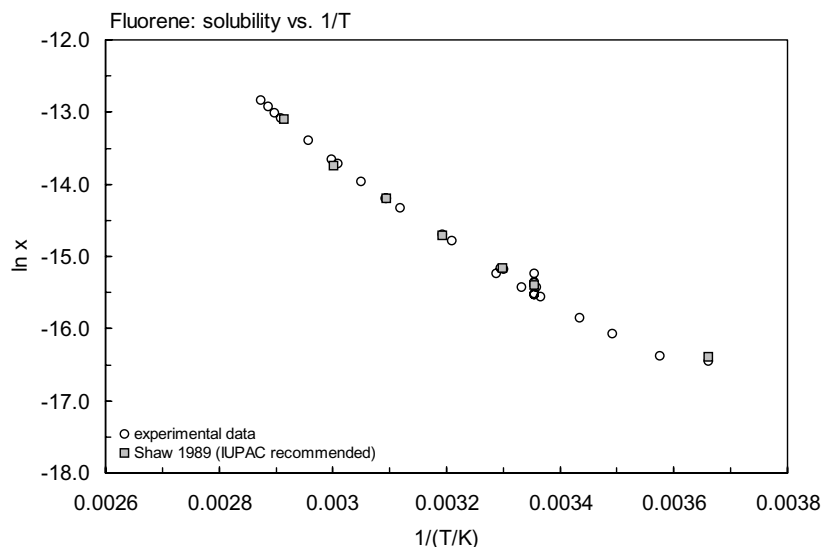
Wauchope & Getzen 1972				May 1980, 1983		Shaw 1989	
shake flask-UV				generator column-HPLC		IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
	experimental		smoothed				
24.6	1.93	0	0.66	6.60	0.7184	0	0.70
24.6	1.87	24.6	1.86	13.2	0.9673	25	1.90
24.6	1.88	25	1.90	18.0	1.203	30	2.40
29.9	2.41	29.9	2.37	24.0	1.616	40	3.80
29.9	2.33	30.3	2.41	27.0	1.845	50	6.30
29.9	2.34	38.4	3.53	31.1	2.248	60	10
30.3	2.10	40.1	3.84			70	19
30.3	2.25	47.5	5.54				
30.3	2.23	50	6.29	temp dependence eq. 2			
38.4	3.72	50.1	6.32	S	μg/kg		
38.4	3.73	50.2	6.35	a	0.0185		
40.1	3.88	54.7	8.02	b	0.4543		
40.1	3.84, 3.85	59.2	10.2	c	22.76		
47.5	5.59, 5.62	60.5	10.9	d	543.3		
47.5	5.68	65.1	14.1				
50.1	6.31, 6.42	70.7	19.2	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 32.97$			
50.1	6.54	71.9	20.6	measured between 5–30°C			
50.2	6.27	73.4	22.5				
54.7	8.31, 8.41	75	24.7				
54.7	8.56						
59.2	10.5						
60.5	10.7	temp dependence eq. 1					
60.5	11.0	ln x	mole fraction				
60.5	11.6	$\Delta H_{\text{fus}}$	$19.54 \pm 0.13$				
65.1	14.2	$10^2 \cdot b$	$3.09 \pm 0.1$				
65.1	14.1	c	$24.2 \pm 0.3$				
70.7	18.5						
70.7	18.9						
71.9	18.8						
73.4	21.5						

 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.54$ 

Empirical temperature dependence equations:

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

$$\text{May et al. (1978): } -S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t_{1/2} + c \cdot t + d \quad (2)$$



**FIGURE 4.1.1.21.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for fluorene.

**TABLE 4.1.1.21.2**

**Reported vapor pressures of fluorene 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)		
$\ln P = A/R - B/[R(T/K)] - (C/R) \cdot \ln [(T/K)/298.15]$ ; R – gas constant			(5)

1.

Mortimer & Murphy 1923		Stull 1947		Bradley & Cleasby 1953		Osborn & Douslin 1975	
isoteniscope-Hg manometer		summary of literature data		effusion		manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
161.0	2400	129.3	666.6	33.3	0.2186	75.0	15.065
202.5	9266	146.0	1333	37.2	0.3333	80.0	22.264
203.0	9399	164.2	2666	40.3	0.4573	85.0	32.263
240.0	27398	185.2	5333	45.0	0.7239	90.0	47.462
241.4	27784	197.8	7999	49.25	1.0906	95.0	68.26
276.6	64995	214.7	13332	34.85	0.2600	100.0	99.19
277.1	65421	240.3	26664	38.45	0.3746	105.0	141.45
295.6	98499	268.6	53329	42.45	0.5546	110.0	199.98
295.7	98499	295.0	101325	47.75	0.9439	114.0	259.04
295.7	98499			49.55	1.1106		
299.8	107231	mp/°C	113				
300.4	108298			eq. 1	P/mmHg	triple point	387.943 K
				A	10.325		
				B	4324	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 81.76$	
eq. 1	P/mmHg			temp range 33–50°C			at bp



TABLE 4.1.1.21.2 (Continued)

Mortimer & Murphy 1923		Stull 1947		Bradley & Cleasby 1953		Osborn & Douslin 1975	
isoteniscope-Hg manometer		summary of literature data		effusion		manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
A	8.059					$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.58$	
B	2957					$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 62.17$	
temp range 161–300°C						at bp	
2.							
Sonnefeld et al. 1983		Sato et al. 1986		Sasse et al. 1988		Verevkin 2004	
gas saturation–HPLC		gas saturation–electrobalance		electronic manometry		transpiration	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
				solid			
10.5	0.0132	34.55	0.297	30.03	0.157	288.8	0.028
10.5	0.0133	36.35	0.360	39.92	0.184	290.4	0.034
10.5	0.013	41.15	0.620	49.88	1.241	292.4	0.044
20.4	0.0425	47.45	1.21	59.92	3.426	289.6	0.031
20.4	0.0438	49.85	1.53	60.03	3.533	296.2	0.067
20.4	0.0451	52.35	1.95	69.93	8.746	298.2	0.086
30.0	0.147	55.45	2.60	79.96	20.67	300.2	0.112
29.97	0.153	57.35	3.07	79.98	20.80	302.2	0.132
29.97	0.146	58.75	3.88	89.99	46.26	304.3	0.166
38.85	0.387	63.25	4.78	89.99	46.40	306.3	0.218
38.85	0.384	64.55	5.88	100.04	97.86	308.3	0.268
38.85	0.382	67.25	7.38	100.08	98.93	310.2	0.328
38.9	0.387	69.75	9.13			313.3	0.449
38.9	0.393	71.25	10.2	eq. 2	P/mmHg	314.3	0.507
25.0	0.080	74.35	13.0	A	11.64431	315.3	0.545
				B	4268.664	317.3	0.666
eq. 1	P/Pa	eq. 3	P/Pa	C	262.656	320.3	0.930
A	14.385	A	17.0935	temp range: 30–100.08°C		323.4	1.245
B	4616.07	B	2815.52			326.5	1.645
		C	–153.984	liquid		329.3	2.223
				110.06	212.5	332.3	3.103
				120.04	352.0	335.3	3.867
				120.04	353.0	338.2	4.838
				129.97	568.6	341.2	6.552
				139.95	894.3	344.2	8.417
				149.86	1369	347.1	11.190
				154.81	1683	350.3	14.497
						353.2	18.302
				eq. 2	P/mmHg	356.3	23.900
				A	7.94839	359.2	30.456
				B	2641.73		
				C	230.963	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.08$	
				temp range: 110–155°C		eq. 5	P/Pa
						A	298.47
						B	95086.65
						C	30.2

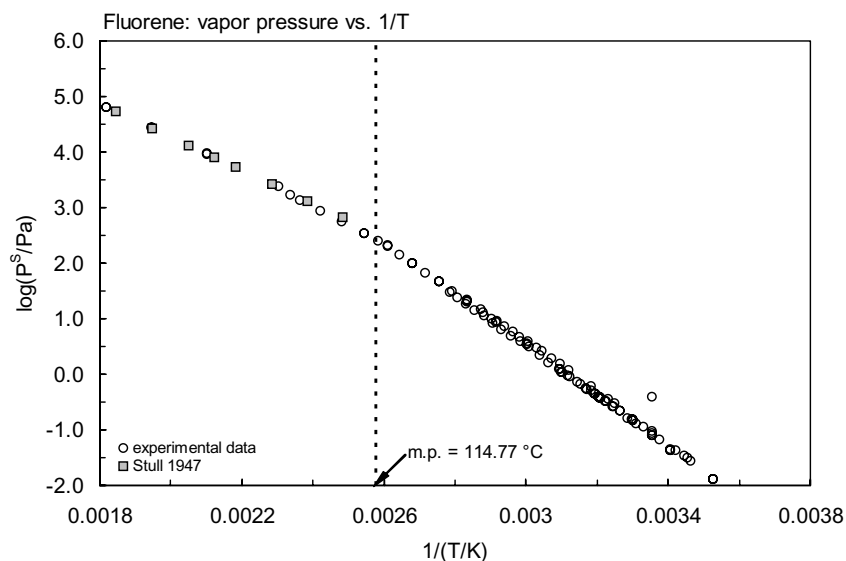
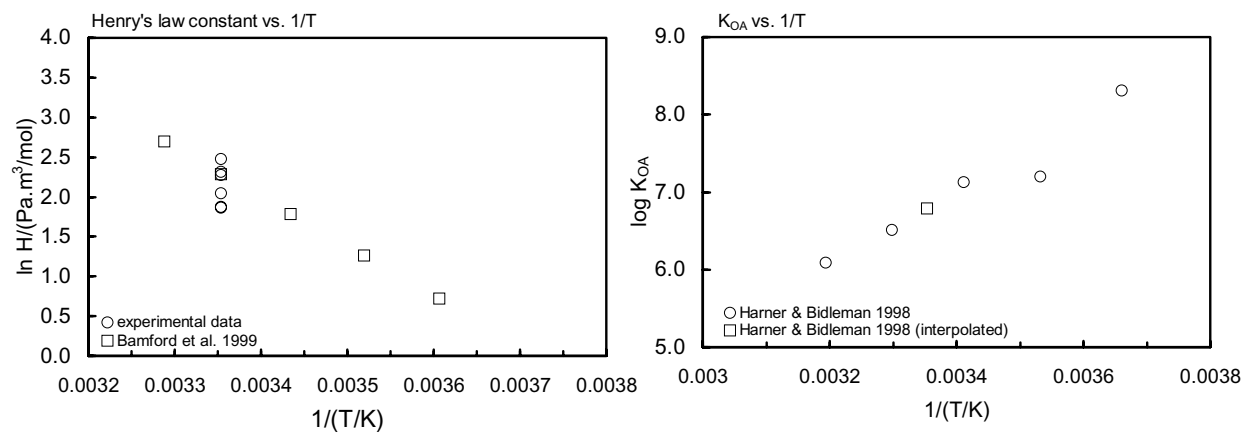


FIGURE 4.1.1.21.2 Logarithm of vapor pressure versus reciprocal temperature for fluorene.

TABLE 4.1.1.21.3

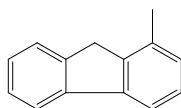
Reported Henry's law constants and octanol–air partition coefficients of fluorene at various temperatures and temperature dependence equations

Henry's law constant			log $K_{OA}$	
Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)	t/°C	log $K_{OA}$
		average		
4.1	1.96, 2.14	2.05	0	8.134
11.0	3.44, 3.65	3.54	10	7.501
18.0	5.81, 6.12	5.96	20	7.130
25.0	9.49, 10.1	9.81	30	6.516
31.0	14.1, 15.4	14.8	40	6.093
			25(exptl)	6.79
			25(calc)	6.59
ln $K_{AW} = A - B/(T/K)$			log $K_{OA} = A + B/(T/K)$	
eq. 1	$K_{AW}$		A	-7.74
A	14.193		B	4332
B	5870			
enthalpy, entropy change:			enthalpy of phase change	
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 48.8 \pm 0.8$			$\Delta H_{OA}/(\text{kJ}\cdot\text{mol}^{-1}) = 82.9$	
$\Delta S/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = 118$				
at 25°C				



**FIGURE 4.1.1.21.3** Logarithm of Henry's law constant and  $K_{OA}$  versus reciprocal temperature for fluorene.

## 4.1.1.22 1-Methylfluorene



Common Name: 1-Methylfluorene

Synonym:

Chemical Name: 1-methylfluorene

CAS Registry No: 1730-37-6

Molecular Formula:  $C_{14}H_{12}$

Molecular Weight: 180.245

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

87 (Lide 2003)

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

318 (Weast 1982)

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

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

177.1 (Ruelle & Kesselring 1997)

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.246 (mp at  $87^{\circ}C$ )

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

1.092, 4.867 (measured, supercooled liquid value, Miller et al. 1985)

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

0.136; 0.0708 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -3711/(T/K) + 11.58$ ;  $\Delta H_{vap} = -71.1 kJ \cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

0.032 ( $24.95^{\circ}C$ , transpiration method, measured range  $298.1-375.3 K$ , Verevkin 2004)

$\ln (P_S/Pa) = 311.78/R - 101590.4/[R(T/K)] - (35.1/R) \cdot \ln [(T/K)/298.15]$ ; temp range  $298.1-359.2 K$  (solid, transpiration method, Verevkin 2004)

$\ln (P_L/Pa) = 330.39/R - 104778.1/[R(T/K)] - (87.5/R) \cdot \ln [(T/K)/298.15]$ ; temp range  $361.2-375.3 K$  (liquid, transpiration method, Verevkin 2004)

Henry's Law Constant ( $Pa m^3/mol$ ):

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

4.97 (calculated, Miller et al. 1985)

4.63 (calculated-solvatochromic parameters and  $V_L$ , Kamlet et al. 1988)

5.7640 (calculated-UNIFAC group contribution, Chen et al. 1993)

4.97 (recommended, Hansch et al. 1995)

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

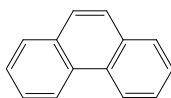
Bioconcentration Factor,  $\log BCF$ :

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

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

Half-Lives in the Environment:

## 4.1.1.23 Phenanthrene



Common Name: Phenanthrene

Synonym: *o*-diphenyleneethylene, phenanthren

Chemical Name: phenanthrene

CAS Registry No: 85-01-8

Molecular Formula: C<sub>14</sub>H<sub>10</sub>

Molecular Weight: 178.229

Melting Point (°C):

99.24 (Lide 2003)

Boiling Point (°C):

340 (Dean 1985; Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.174 (Dean 1985)

0.980 (4°C, Weast 1982–83; Lide 2003)

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

182.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

18.62 (Parks & Huffman 1931; Tsonopoulos & Prausnitz 1971; Fu & Luthy 1985)

16.28 (differential calorimetry, Wauchope & Getzen 1972)

16.44 (calorimetry, Osborn & Douslin 1975)

0.22, 16.46; 15.58 (74.35, 99.25°C; total phase change enthalpy, Chickos et al. 1999)

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

42.68 (Wauchope & Getzen 1972)

45.19 (Casellato et al. 1973)

50.63 (Ubbelohde 1978)

47.70 (De Kruif 1980)

44.83, 44.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming  $\Delta S_{\text{fus}} = 56$  J/mol K), F: 0.187 (mp at 99.24°C)

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

1.65 (shake flask-nephelometry, Davis & Parker 1942)

1.60 (27°C, nephelometry, Davis et al. 1942)

0.994 (shake flask-UV, Andrews & Keefer 1949)

1.60 (shake flask-UV, Kleven 1950)

1.18 (Pierotti et al. 1959)

0.71 (shake flask, binding to bovine serum albumin, Sahyun 1966)

1.60 (shake flask-UV/fluorescence, Barone et al. 1967)

2.67 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)

1.18\* (shake flask-UV, measured range 24.6–73.4°C, Wauchope & Getzen 1972)

$R \cdot \ln x = -3890/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 27.9 + 0.0374 \cdot (T/K)$ ; temp range 24.6–73.4°C

(shake flask-UV measurements, Wauchope & Getzen 1972)

3.03, 2.85 (20°C, HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

1.21 (shake flask-UV, Vesala 1974)

1.07 (shake flask-GC, Eganhouse & Calder 1976)

1.29 (shake flask-fluorescence, Mackay & Shiu 1977)

1.002 (Rossi 1977; Neff 1979)

1.151\* (shake flask-UV, measured range 8.4–31.8°C, Schwarz 1977)

- 1.002\* (generator column-HPLC/UV, measured range 4–29°C, May et al. 1978, 1983)  
 $S/(\mu\text{g/kg}) = 324.0 + 5.413 \cdot (t/^\circ) + 0.8059 \cdot (t/^\circ\text{C})^2 + 0.0025 \cdot (t/^\circ\text{C})^3$ ; temp range 4–29°C (generator column-HPLC/UV, May et al. 1978)
- 0.955\* (24.3°C, generator column-HPLC, measured range 4.0–29.9°C, May 1980)
- 0.816 (quoted, Verschueren 1983)
- 1.0 (generator column-HPLC/UV, Wasik et al. 1983)
- 1.28 (average lit. value, Pearlman et al. 1984)
- 1.29 (generator column-HPLC/fluorescence, Walters & Luthy 1984)
- 1.10\* (generator column-HPLC/UV, measured range 4.6–25.3°C, Whitehouse 1984)
- 1.69 (29°C, shake flask-GC/FID, Stucki & Alexander 1987)
- 0.0446 (vapor saturation-UV, Akiyoshi et al. 1987)
- 1.08 (generator column-HPLC, Billington et al. 1988)
- 1.10\* (recommended, IUPAC Solubility Data Series, Shaw 1989)
- 1.0 (generator column-HPLC, Vadas et al. 1991)
- 1.03 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
- 0.823 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
- 1.20 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
- $\log S_L (\text{mol/L}) = 0.930 - 861.6/(T/K)$  (supercooled liquid, Passivirta et al. 1999)
- $\ln x = -2.546051 - 4053/(T/K)$ ; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

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

- 7773\* (230°C, isoteniscope-Hg, measured range 230–340°C, Nelson & Senseman 1922)
- 3626\* (203.6°C, isoteniscope-Hg manometer, measured range 203.6–346.8°C, Mortimer & Murphy 1923)
- $\log (P/\text{mmHg}) = 7.771 - 2990/(T/K)$ ; temp range 203.6–346.8°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)
- 133.3\* (118.2°C, summary of literature data, temp range 118.2–340.2°C, Stull 1947)
- 0.0997 (effusion method, Inokuchi et al. 1952)
- 0.0227\* (effusion method, Bradley & Cleasby 1953)
- $\log (P/\text{cmHg}) = 10.388 - 4519/(T/K)$ ; temp range 36.7–49.65°C (Antoine eq., Bradley & Cleasby 1953)
- $\log (P/\text{mmHg}) = 16.0 - 5008/(T/K)$ ; temp range 0–60°C (Knudsen effusion method, Hoyer & Peperle 1958)
- 0.464 (extrapolated from Antoine eq. of liquid state  $P_L$ , Weast 1972–73)
- $\log (P/\text{mmHg}) = [-0.2185 \times 14184.0/(T/K)] + 7.936781$ ; temp range 118.2–340°C (Antoine eq., Weast 1972–73)
- 0.159 (extrapolated from Antoine eq. of liquid state  $P_L$ , Boublik et al. 1973)
- 30.4\* (100.0°C, inclined-piston manometry, measured range 100.0–150.0°C, Osborn & Douslin 1975)
- 0.0187 (lit. average-interpolated, API 1979)
- 0.0263\* (gas saturation, Macknick & Prausnitz 1979)
- 0.0267 (extrapolated-Clapeyron eq., Macknick & Prausnitz 1979)
- $\log (P/\text{mmHg}) = 26.648 - 10484/(T/K)$ ; temp range 51.6–90.3°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
- 0.018\* (effusion, De Kruif 1980)
- 0.0161\* (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
- $\log (P/\text{Pa}) = 14.852 - 4962.77/(T/K)$ ; temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)
- 0.016 (generator column-HPLC/UV, Wasik et al. 1983)
- 0.111, 0.0688 ( $P_{GC}$  by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
- 0.134 (supercooled liquid  $P_L$  converted from literature  $P_s$ , Bidleman 1984)
- $\log (P_L/\text{kPa}) = 6.61335 - 2593.134/(224.402 + t/^\circ\text{C})$ ; temp range 203.6–346.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P_L/\text{kPa}) = 6.01392 - 2039.351/(168.569 + t/^\circ\text{C})$ ; temp range 230–340°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P/\text{mmHg}) = 7.26082 - 2379.04/(203.76 + t/^\circ\text{C})$ ; temp range 176–379°C (Antoine eq., Dean 1985, 1992)
- 0.070 (Yamasaki et al. 1984)
- 0.0149 (selected, Howard et al. 1986)

- 0.012\* (gas saturation, extrapolated-Antoine eq. from exptl. data, temp range 49–74°C, Sato et al. 1986)  
 $\ln (P/\text{Pa}) = 20.3950 - 2931.20/(T/\text{K} - 139.743)$ ; temp range: 322.9–347.8 K (Antoine eq., gas saturation, Sato et al. 1986)
- 0.025 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_s/\text{kPa}) = 10.305 - 4444/(T/\text{K})$ ; temp range 296–315 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_s/\text{kPa}) = 10.70162 - 4554.38/(T/\text{K})$ ; temp range 313–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.64812 - 2513.134/(-65.345 + T/\text{K})$ ; temp range 373–423 K (Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.17186 - 3235.19/(12.908 + T/\text{K})$ ; temp range 391–613 K (Antoine eq., Stephenson & Malanowski 1987)
- 0.0127, 0.0827 (literature mean  $P_s$ , supercooled liquid  $P_L$ , Bidleman & Foreman 1987)
- 0.111, 0.0556 ( $P_{GC}$ , GC-RT correlation with different reference standards, Hinckley et al. 1990)
- 0.134, 0.10 (supercooled liquid  $P_L$  converted from literature  $P_s$  with different  $\Delta S_{fus}$  values, Hinckley et al. 1990)  
 $\log (P_L/\text{Pa}) = 11.46 - 3716/(T/\text{K})$  (GC-RT correlation, Hinckley et al. 1990)  
 $\log (P/\text{mmHg}) = 50.2858 - 5.7409 \times 10^3/(T/\text{K}) - 13.935 \cdot \log (T/\text{K}) - 8.852 \times 10^{-10} \cdot (T/\text{K}) + 2.11343 \times 10^{-6} \cdot (T/\text{K})^2$ ;  
temp range 372–869 K (vapor pressure eq., Yaws 1994)
- 0.0708 (supercooled liquid  $P_L$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
- 0.0251, 0.0227, 0.018, 0.0186; 0.0267, 0.0161 (quoted exptl.: effusion method, gas saturation, Delle Site 1997)
- 0.0288, 0.0227, 0.0181; 0.0196, 0.0122, 0.0173 (quoted lit.: calculated; from GC-RT correlation, Delle Site 1997)
- 0.0197\* (Knudsen effusion/thermogravimetry technique, extrapolated Clausius-Clapeyron eq., Oja & Suuberg 1998)  
 $\log (P/\text{Pa}) = 34.387 - 11423/(T/\text{K})$ ; temp range: 303–333 K (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)
- 0.115; 0.0306 (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_s$  with fugacity ratio  $F$ , Passivirta et al. 1999)  
 $\log (P_s/\text{Pa}) = 11.38 - 3842/(T/\text{K})$  (solid, Passivirta et al. 1999)  
 $\log (P_L/\text{Pa}) = 9.07 - 2982/(T/\text{K})$  (supercooled liquid, Passivirta et al. 1999)
- 0.0163  $\pm$  0.004 (gas saturation-HPLC/fluorescence; de Seze et al. 2000)  
 $\log (P/\text{Pa}) = 14.852 - 4962.77/(T/\text{K})$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.0799; 0.0475 (supercooled liquid  $P_L$ , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)  
 $\log (P_L/\text{Pa}) = -3768/(T/\text{K}) + 11.54$ ;  $\Delta H_{vap} = -72.2 \text{ kJ} \cdot \text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)
- 0.0202 (solid  $P_s$ , gas saturation-GC/MS, Mader & Pankow 2003)
- 0.0966 (supercooled liquid  $P_L$ , calculated from  $P_s$  assuming  $\Delta S_{fus} = 56 \text{ J/mol K}$ , Mader & Pankow 2003)

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

- 5.55 (gas stripping-GC, Southworth 1979)
- 3.981 (gas stripping-GC, Mackay et al. 1979; Mackay & Shiu 1981; Mackay et al. 1982)
- 3.65 (gas stripping-GC, Mackay & Shiu 1981; Mackay et al. 1982)
- 2.38 (wetted-wall column-GC, Fendinger & Glotfelty 1990; quoted, Shiu & Mackay 1997; Shiu et al. 1999)
- 3.97 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
- 4.68\* (gas stripping-GC, measured range 5.9–34.7°C, Alaei et al. 1996)  
 $\ln K_{AW} = 6.0314 - 3524.18/(T/\text{K})$ ; temp range 5.9–34.7°C (gas stripping-GC, Alaei et al. 1996)
- 3.61 (gas stripping-GC, Shiu & Mackay 1997)
- 2.90 (gas stripping-HPLC/fluor., De Maagd et al. 1998)
- 4.29\* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)  
 $\ln K_{AW} = -5689.2/(T/\text{K}) + 12.75$ ,  $\Delta H = 47.3 \text{ kJ} \cdot \text{mol}^{-1}$ ; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
- $\log (H/(\text{Pa m}^3/\text{mol})) = 8.14 - 2120/(T/\text{K})$  (Passivirta et al. 1999)
- 3.85 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 2001)  
 $\log K_{AW} = 2.417 - 1530/(T/\text{K})$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log  $K_{ow}$  at 25°C or as indicated:

- 4.46 (Hansch & Fujita 1964; Leo et al. 1971; Hansch et al. 1973; Hansch & Leo 1979)
- 4.66 (calculated-molecular connectivity indices MCI, Kier et al. 1971)
- 4.67 (calculated-fragment const., Rekker 1977)
- 4.57 (shake flask-UV, concn ratio, Karickhoff et al. 1979)
- 4.45 (HPLC- $k'$  correlation, McDuffie 1981)
- 4.63 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)
- 4.53 (HPLC- $k'$  correlation, Hammers et al. 1982)
- 4.52; 4.31 (shake flask; HPLC correlation, Eadsforth & Moser 1983)
- 4.46 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)
- 4.28 (HPLC- $k'$  correlation, Haky & Young 1984)
- 4.39 (RP-HPLC-RT correlation, Chin et al. 1986)
- 4.50 (HPLC-RT correlation, Wang et al. 1986)
- 4.56 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
- 4.52  $\pm$  0.15 (recommended, Sangster 1989, 1993)
- 4.374  $\pm$  0.034, 4.562  $\pm$  0.006 (shake flask/slow stirring-GC/HPLC, interlaboratory studies, Brooke et al. 1990)
- 4.30 (centrifugal partition chromatography, Berthod et al. 1992)
- 4.46 (shake flask-UV spectroscopy, pH 7.4, Alcron et al. 1993)
- 4.46 (recommended, Hansch et al. 1995)
- 4.53, 4.83 (26°C, 4°C, quoted, Piatt et al. 1996)
- 4.48  $\pm$  0.19, 4.54  $\pm$  0.61 (HPLC- $k'$  correlation: ODS column, Diol column, Helweg et al. 1997)
- 4.57, 4.49–4.64 (shake flask/slow stirring-HPLC/fluor., mean value, De Maagd et al. 1998)
- 4.60 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
- 4.50; 4.65, 4.52 (shake flask-SPME solid-phase micro-extraction; quoted lit. values, Paschke et al. 1999)

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

- 7.45 (calculated, Finizio et al. 1997)
- 7.57\*; 7.41 (generator column-GC; calculated-concn ratio  $C_o/C_A$ , measured range 0–40°C, Harner & Bidleman 1998)
- log  $K_{OA}$  =  $-5.62 + 3942/(T/K)$ ; temp range 0–40°C,  $\Delta H_{OA}$  = 63.3 kJ/mol (generator column-GC, Harner & Bidleman 1998)
- 7.52 (calculated- $S_{oct}$  and vapor pressure  $P$ , Abraham et al. 2001)
- 7.88 (solid-phase microextraction SPME-GC, Treves et al. 2001)

Bioconcentration Factor, log BCF:

- 3.42 (fathead minnow, Carlson et al. 1978)
- 2.51 (*Daphnia pulex*, Southworth et al. 1978)
- 2.57 (kinetic estimation, Southworth et al. 1978)
- 3.80 (mixed microbial population, Steen & Karickhoff 1981)
- 4.28 (*P. hoyi*, Eadie et al. 1982)
- 3.67 (microorganisms-water, Mabey et al. 1982)
- 4.38, 4.03, 4.57 (average, *Selenastum capricornutum*-dosed singly, dosed simultaneously, Casserly et al. 1983)
- 3.25 (*Chlorella fusca*; Geyer et al. 1984)
- 2.51 (fish, Govers et al. 1984)
- 2.97, 3.25, 3.25 (activated sludge, algae, fish, Freitag et al. 1985)
- 4.18; 4.28 (*P. hoyi* of Lake Michigan interstitial waters; of high sediment study site, Landrum et al. 1985)
- 2.51 (*Daphnia magna*, Newsted & Giesy 1987)
- 3.21 (10–20°C, *h. limbata*, rate constant ratio  $k_1/k_2$ , Landrum & Poore 1988)
- 4.45; 3.77; 3.43 (4°C, *P. hoyi*; *S. heringianus*; *Mysis relicta*, quoted, Landrum & Poore 1988)
- 0.756, 1.487 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)



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

- 4.36 (natural sediment, average of sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
- 4.08 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
- 4.60 (fluorescence quenching interaction with AB humic acid, Gauthier et al. 1986)
- 4.28 (sediment from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
- 4.00 (Aldrich and Fluka humic acids, Chin et al. 1989)
- 6.12 (sediments average, Kayal & Connell 1990)
- 4.22, 4.28 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo 1990b)
- 4.42 (sandy surface soil, batch equilibrium-sorption isotherm, Wood et al. 1990)
- 4.07 (Quarry dark sand, batch equilibrium-sorption isotherm, Magee et al. 1991)
- 4.64 (DOM derived from soil, fluorescence quenching method, Magee et al. 1991)
- 4.42, 4.30 (marine porewater organic colloids; marine sediment, Fort Point Channel FPC 25–29 cm, Chin & Gschwend 1992)
- 4.17; 4.18, 4.17 (sediment: concn ratio  $C_{sed}/C_w$ ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
- 4.50 (Rotterdam Harbor sediment 4.6% OC, batch sorption equilibrium, Hegeman et al. 1995)
- 4.37 (Speyer soil 1.08% OC, batch sorption equilibrium, Ou et al. 1995)
- 6.07, 7.03, 6.39; 4.12 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island; quoted lit., McGroddy & Farrington 1995)
- 5.77 (marine sediments: Fort Point Channel FPC 25–29 cm, McGroddy & Farrington 1995)
- 4.28, 4.12, 4.23 (RP-HPLC- $k'$  correlation on different stationary phases, Szabo et al. 1995)
- 4.09; 4.32 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 4.18 (range 4.13–4.20); 3.56 (range 3.54–3.56) (4°C, low organic carbon sediment  $f_{OC} = 0.0002$ , batch equilibrium; column exptl., Piatt et al. 1996)
- 4.13 (range 4.06–4.19); 3.48 (range 3.47–3.48) (26°C, low organic carbon sediment  $f_{OC} = 0.0002$ , batch equilibrium; column exptl., Piatt et al. 1996)
- 4.65;  $4.81 \pm 0.16$  (humic acid, HPLC- $k'$  correlation; quoted lit., Nielsen et al. 1997)
- 2.42–2.56 (5 soils, 20°C, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
- 4.27, 4.27, 4.12, 4.27, 4.10; mean  $4.12 \pm 0.088$  (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
- 4.38, 4.45, 4.53, 4.33, 4.42, 4.62, 4.64  $\pm 0.087$  (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
- 4.48 (4.46–4.50), 4.22 (4.20–4.23) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 3.67; 3.29, 4.04, 3.27, 4.37, 4.21 (calculated- $K_{OW}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 4.31–6.02 (range, calculated from sequential desorption of 11 urban soils; Krauss & Wilcke 2001)
- 5.34; 5.23, 4.82, 4.98 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 4.39 - algae, 4.66 - degraded algae, 3.33 - cellulose, 4.72 - collagen, 4.50 - cuticle, 4.18 - lignin, 4.67 - humic acid, 4.56 - oxidized humic acid, 4.64 - Green River kerogen, 4.88 - Pula kerogen (aliphatic-rich sedimentary organic matter, batch experiments, Salloum et al. 2002)
- 4.28 (Askov soil - a Danish agricultural soil, Sverdrup et al. 2000)
- 4.03, 4.08 (soils: organic carbon OC  $\geq 0.1\%$ , OC  $\geq 0.5\%$ , average, Delle Site 2001)
- 4.34 (average values for sediment OC  $\geq 0.5\%$ , Delle Site 2001)
- 4.70 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)
- 4.66–4.90 (sediment/water, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluor., ten Hulscher et al. 2003)
- 5.29–5.92, 5.98 (NIST SRM diesel particulate matter: flocculation-based batch equilibrium method with 59-d equilibration time, air-bridge equilibrium with 123-d equilibration time, Nguyen et al. 2004)

- 4.30–5.3, 5.2–5.5 (sediments of 5 lakes with OC ranges from 0.12–21.03%, solute concn at 1 mg/L, at 1 ng/L, sorption isotherms, Cornelissen et al. 2004)
- 4.80, 4.80, 4.50, 4.84 (sediment free of BC “black carbon”: Lake Varparanta OC 0.12%, Lake Kuorinka OC 1.39%, Lake Höytiäinen OC 3.3%, Lake Ketelmeer OC 5.51%, equilibrium sorption isotherm, Cornelissen et al. 2004)

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

Volatilization: half-lives from solution: 97, 108 min (exptl., calculated, Mackay et al. 1983).

Photolysis: calculated  $t_{1/2} = 8.4$  h for direct sunlight photolysis at 40°N latitude of midday in midsummer, near surface water and  $t_{1/2} = 59$  d (inland water) and  $t_{1/2} = 69$  d for inland water with sediment partitioning in a 5-m deep inland water body (Zepp & Schlotzhauer 1979)

$t_{1/2} = 3$  h, atmospheric and aqueous half-life, based on measured aqueous photolysis quantum yields and calculated for midday summer sunlight at 40°N latitude and  $t_{1/2} = 25$  h after adjusting for approximate winter sunlight intensity (Howard et al. 1991);

half-lives on different atmospheric particulate substrates (appr. 25  $\mu\text{g/g}$  on substrate):  $t_{1/2} = 150$  h on silica gel,  $t_{1/2} = 45$  h on alumina and  $t_{1/2} = 49$  h on fly ash (Behymer & Hites 1985);

$t_{1/2} = 59$  d under sunlight (Mill & Mabey 1985);

$k = 0.11 \text{ h}^{-1}$  with  $t_{1/2} = 6.3$  h in distilled water (Fukuda et al. 1988);

photodegradation  $k = 6.53 \times 10^{-3} \text{ min}^{-1}$  and  $t_{1/2} = 1.78$  h in methanol-water (2:3, v/v) solution with an initial concn of 5.0 ppm under high pressure mercury lamp or sunlight (Wang et al. 1991)

$k(\text{expt}) = 0.00653 \text{ min}^{-1}$  pseudo-first-order direct photolysis rate constant with the calculated  $t_{1/2} = 1.78$  h and the predicted  $k = 0.00165 \text{ min}^{-1}$  calculated by QSPR, in aqueous solution when irradiated with a 500-W medium pressure mercury lamp (Chen et al. 1996);

direct photolysis  $t_{1/2} = 4.62$  h (observed),  $t_{1/2} = 3.89$  h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001);

photochemical degradation under atmospheric conditions:  $k = (4.49 \pm 0.68) \times 10^{-5} \text{ s}^{-1}$  and  $t_{1/2} = (4.29 \pm 0.57) \text{ h}$  in diesel particulate matter,  $k = (2.11 \pm 0.04) \times 10^{-5} \text{ s}^{-1}$  and  $t_{1/2} = (9.1 \pm 0.19) \text{ h}$  in diesel particulate matter/soil mixture, and  $t_{1/2} = 17 - 4.97$  h in various soil components using a 900-W photo-irradiator as light source;  $k = (3.17 \pm 0.06) \times 10^{-6} \text{ s}^{-1}$  and  $t_{1/2} = (60.63 \pm 1.33) \text{ h}$  in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation  $k = 0.09 \times 10^{-4} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

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

$k$  (aquatic fate rate)  $= 0.01 \text{ L M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 8 \times 10^6 \text{ d}$  (Callahan et al. 1979)

$k$  (calc)  $< 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k < 36 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)

$k = (1.33 - 1.57) \times 10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  over the pH range 1–7 for the reaction with  $\text{O}_3$  in water at 25°C,  $t_{1/2} = 0.44 \text{ s}$  in presence of  $10^{-4} \text{ M}$  ozone at pH 7 (Butković et al. 1983)

$k_{\text{OH}} = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 1 \text{ K}$ ,  $k_{\text{OH}} = 2.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $319 \pm 1 \text{ K}$  (relative rate method, Biermann et al. 1985)

$k_{\text{OH}}^* = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (review, Atkinson 1989)

$k_{\text{OH}} = 25.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}}^* = 27 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 346–386 K with a calculated atmospheric lifetime of 11 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: 100% degradation within 7 d for a domestic sewage of an average of three static-flask screening test (Tabak et al. 1981);

$t_{1/2}(\text{aerobic}) = 384\text{--}4800 \text{ h}$ , based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$k = 0.0447 \text{ d}^{-1}$  with  $t_{1/2} = 16 \text{ d}$  for Kidman sandy loam and  $k = 0.0196 \text{ d}^{-1}$  with  $t_{1/2} = 35 \text{ d}$  for McLarin sandy loam all at  $-0.33 \text{ bar}$  soil moisture (Park et al. 1990);

$t_{1/2}(\text{anaerobic}) = 1536\text{--}19200 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 4$  d in inorganic solution and  $t_{1/2} = 11$  d in Kendaia soil (Manilal & Alexander 1991)

removal rate of 1.10 and 0.12 mg (g of volatile suspended solid d)<sup>-1</sup>, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers respectively under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

first-order  $k = 0.033$  to  $0.139$  L mg<sup>-1</sup> d<sup>-1</sup> for a marine PAH-degrading enrichment without sediment, the degradation rate was 2.1 to 3.5 times faster with sediment present (Poeton et al. 1999)

Biotransformation: for bacteria,  $1.6 \times 10^{-7}$  mL cell<sup>-1</sup> h<sup>-1</sup> (Paris et al. 1980; quoted, Mabey et al. 1982)

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

$k_1 = 203$  h<sup>-1</sup>;  $k_2 = 0.543$  h<sup>-1</sup> (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.31$  h<sup>-1</sup>;  $\log k_2 = -0.27$  h<sup>-1</sup> (*Daphnia pulex*, as per the correlation of Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 129.0$  mL g<sup>-1</sup> h<sup>-1</sup>;  $k_2 = 0.0046$  h<sup>-1</sup> (4°C, *p. hoyi*, Landrum 1988; quoted, Landrum & Poore 1988)

$k_1 = 52.5$  h<sup>-1</sup>;  $k_2 = 0.032$  h<sup>-1</sup> (10–20°C, *H. limbata*, Landrum & Poore 1988)

$k_1 = 94.0$  h<sup>-1</sup>;  $k_2 = 0.016$  h<sup>-1</sup> (4°C, *S. heringianus*, quoted, Landrum & Poore 1988)

$k_1 = 32.0$  h<sup>-1</sup>;  $k_2 = 0.012$  h<sup>-1</sup> (4°C, *Mysis relicta*, quoted, Landrum & Poore 1988)

$k_1 = 8.8$  mg g<sup>-1</sup> h<sup>-1</sup>;  $k_2 = 0.045$  h<sup>-1</sup> (freshwater oligochaete from sediment, Van Hoof et al. 2001)

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 6$  h with a steady-state concn of tropospheric ozone of  $2 \times 10^{-9}$  M in clean air (Butković et al. 1983)

$t_{1/2} = 2.01$ – $20.1$  h, based on photooxidation half-life in air (Howard et al. 1991);

calculated atmospheric lifetime of 11 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: computed near-surface of a water body,  $t_{1/2} = 8.4$  h for direct photochemical transformation at latitude 40°N, midday, midsummer with  $t_{1/2} = 59$  d (no sediment-water partitioning),  $t_{1/2} = 69$  d (with sediment-water partitioning) on direct photolysis in a 5-m deep inland water body (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.44$  s in presence of  $10^{-4}$  M ozone at pH 7 (Butković et al. 1983);

calculated  $t_{1/2} = 59$  d under sunlight for summer at 40°N latitude (Mill & Mabey 1985);

$t_{1/2} = 3$ – $25$  h, based on aqueous photolysis half-life (Howard et al. 1991);

photolysis  $t_{1/2} = 1.78$  h in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:  $t_{1/2} = 768$ – $9600$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction  $t_{1/2}(\text{est.}) = 1196$  h,  $t_{1/2}(\text{exptl}) = 825$  h for chemical available phenanthrene and  $t_{1/2} = 151$  h for bioavailable phenanthrene for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C. The average uptake clearance from sediment was  $(0.041 \pm 0.023)$  g of dry sediment·g<sup>-1</sup> of organism·h<sup>-1</sup>, and the rate constants to become biologically unavailable was  $(0.0055 \pm 0.003)$  h<sup>-1</sup> resulting a bioavailable  $t_{1/2} = 126$  h (Landrum 1989); desorption  $t_{1/2} = 8.6$  d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil:  $t_{1/2} = 2.5$ – $26$  d (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 9.7$  d for 5 mg/kg treatment and  $t_{1/2} = 14$  d for 50 mg/kg (Bulman et al. 1987);

biodegradation  $k = 0.0447$  d<sup>-1</sup> with  $t_{1/2} = 16$  d in Kidman sandy loam soil and  $k = 0.0196$  d<sup>-1</sup> with  $t_{1/2} = 35$  d in McLaurin sandy loam soil (Park et al. 1990);

biodegradation  $t_{1/2} = 11$  d in Kendaia soil (Manilal & Alexander 1991);

$t_{1/2} = 384$ – $4800$  h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} > 50$  d (Ryan et al. 1988);

$t_{1/2} = 0.4$ – $26$  wk, 5.7 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: depuration  $t_{1/2} = 40.9$  h in *S. heringianus* (Frank et al. 1986);

elimination  $t_{1/2} = 9$  d from rainbow trout,  $t_{1/2} = 8.4$  d from clam *Mya arenaria*,  $t_{1/2} = 1.9$  d from mussel *Mytilus edulis*;  $t_{1/2} = 7$  d from polychaete *Abarenicola pacifica*,  $t_{1/2} = 3.4$  d from Oyster,  $t_{1/2} = 0.9$  d from shrimp,  $t_{1/2} = 4.8$  d from polychaete *Nereis virens*,  $t_{1/2} = 6.1$  d from clam *Mercenaria mercenaria* (Meador et al. 1995).

TABLE 4.1.1.23.1

Reported aqueous solubilities of phenanthrene at various temperatures

1.

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
	experimental		smoothed				
24.6	1.12	0	0.39	8.4	0.501	8.5	0.423
24.6	1.11	24.8	1.16	11.1	0.5507	10.0	0.468
29.9	1.49	25	1.18	14.0	0.640	12.5	0.512
29.9	1.49	29.9	1.49	17.5	0.784	15.0	0.601
30.3	1.47	30.3	1.52	20.2	0.881	21.0	0.816
30.3	1.48	38.4	2.27	23.3	1.085	24.3	0.995
38.4	2.44, 2.45	40.1	2.47	25.0	1.151	29.9	1.277
40.1	2.27, 2.28	47.5	3.63	29.3	1.372		
40.1	2.25	50	4.14	34.6	1.627	temp dependence eq. 2	
47.5	3.87, 3.88	50.1	4.16	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 36.32$		S	μg/kg
47.5	3.87	50.2	4.19			a	0.0025
50.1	4.30, 4.38	54.7	5.34			b	0.8059
50.1	4.32	59.2	6.85			c	5.413
50.2	4.08, 4.04	60.5	7.30			d	324
50.2	4.11	65.1	9.60				
54.7	5.66, 5.64	70.7	13.3			May et al. 1978b	
54.7	5.63	71.9	14.2			generator column-HPLC	
59.2	7.17, 7.19	73.4	15.6			t/°C	S/g·m <sup>-3</sup>
59.2	7.21	75	17.2			25	1.002
60.5	7.20, 7.60					29	1.220
65.1	9.80	temp dependence eq. 1				temp dependence eq. 2	
65.1	9.70	ln x	mole fraction			S	μg/kg
65.1	9.80	$\Delta H_{\text{fus}}$	$16.28 \pm 0.08$			a	0.0025
70.7	12.4	$10^2 \cdot b$	$3.74 \pm 0.13$			b	0.8059
70.7	12.6	c	$27.9 \pm 0.4$			c	5.413
70.7	12.4					d	324
71.9	18.8						
73.4	21.5						

 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 16.28$  $\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.81$   
for temp range 5–30°C

Empirical temperature dependence equations:

Wauchope & Getzen (1972):  $R \cdot \ln x = -[H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K)$  (1)May et al. (1978):  $S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t_{1/2} + c \cdot t + d$  (2)

TABLE 4.1.1.23.1 (Continued)

2.

May 1980		May et al. 1983		Whitehouse 1984		Shaw 1989	
generator column-HPLC		generator column-HPLC		generator column-HPLC/UV		IUPAC recommended	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
4.0	0.361	4.0	0.361	4.6	0.358	0	0.40
8.5	0.423	8.5	0.423	8.8	0.437	10	0.50
10	0.468	10.0	0.468	12.9	0.556	20	0.85
12.5	0.512	12.5	0.512	17.0	0.720	25	1.10
15	0.601	15.5	0.602	21.1	0.880	30	1.40
20	0.787	20.0	0.788	25.3	1.10	40	2.50
21	0.816	21.0	0.817			50	4.10
24.3	0.955	24.3	0.956			50	7.20
29.9	1.227	29.9	1.188			70	13.0
						75	17.0

temp dependence eq. 2

S	μg/kg
a	0.0025
b	0.8059
c	5.412
d	324

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.81$   
for temp range 5–30°C

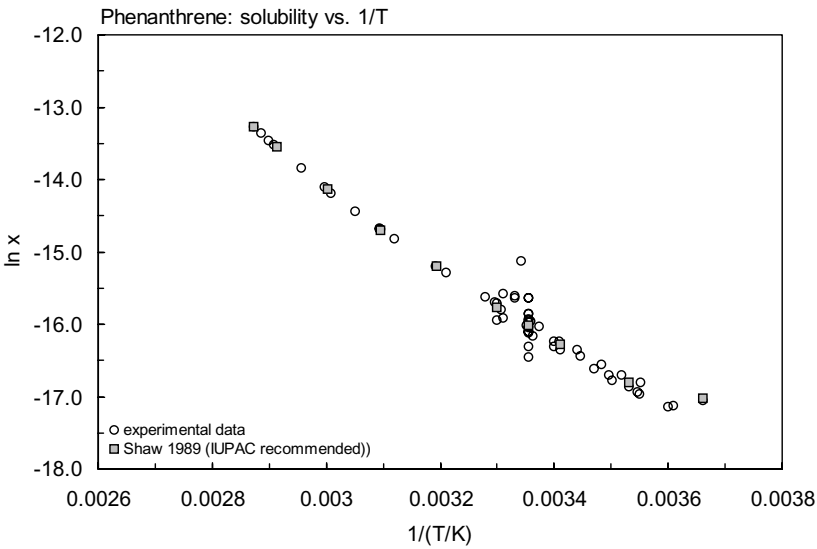


FIGURE 4.1.1.23.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for phenanthrene.

TABLE 4.1.1.23.2

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

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

## 1.

Nelson & Senseman 1922		Mortimer & Murphy 1923		Stull 1947		Bradley & Cleasby 1953	
isoteniscope-Hg manometer		isoteniscope-Hg manometer		summary of literature data		effusion	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
230	7773	203.6	3626	118.2	133.3	36.7	0.0853
235	9079	233.8	8999	154.3	666.6	39.85	0.1187
240	10532	246.0	12572	173.0	1333	42.0	0.160
245	12146	271.5	24265	193.7	2666	46.7	0.2466
250	13919	271.5	24398	215.8	5333	48.8	0.2973
255	15892	293.1	39957	229.0	7999	48.8	0.3000
260	18065	293.2	39970	249.0	13332	39.15	0.1080
265	20492	293.2	39983	277.1	26664	42.1	0.1480
270	23145	306.4	53222	308.0	53329	44.62	0.1933
275	26091	324.5	53289	340.2	101325	46.7	0.2426
280	18331	324.9	77954			49.65	0.3213
285	32891	325.4	78487	mp/ $^{\circ}\text{C}$	99.5		
290	36810	337.1	79007			eq. 2	P/mmHg
300	45823	337.1	98792			A	10.388
310	56529	345.1	115244			B	4519
320	69169	245.7	116110				
330	83913	346.8	117844				
340	100925						

## 2.

Hoyer & Peperle 1958		Osborn & Douslin 1975		Macknick & Prausnitz 1979		de Kruif 1980	
effusion		inclined-piston manometry		gas saturation-GC		effusion	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
data presented in		100.0	30.4	51.60	0.465	38.96	0.1
eq. 1	P/mmHg	105.0	41.20	57.70	0.813	45.29	0.2
A	16.0	110.0	54.66	61.85	1.321	49.11	0.3
B	5998	115.0	73.59	67.35	2.120	51.88	0.4
for temp range 0–60 $^{\circ}\text{C}$		120.0	95.99	71.80	3.093	54.06	0.5
		125.0	124.79	78.90	5.653	55.86	0.6
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.90$		130.0	161.05	83.40	8.892	57.40	0.7
		135.0	207.18	90.30	14.52	58.75	0.8
		140.0	264.91			9.95	0.9
		145.0	335.30	eq. 1a	P/mmHg	61.02	1.0
		150.0	420.76	A	26.648	25.0	0.18
				B	10.484		
		triple pt. tp/K	372.385			$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 90.5$	

TABLE 4.1.1.23.2 (Continued)

Hoyer & Peperle 1958		Osborn & Douslin 1975		Macknick & Prausnitz 1979		de Kruif 1980	
effusion		inclined-piston manometry		gas saturation-GC		effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
<div><div><math>\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) =</math> at 398.15 K68.58 at tp70.79</div><div><math>\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 87.24</math> at tp</div><div><math>\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 16.44</math></div></div>							
3.							
Sonnefeld et al. 1983		Sato et al. 1986		Oja & Suuberg 1998			
generator column-HPLC		gas saturation-electrobalance		Knudsen effusion			
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa		
10.35	0.00219	322.9	0.340	30.34	0.0357		
10.35	0.00222	324.6	0.420	37.22	0.0909		
10.35	0.00211	328.5	0.655	40.77	0.140		
10.35	0.00238	333.0	1.05	44.79	0.227		
18.85	0.00738	335.2	1.34	40.1	0.323		
18.85	0.00731	337.8	1.73	59.78	0.998		
18.85	0.00749	339.5	2.03				
29.5	0.0262	343.2	2.98	eq. 1a	P/Pa		
29.5	0.0271	346.0	3.75	A	11.423		
29.5	0.0268	347.8	4.42	B	33.387		
38.65	0.0899					$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.0$	
38.65	0.0917	eq. 3a	P/Pa				
3865	0.0889	A	20.3950				
38.65	0.0849	B	3931.20				
38.80	0.0863	C	−139.743				
38.80	0.0844						
38.88	0.0902	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 96.5$					
38.90	0.0902						
38.90	0.0922						
38.90	0.0906						
25.0	0.0161						
eq. 1	P/Pa						
A	14.852						
B	4962.77						
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.0$							

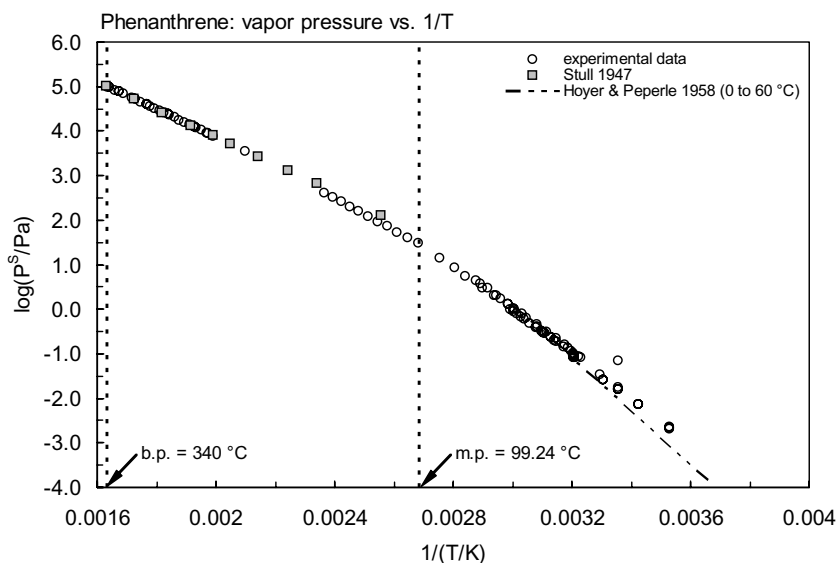
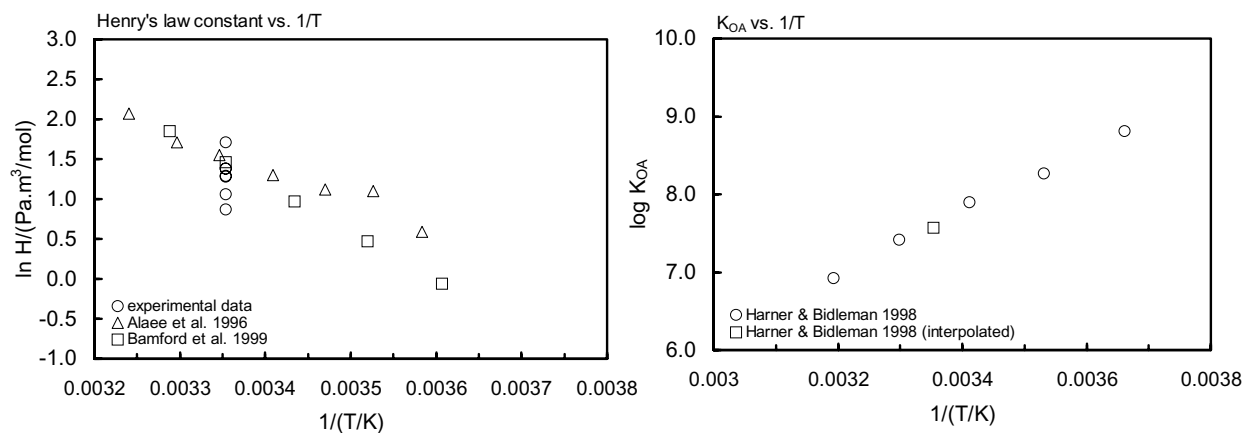


FIGURE 4.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for phenanthrene.

TABLE 4.1.1.23.3  
 Reported Henry's law constants and octanol-air partition coefficients of phenanthrene at various temperatures and temperature dependence equations

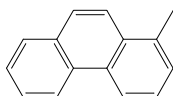
$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)	
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)	
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)				
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)	
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)				
Henry's law constant					$\log K_{OA}$	
Alaee et al. 1996		Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-GC		gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)	t/°C	$\log K_{OA}$
				average		
5.9	1.81	4.1	0.88, 1.00	0.94	0	8.808
10.4	2.99	11.0	1.53, 1.67	1.60	10	8.267
15.0	3.06	18.0	2.55, 2.70	2.65	20	7.898
20.2	3.66	25.0	4.08, 4.51	4.29	30	7.418
25.7	4.73	31.0	5.97, 6.82	6.38	40	6.926
30.2	5.54				25(exptl)	7.57
34.7	7.90				25(calc)	7.41
$\ln K_{AW} = A - B/(T/K)$		$\ln K_{AW} = A - B/(T/K)$			$\log K_{OA} = A + B/(T/K)$	
A	6.0313	A	14.1293		A	-5.62
B	3524.2	B	5689.2		B	3942
enthalpy of volatilization:		enthalpy, entropy change:			enthalpy of phase change	
$\Delta H_{vol}/(\text{kJ}\cdot\text{mol}^{-1}) = 29.3$		$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 47.3 \pm 1.2$			$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 75.5$	
at 20°C		$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 118$				
		at 25°C				





**FIGURE 4.1.1.23.3** Logarithm of Henry's law constant and  $K_{OA}$  versus reciprocal temperature for phenanthrene.

## 4.1.1.24 1-Methylphenanthrene



Common Name: 1-Methylphenanthrene

Synonym:

Chemical Name: 1-methylphenanthrene

CAS Registry No: 832-69-6

Molecular Formula:  $C_{15}H_{12}$

Molecular Weight: 192.256

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

123 (Weast 1982–83; Lide 2003)

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

354 (Lide 2003)

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

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

188.0 (Ruelle & Kesselring 1997)

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.109 (mp at  $123^{\circ}C$ )

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):

0.255\* ( $24.1^{\circ}C$ , generator column-HPLC/UV, measured range  $6.6$ – $29.9^{\circ}C$ , May et al. 1978a, 1983)

0.269 (generator column-HPLC, May et al. 1978b)

$S/(\mu g/kg) = 55.42 + 6.8016 \cdot (t/^{\circ}C) - 0.1301 \cdot (t/^{\circ}C)^2 + 0.0080 \cdot (t/^{\circ}C)^3$ ; temp range  $6.6$ – $29.9^{\circ}C$  (generator column-HPLC/UV, May et al. 1978)

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

0.0186; 0.0160 (supercooled liquid  $P_L$ , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -3987/(T/K) + 11.64$ ;  $\Delta H_{vap} = -76.3$  kJ $\cdot$ mol $^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

5.0\* (gas stripping-GC, measured range  $4.1$ – $31^{\circ}C$ , Bamford et al. 1999)

$\ln K_{AW} = -4257.88/(T/K) + 8.0587$ ,  $\Delta H = 35.4$  kJ mol $^{-1}$ ; measured range  $4.1$ – $31^{\circ}C$  (gas stripping-GC, Bamford et al. 1999)

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

5.08 (HPLC-RT correlation, Wang et al. 1986)

5.08 (recommended, Sangster 1989, 1994)

5.08 (recommended, Hansch et al. 1995)

5.10–5.20; 5.15 (quoted lit. range; lit. mean, Meador 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: photodegradation of 5 ppm initial concentration in methanol-water (3:7, v/v) by high pressure mercury lamp or sunlight with a rate constant  $k = 1.84 \times 10^{-3}$  min $^{-1}$  and  $t_{1/2} = 6.27$  h (Wang et al. 1991); the

pseudo-first-order direct photolysis  $k(\text{exptl}) = 0.00184 \text{ min}^{-1}$  with the calculated  $t_{1/2} = 6.27 \text{ h}$  and the predicted  $k = 0.0026 \text{ min}^{-1}$  calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

direct photolysis  $t_{1/2} = 3.10 \text{ h}$  (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: direct photolysis  $t_{1/2} = 3.10 \text{ h}$  (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis  $t_{1/2} = 6.27 \text{ h}$  in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:

Sediment:

Soil:

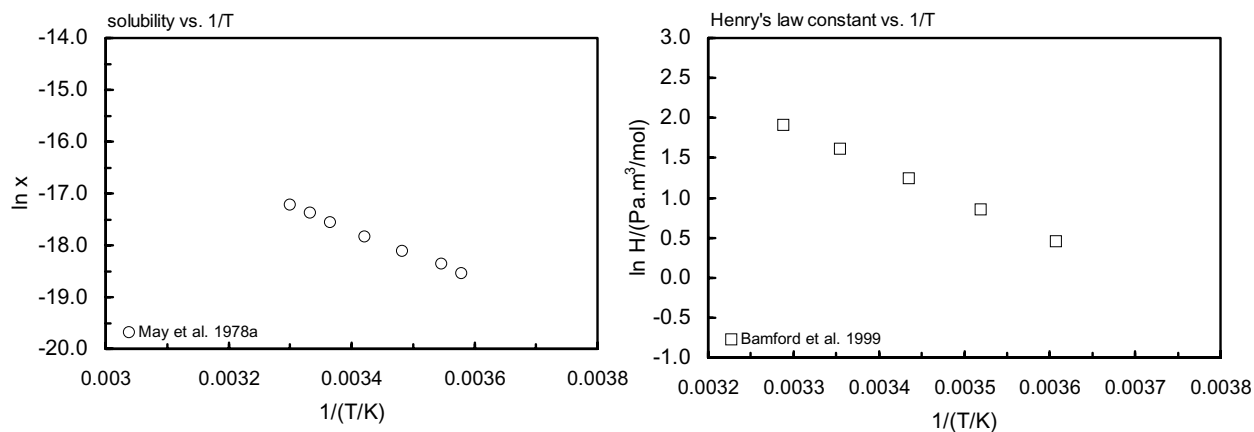
Biota: elimination  $t_{1/2} = 6.7 \text{ d}$  from Oyster, 6.0 d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.24.1

Reported aqueous solubilities and Henry's law constant of 1-methylphenanthrene at various temperature and the empirical temperature dependence equations

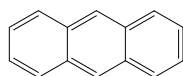
$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

Aqueous solubility						Henry's law constant	
May et al. 1978a		May et al. 1978b		May 1980, 1983		Bamford et al. 1999	
generator column-HPLC		generator column-HPLC		generator column-HPLC		gas stripping-GC/MS	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	H/(Pa m <sup>3</sup> /mol)
6.6	0.0952	25.0	0.269	6.6	0.0952	4.1	1.42, 1.75
8.9	0.114			8.9	0.114		av. 1.58
14.0	0.147	temp dependence eq. 1		14.0	0.147	11.0	2.20, 2.53
19.2	0.193	S	μg/kg	19.2	0.193		av. 2.36
24.1	0.255	a	0.0080	24.1	0.255	18.0	3.26, 3.69
26.9	0.304	b	0.1301	26.9	0.304		av. 3.47
29.9	0.355	c	6.8016	29.9	0.355	25.0	4.62, 5.42
		d	55.42				av. 5.00
data of May et al. 1978a				data of May 1980 fitted to		31.0	6.09, 7.52
temp dependence eq. 1		ΔH <sub>sol</sub> /(kJ mol <sup>-1</sup> ) = 30.08		temp dependence eq. 1			av. 6.77
S		measured between 5–30°C		S			
a				a		ln K <sub>AW</sub> = A – B/(T/K)	
b				b		A	8.0587
c				c		B	4257.88
d				d			
						enthalpy, entropy change:	
						ΔH/(kJ·mol <sup>-1</sup> ) = 35.4 ± 1.9	
						ΔS/(J·K <sup>-1</sup> mol <sup>-1</sup> ) = 67	
						at 25°C	



**FIGURE 4.1.1.24.1** Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1-methylphenanthrene.

## 4.1.1.25 Anthracene



Common Name: Anthracene

Synonym: paranaphthalene, green oil, tetra olive NZG

Chemical Name: anthracene

CAS Registry No: 120-12-7

Molecular Formula:  $C_{14}H_{10}$

Molecular Weight: 178.229

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

215.76 (Lide 2003)

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

339.9 (Lide 2003)

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

1.25 ( $27^{\circ}C$ , Dean 1985)

1.28 ( $25^{\circ}C$ , Lide 2003)

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

139 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

28.83 (Parks & Huffman 1931)

28.87 (Tsonopoulos & Prausnitz 1971; Ruelle & Kesselring 1997)

29.37 (Chickos et al. 1999)

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

58.99 (Tsonopoulos & Prausnitz 1971; Wauchope & Getzen 1972; Ubbelohde 1978)

58.58 (Casellato et al. 1973)

55.65 (De Kruif 1980)

60.08, 44.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0134 (mp at  $215.76^{\circ}C$ )

0.0101 (calculated,  $\Delta S_{fus} = 58.6 J/mol K$ , Passivirta et al. 1999)

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

0.075 ( $27^{\circ}C$ , shake flask-nephelometry, Davis et al. 1942)

0.075 (shake flask-UV, Klevens 1950)

0.075 (Pierotti et al. 1959; Weimer & Prausnitz 1965)

0.112 (shake flask, binding to bovine serum albumin-UV, Sahyun 1966)

0.080 (shake flask-UV/fluorescence, Barone et al. 1967)

0.043 ( $20^{\circ}C$ , shake flask-UV, Eisenbrand & Baumann 1970)

0.040 (shake flask-UV, Eisenbrand & Baumann 1970)

0.171, 0.0392 ( $20^{\circ}C$ , HPLC-relative retention correlation, different stationary or mobile phases, Locke 1974)

0.075\* (extrapolated value, shake flask-UV, measured range  $25-74.7^{\circ}C$ , Wauchope & Getzen 1972)

$R \cdot \ln x = -6930/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 19.3 + 0.0181 \cdot (T/K)$ , temp range  $35.4-73.4^{\circ}C$  (shake flask-UV measurements, Wauchope & Getzen 1972)

0.030 (fluorescence/UV, Schwarz & Wasik 1976)

0.073 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0446 (Rossi 1977; Neff 1979)

0.041\* (shake flask-UV, measured range  $8.6-31.3^{\circ}C$ , Schwarz 1977)

0.074 (Lu et al. 1978)

0.0446\* (generator column-HPLC/UV, measured range  $5.2-29.3^{\circ}C$ , May et al. 1978)

0.0434\* ( $24.6^{\circ}C$ , generator column-HPLC, measured range  $5.2-28.7^{\circ}C$ , May 1980)

$S/(\mu\text{g/kg}) = 8.21 + 0.8861 \cdot (t/^\circ\text{C}) + 0.0097 \cdot (t/^\circ\text{C})^2 + 0.0013 \cdot (t/^\circ\text{C})^3$ ; temp range 5.2–29.3°C (generator column-HPLC/UV, May et al. 1978)

- 0.033 (20°C, generator column-fluorescence, Hashimoto et al. 1982)  
 0.0434\* (24.6°C, generator column-HPLC, measured range 5.6–29.3°C, May et al. 1983)  
 0.030, 0.051 (generator column-HPLC/UV, Swann et al. 1983)  
 0.04257\* (generator column-spectrofluorimetry, measured range 10–30°C, Velapoldi et al. 1983)  
 0.0446 (generator column-HPLC/UV, Wasik et al. 1983)  
 0.066 (average lit. value, Pearlman et al. 1984)  
 0.0698 (generator column-HPLC/fluorescence, Walters & Luthy 1984)  
 0.0442\* (generator column-HPLC/UV, measured range 4.6–25.3°C, Whitehouse 1984)  
 0.0446 (vapor saturation-UV, Akiyoshi et al. 1987)  
 0.0443, 0.034 (generator column-HPLC/UV, Billington et al. 1988)  
 0.041 (20°C, shake flask/UV, ring test, Kishi & Hashimoto 1989)  
 0.062\* (recommended, IUPAC Solubility Data Series, Shaw 1989)  
 0.070 (23°C, shake flask-HPLC/UV/fluorescence, Pinal et al. 1991)  
 0.058 (generator column-HPLC, Vadas et al. 1991)  
 0.0488 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)  
 0.043 (shake flask-HPLC, Haines & Sandler 1996)  
 0.0796; 0.138, 0.0743 (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)  
 0.093 (generator column-HPLC/fluorescence, De Maagd et al. 1998)  
 0.070 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)  
 $\log [S_L/(\text{mol/L})] = 1.679 - 1509/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $\ln x = -1.43611 - 5307.35/(T/K)$ ; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)  
 0.0434\* (24.61°C, generator column-HPLC/fluoro., Reza et al. 2002)  
 $\ln x = (0.50 \pm 0.45) + [(-5876 \pm 135)/(T/K)]$ ; temp range 282.09–323.07 K (Reza et al. 2002)  
 0.0438\* (generator column-HPLC/UV, measured range 0–50°C, Dohányosová et al. 2003)  
 $\ln x = -33.7547 + 14.5018/\tau + C \ln \tau$ ,  $\tau = (T/K)/298.15$  K; temp range 0–50°C (generator column-HPLC/UV, temp range 0–50°C, Dohányosová et al. 2003)

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

- 5680\* (220°C, isoteniscope-Hg, measured range 220–342°C, Nelson & Senseman 1922)  
 6399\* (223.3°C, isoteniscope-Hg manometer, measured range 223.3–340.5°C, Mortimer & Murphy 1923)  
 $\log (P_s/\text{mmHg}) = 10.972 - 4595/(T/K)$ ; temp range 100–210°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)  
 $\log (P_L/\text{mmHg}) = 7.910 - 3093/(T/K)$ ; temp range 223.2–340.5°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)  
 133.3\* (145.0°C, summary of literature data, temp range 145.0–342.0°C, Stull 1947)  
 0.001014 (static method-Rodebush gauge, Sears & Hopke 1949)  
 $\log (P/\text{mmHg}) = 12.0072 - 5102.6/(T/K)$ ; temp range 378–398 K (Rodebush gauge, Sears & Hopke 1949)  
 $3.60 \times 10^{-3}$  (effusion method, Inokuchi et al. 1952; quoted, Bidleman 1984)  
 $8.31 \times 10^{-4}$ \* (effusion method, Bradley & Cleasby 1953)  
 $\log (P/\text{cmHg}) = 11.638 - 5320/(T/K)$ ; temp range 65.7–80.4°C (Antoine eq., Bradley & Cleasby 1953)  
 $1.04 \times 10^{-3}$  (fluorescence spectroscopy, Stevens 1953)  
 $\log (P/\text{mmHg}) = 12.002 - 5102/(T/K)$ ; temp range 396–421 K (fluorescence, Stevens 1953)  
 $\log (P/\text{mmHg}) = 11.15 - 5401/(T/K)$ ; temp range 30–100°C, (Knudsen effusion method, Hoyer & Peperle 1958)  
 $8.62 \times 10^{-4}$  (effusion method, Kelley & Rice 1964)  
 $\log (P/\text{mmHg}) = 12.068 - 5145/(T/K)$ ; temp range 69–86°C (effusion method, Kelley & Rice 1964)  
 $3.87 \times 10^{-7}$  (Wakayama & Inokuchi 1967)  
 0.0024\* (effusion method-interpolated, measured range 290.1–358 K, Wiedemann & Vaughan 1969, Wiedemann 1972)

- $\log (P/\text{mmHg}) = 10.0216 - 4397.60/(T/K)$ ; temp range 290.1–358 K (Knudsen method, Wiedemann & Vaughan 1969, Wiedemann 1972)
- $\log (P/\text{mmHg}) = 7.67401 - 2819.63/(247.02 + t/^{\circ}\text{C})$ ; temp range: 175.5–380°C (liquid state, Antoine eq., Zwolinski & Wilhoit 1971)
- $\log (P/\text{mmHg}) = [-0.2185 \times 16823.6/(T/K)] + 8.70760$ ; temp range 100–600°C (Antoine eq., Weast 1972–73)  $1.113 \times 10^{-3}$ \* (Knudsen effusion weight-loss method, extrapolated Malaspina et al. 1973)
- $\log (P/\text{torr}) = 12.616 - 5277/(T/K)$ ; temp range 352.7–432.3 K (Knudsen method, Malaspina et al. 1973)  $1.47 \times 10^{-5}$  (effusion method, Murray et al. 1974)
- 0.026 (20°C, Radding et al. 1976)
- $9.04 \times 10^{-4}$  (effusion method, Taylor & Crooks 1976)
- $5.59 \times 10^{-3}$  (gas saturation, Power et al. 1977)
- $1.41 \times 10^{-3}$ \* (gas saturation, extrapolated-Clapeyron eq., measured range 85.25–119.95°C, Macknick & Prausnitz 1979)
- $\log (P/\text{mmHg}) = 26.805 - 11402/(T/K)$ ; temp range 85.25–119.95°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
- $7.50 \times 10^{-4}$ \* (effusion methods, extrapolated, measured range 64.44–87.74°C, De Kruif 1980)
- $4.90 \times 10^{-4}$  (calculated-TSA, Amidon & Anik 1981)
- $1.83 \times 10^{-3}$ \* (gas saturation, extrapolated-Antoine eq., measured range 50–85°C, Grayson & Fosbraey 1982)
- $1.44 \times 10^{-3}$ \* (gas saturation, extrapolated-Antoine eq. measured range 80–125°C, Bender et al. 1983)
- $\ln (P/\text{Pa}) = 31.620 - 11378/(T/K)$ ; temp range 353.6–398.6 K (Antoine eq., Bender et al. 1983)
- $8.0 \times 10^{-4}$ \* (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)
- $\log (P/\text{Pa}) = 12.977 - 4791.87/(T/K)$ ; temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)
- $8.0 \times 10^{-4}$  (gas saturation-HPLC, Wasik et al. 1983)
- 0.10, 0.0638 ( $P_{\text{GC}}$  by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
- 0.0865 (supercooled liquid  $P_{\text{L}}$ , converted from literature  $P_{\text{S}}$  with  $\Delta S_{\text{fus}}$  Bidleman 1984)
- $\log (P_{\text{L}}/\text{kPa}) = 6.53182 - 2550.737/(221.756 + t/^{\circ}\text{C})$ ; temp range 223.2–340.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P_{\text{L}}/\text{kPa}) = 6.66266 - 2659.55/(230.119 + t/^{\circ}\text{C})$ ; temp range 220–310°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P/\text{mmHg}) = 8.91 - 3761/(T/K)$ ; temp range: 100–160°C (Antoine eq., Dean 1985, 1992)
- $\log (P/\text{mmHg}) = 7.67401 - 2819.63/(247.02 + t/^{\circ}\text{C})$ ; temp range: 176–380°C (Antoine eq., Dean 1985, 1992)
- $1.06 \times 10^{-3}$ \* (gas saturation-GC, Rordorf 1985)
- $8.05 \times 10^{-4}$ \* (extrapolated-Clausius-Clapeyron eq. on gas saturation data, Hansen & Eckert 1986)
- $\log (P/\text{mPa}) = 17.88 - 5359/(T/K)$ ; temp range 313–363 K (Clausius-Clapeyron eq., Hansen & Eckert 1986)
- $1.14 \times 10^{-3}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log (P_{\text{S}}/\text{kPa}) = 10.58991 - 4903.3/(-1.58 + T/K)$ ; temp range 299–439 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_{\text{S}}/\text{kPa}) = 11.76139 - 5315.532/(T/K)$ ; temp range 313–363 K, (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_{\text{S}}/\text{kPa}) = 10.75544 - 4947.751/(T/K)$ ; temp range 363–393 K (solid, Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log (P_{\text{L}}/\text{kPa}) = 7.47799 - 3612.44/(-44.906 + T/K)$ ; temp range 504–615 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)
- $5.73 \times 10^{-4}$ ;  $5.60 \times 10^{-3}$  (literature mean solid  $P_{\text{S}}$ , supercooled liquid  $P_{\text{L}}$ , Bidleman & Foreman 1987)
- 0.086, 0.0940 (supercooled  $P_{\text{L}}$ , converted from literature  $P_{\text{S}}$  with different  $\Delta S_{\text{fus}}$  values, Hinckley et al. 1990)
- 0.100, 0.0689 ( $P_{\text{GC}}$  by GC-RT correlation with different reference standards, Hinckley et al. 1990)
- $\log P_{\text{L}}/\text{Pa} = 11.18 - 3642/(T/K)$  (GC-RT correlation, Hinckley et al. 1990)
- $\log (P/\text{mmHg}) = -120.0992 + 4.478/(T/K) + 52.574 \cdot \log (T/K) - 4.7697 \times 10^{-2} \cdot (T/K) + 1.5020 \times 10^{-5} \cdot (T/K)^2$ ; temp range 489–873 K (vapor pressure eq., Yaws 1994)
- 0.0162;  $7.64 \times 10^{-4}$ , 0.0617 (liquid  $P_{\text{L}}$  by GC-RT correlation; quoted  $P_{\text{S}}$ , converted to  $P_{\text{L}}$ , Donovan 1996)
- 0.0661 (supercooled liquid  $P_{\text{L}}$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
- 0.000144–0.00313; 0.000804–0.00511; 0.000683–0.00484 (quoted exptl. values measured by: effusion, gas saturation; manometry, Delle Site 1997)
- 0.0049–0.00125; 0.000925–0.00129 (quoted lit. values by: calculation; from GC-RT relation, Delle Site 1997)

$8.69 \times 10^{-4}$ \* (Knudsen effusion, extrapolated-Antoine eq. derived from exptl. data, temp range 30–60°C, Oja & Suuberg 1998)  
 $\log(P/\text{Pa}) = 33.281 - 12024/(T/\text{K})$ ; temp range 318–363 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)  
 $9.01 \times 10^{-2}$ ;  $9.08 \times 10^{-4}$  (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_S$  with fugacity ratio F, Passivirta et al. 1999)  
 $\log(P_S/\text{Pa}) = 11.66 - 4380/(T/\text{K})$  (solid, Passivirta et al. 1999)  
 $\log(P_L/\text{Pa}) = 8.39 - 2872/(T/\text{K})$  (supercooled liquid value, Passivirta et al. 1999)  
 $\log(P/\text{Pa}) = 12.977 - 4791.89/(T/\text{K})$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)  
0.0724; 0.0442 (supercooled liquid  $P_L$ , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)  
 $\log(P_L/\text{Pa}) = -3780/(T/\text{K}) + 11.54$ ;  $\Delta H_{\text{vap}} = -72.4 \text{ kJ}\cdot\text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)  
0.0014 (solid  $P_S$ , gas saturation-GC/MS, Mader & Pankow 2003)  
0.0922 (supercooled liquid  $P_L$ , calculated from  $P_S$  assuming  $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$ , Mader & Pankow 2003)  
 $\ln(P/\text{Pa}) = 34.261 - 12339/(T/\text{K})$ ; temp range 313–363 K (regression eq. of Hansen & Eckert 1986 data, Li et al. 2004)  
 $\ln(P/\text{Pa}) = (34.199 \pm 0.641) - (12332 \pm 229)/(T/\text{K})$ ; temp range 348–368 K (Knudsen effusion technique, Li et al. 2004)

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

6.59 (gas stripping-GC, Southworth 1977, 1979)  
7.19 (gas stripping-GC, Mackay & Shiu 1981)  
1.96 (wetted-wall column/GC, Fendinger & Glotfelty 1990)  
3.30 (gas stripping-GC, Friesen et al. 1993)  
8.68 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)  
4.94\* (gas stripping-GC, measured range 4.1–31°C, Alaei et al. 1996)  
 $\ln K_{\text{AW}} = 4.6774 - 3235.5/(T/\text{K})$ ; temp range: 5.4–35.3°C (gas stripping-GC, Alaei et al. 1996)  
5.64\* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)  
 $\ln K_{\text{AW}} = -5629.06/(T/\text{K}) + 12.75$ ,  $\Delta H = 46.8 \text{ kJ mol}^{-1}$ , measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)  
 $\log[H/(\text{Pa m}^3/\text{mol})] = 6.91 - 1363/(T/\text{K})$ , (Passivirta et al. 1999)  
4.58 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 2001)  
 $\log K_{\text{AW}} = 2.065 - 1404/(T/\text{K})$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

4.45 (Hansch & Fujita 1964; Leo et al. 1971; Hansch & Leo 1979)  
4.67 (calculated-fragment const., Rekker 1977)  
4.45 (calculated from Leo 1975, Southworth et al. 1978)  
4.54 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)  
3.45 (HPLC-RT correlation, Veith 1979a)  
4.34 (Kenaga & Goring 1980)  
4.49 (HPLC- $k'$  correlation, McDuffie 1981)  
4.38 (HPLC- $k'$  correlation, Hanai et al. 1981)  
4.63 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)  
4.20 (HPLC- $k'$  correlation, D'Amboise 1982)  
4.45 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)  
4.45 (RP-HPLC-RT correlation, Rapaport et al. 1984)  
4.45 (shake flask-GC, Haky & Leja 1986)  
4.51 (HPLC-RT correlation, Eadsforth 1986)  
4.63 (HPLC-RT correlation, Wang et al. 1986)  
4.80 (HPLC-RT correlation, De Kock & Lord 1987)  
 $4.50 \pm 0.15$  (recommended, Sangster 1989, 1993)  
4.57 (TLC-RT correlation, De Voogt et al. 1990)  
4.45 (recommended, Hansch et al. 1995)  
 $4.53 \pm 0.19$ ,  $4.55 \pm 0.61$  (HPLC- $k'$  correlation: ODS column, Diol column, Helweg et al. 1997)



- 4.68 (range 4.55–4.79) (shake flask-HPLC/fluo., De Maagd et al. 1998)  
 5.34 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

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

- 7.30 (calculated- $K_{OW}/K_{AW}$ , Wania & Mackay 1996)  
 7.34 (calculated, Finizio et al. 1997)  
 7.55 (calculated- $S_{oct}$  and vapor pressure  $P$ , Abraham et al. 2001)

## Bioconcentration Factor, log BCF:

- 3.08, 2.68 (*Daphnia pimephales*, Southworth 1977)  
 2.88 (*Daphnia pulex*, Herbes & Risi 1978)  
 2.96 (*Daphnia pulex*, Southworth et al. 1978)  
 3.08 (kinetic estimation, Southworth et al. 1978)  
 3.89 (algae, Geyer et al. 1981)  
 4.22 (*P. hoyi*, Eadie et al. 1982)  
 3.67 (microorganisms-water, Mabey et al. 1982)  
 2.83 (bluegill sunfish, Spacie et al. 1983)  
 3.83 (activated, sludge, Freitag et al. 1984)  
 3.89 (algae, Geyer et al. 1984)  
 2.21 (goldfish, Ogata et al. 1984)  
 2.96, 3.89, 3.83 (fish, algae, activated sludge, Freitag et al. 1985)  
 2.99 (*Daphnia magna*, Newsted & Giesy 1987)  
 0.820, 1.373 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

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

- 4.42 (natural sediment, average of sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)  
 3.74 (22°C, suspended particulates, Herbes et al. 1980)  
 4.204 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)  
 4.20 (soil, shake flask-UV, Karickhoff 1981)  
 3.95, 4.46 (Aldrich humic acid 9.4 mg/L DOC, RP-HPLC separation, equilibrium dialysis, Landrum et al. 1984)  
 3.95, 4.73 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/L DOC: Landrum et al. 1984)  
 4.87, 5.70 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)  
 3.81, 4.87, 4.62, 4.20 (humic materials in natural water: Huron River 6.1% DOC spring, Huron river 6.7% DOC winter, Grand River 10.7% DOC spring, Lake Michigan 5.5% DOC spring, Lake Erie 9.6% DOC spring, RP-HPLC separation method, Landrum et al. 1984)  
 4.20 (soil, shake flask-LSC, Nkedi-Kizza 1985)  
 4.93 (fluorescence quenching interaction with AB humic acid, Gauthier et al. 1986)  
 4.38 (HPLC- $k'$  correlation, Hodson & Williams 1988)  
 4.21  $\pm$  0.11 (Aldrich and Fluka humic acids, observed; Chin et al. 1989)  
 4.11 (soil-fine sand 0.2% OC, dynamic soil column studies, Enfield et al. 1989)  
 5.76 (sediments average, Kayal & Connell 1990)  
 4.41 (RP-HPLC correlation, Pussemier et al. 1990)  
 4.53, 4.42 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)  
 4.34, 4.38, 4.32 (RP-HPLC- $k'$  correlation on different stationary phases, Szabo et al. 1995)  
 4.65 (humic acid, HPLC- $k'$  correlation; Nielsen et al. 1997)  
 4.62 (4.60–4.64) (sediment from Lake Oostvaardersplassen, shake flask-HPLC/UV, de Maagd et al. 1998)  
 4.40; 4.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)  
 4.36–5.97; 4.20–6.90 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)  
 5.31; 5.33, 5.12, 4.92 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)  
 4.34; 4.26; 3.95–5.70 (calculated- $K_{OW}$ ; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)

- 4.375 at pH 4, 4.42 at pH 7, 4.39 at pH 10 in 0.001 M NaCl; 4.415 at pH 4, 4.37 at pH 7, 4.30 at pH 10 in 0.01 M NaCl; 4.50 at pH 4, 4.24 at pH 7, 4.27 at pH 10 in 0.1 M NaCl; 4.38 at pH 4, 4.40 at pH 7, 4.12 at pH 10 in 1 mM  $\text{Ca}^{2+}$  in 0.1 M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautman & Morgan 1993a)
- 4.28 at pH 4, 4.18 at pH 7, 4.24 at pH 10 in 0.001 M NaCl; 4.285 at pH 4, 4.15 at pH 7, 4.22 at pH 10 in 0.01 M NaCl; 4.23 at pH 4, 4.12 at pH 7, 4.20 at pH 10 in 0.1 M NaCl; 4.21 at pH 4, 4.19 at pH 7, 4.24 at pH 10 in 1 mM  $\text{Ca}^{2+}$  in 0.1 M total ionic strength solutions (shake flask/fluorescence, fulvic acid; Schlautman & Morgan 1993a)

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

- Volatilization:** removal rate constants from the water column at 25°C in midsummer sunlight were:  $k = 0.002 \text{ h}^{-1}$  in deep, slow, somewhat turbid water;  $k = 0.001 \text{ h}^{-1}$  in deep, slow muddy water;  $k = 0.002 \text{ h}^{-1}$  in deep slow, clear water;  $k = 0.042 \text{ h}^{-1}$  in shallow, fast, clear water; and  $k = 0.179 \text{ h}^{-1}$  in very shallow, fast, clear water (Southworth 1977);
- aquatic  $t_{1/2} = 18\text{--}300 \text{ h}$  (Callahan et al. 1979);
- calculated  $t_{1/2} = 62 \text{ h}$  for a river 1-m deep with water velocity of 0.5 m/s and wind velocity of 1 m/s (Southworth 1979; quoted, Herbes et al. 1980; Hallett & Brecher 1984).
- Photolysis:** removal rate constants from the water at 25°C in midsummer sunlight were:  $k = 0.004 \text{ h}^{-1}$  in deep, slow somewhat turbid water;  $k < 0.001 \text{ h}^{-1}$  in deep, slow, muddy water;  $k = 0.018 \text{ h}^{-1}$  in deep, slow, clear water;  $k = 0.086 \text{ h}^{-1}$  in shallow, fast, clear water; and  $k = 0.238 \text{ h}^{-1}$  in very shallow, fast, clear water (Southworth 1977)
- 24-h photolytic  $t_{1/2} \sim 1.6 \text{ h}$  in summer and  $t_{1/2} = 4.8 \text{ h}$  in winter at 35°N latitude (Southworth 1977)
- direct sunlight  $k = 0.15 \text{ h}^{-1}$  in winter at 35°N latitude (Callahan et al. 1979)
- $t_{1/2}(\text{calc}) = 0.75 \text{ h}$  near surface water for direct sunlight photolysis at 40°N latitude of midday in midsummer (quoted, Herbes et al. 1980; Harris 1982)
- $t_{1/2} = 4.5 \text{ d}$  in inland water, and  $t_{1/2} = 5.2 \text{ d}$  in inland water with sediment partitioning and  $t_{1/2} = 0.75 \text{ h}$  for direct photochemical transformation near water surface (Zepp & Schlottzauer 1979)
- atmospheric and aqueous photolysis  $t_{1/2} = 0.58 \text{ h}$ , based on measured aqueous photolysis rate constant for midday summer sunlight at 35°N latitude (Southworth 1979; quoted, Howard et al. 1991) and adjusted for approximate winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
- half-lives on different atmospheric particulate substrates (appr. 25  $\mu\text{g/g}$  on substrate):  $t_{1/2} = 2.9 \text{ h}$  on silica gel,  $t_{1/2} = 0.5 \text{ h}$  on alumina and  $t_{1/2} = 48 \text{ h}$  on flyash (Behymer & Hites 1985)
- $t_{1/2} = 4.5 \text{ d}$  for summer at 40°N latitude under sunlight in surface water (Mill & Mabey 1985)
- $k = 0.66 \text{ h}^{-1}$  in distilled water with  $t_{1/2} = 1.0 \text{ h}$  (Fukuda et al. 1988)
- photodegradation  $k = 0.023 \text{ min}^{-1}$  and  $t_{1/2} = 0.50 \text{ h}$  for initial concentration of 5 ppm in methanol-water (1:1, v/v) solution by high pressure mercury lamp or sunlight (Wang et al. 1991)
- pseudo-first-order direct photolysis rate constants,  $k(\text{exptl}) = 0.023 \text{ min}^{-1}$  with the calculated  $t_{1/2} = 0.50 \text{ h}$ , and the predicted  $k = 0.030 \text{ min}^{-1}$  calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
- $k = 0.0503\text{--}0.0521 \text{ min}^{-1}$  in natural water system by UV and sunlight (Yu et al. 1999)
- direct photolysis  $t_{1/2}(\text{calc}) = 3.10 \text{ h}$ , predicted by QSPR, in atmospheric aerosol (Chen et al. 2001)
- Photodegradation  $k = 4.7 \times 10^{-4} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)
- Oxidation:** rate constant  $k$ , for gas-phase second order rate constants,  $k_{\text{OH}}$  for reaction with OH radical,  $k_{\text{NO}_3}$  with  $\text{NO}_3$  radical and  $k_{\text{O}_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures see reference:
- photooxidation  $t_{1/2} = 1111\text{--}38500 \text{ h}$ , based on measured rate constant for reaction with hydroxyl radical in water (Radding et al. 1976; quoted, Howard et al. 1991)
- $k(\text{aquatic})$  fate rate of 50  $\text{L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 1600 \text{ d}$  (Callahan et al. 1979)
- $k(\text{calc}) = 5.0 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for singlet  $\text{O}_2$  and  $2.2 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)
- $k(\text{aq.}) = 3.3 \times 10^{-4} \text{ s}^{-1}$  with  $t_{1/2} = 0.6 \text{ h}$  under natural sunlight conditions (NRCC 1983)
- $k_{\text{OH}} = 110 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $325 \pm 1 \text{ K}$  (relative rate technique for propene, (Biermann et al. 1985; Atkinson 1989)
- photooxidation  $t_{1/2} = 0.501\text{--}5.01 \text{ h}$ , based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987)
- $k_{\text{OH}}(\text{calc}) = 203 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1996)

$k = 3.5 \times 10^{-5} \text{ s}^{-1}$ , indirect total photoreaction rate constant in surface waters (Mill 1999)

$k_{\text{OH}}^* = 190 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 306–366 K with a calculated atmospheric lifetime of 1.5 h based on gas-phase OH reaction (Brubaker & Hites 1998)

Hydrolysis:  $k < 0.001 \text{ h}^{-1}$  at 25°C (Southworth 1977); not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$k = 0.061 \text{ h}^{-1}$  for microbial degradation in Third Creek water incubated 18 h at 25°C; removal rate constants from water column at 25°C in midsummer sunlight were:  $k = 0.060 \text{ h}^{-1}$  in deep, slow, somewhat turbid water;  $k = 0.030 \text{ h}^{-1}$  in deep, slow, muddy water;  $k = 0.061 \text{ h}^{-1}$  in deep, slow, clear water;  $k = 0.061 \text{ h}^{-1}$  in shallow, fast, clear water; and  $k = 0.061 \text{ h}^{-1}$  in very shallow, fast, clear water (Southworth 1977)

$k = 0.035 \text{ h}^{-1}$  for microbial degradation (Herbes et al. 1980; quoted, Hallett & Brecher 1984)

significant degradation in 7 d with rapid adaptation for an average of three static-flask screening test (Tabak et al. 1981)

$k = 2.5 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 12 \text{ d}$  and  $k = 2.5 \times 10^{-4} \text{ h}^{-1}$  with  $t_{1/2} = 115 \text{ d}$  for mixed bacterial populations in oil-contaminated and pristine stream sediments (Herbes & Schwall 1978, NRCC 1983)

$t_{1/2}(\text{aq. aerobic}) = 1200\text{--}11040 \text{ h}$ , based on aerobic soil die-away test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991)

$k = 0.0052 \text{ d}^{-1}$  with  $t_{1/2} = 134 \text{ d}$  for Kidman sandy loam and  $k = 0.0138 \text{ d}^{-1}$  with  $t_{1/2} = 50 \text{ d}$  for McLarin sandy loam all at  $-0.33 \text{ bar}$  soil moisture (Park et al. 1990)

$t_{1/2}(\text{aq. anaerobic}) = 4800\text{--}44160 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: aquatic fate rate,  $k < 0.0612 \text{ h}^{-1}$  with  $t_{1/2} > 11.3 \text{ h}$  (Callahan et al. 1979); estimated rate constant for bacteria of  $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$  (Mabey et al. 1982).

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

$\log k_1 = 2.89 \text{ h}^{-1}$ ;  $\log k_2 = 0.0043 \text{ h}^{-1}$  (*Daphnia pulex*, Herbes & Risi 1978)

$k_1 = 702 \text{ h}^{-1}$ ;  $k_2 = 0.589 \text{ h}^{-1}$  (*Daphnia pulex*, Southworth et al. 1978)

$k_1 = (1.73 \times 10^{-3} - 36) \text{ h}^{-1}$ ;  $k_2 = 0.040 \text{ h}^{-1}$  (average, bluegill sunfish, Spacie et al. 1983)

$\log k_1 = 2.85 \text{ h}^{-1}$ ;  $\log k_2 = -0.23 \text{ h}^{-1}$  (*Daphnia pulex*, correlated to Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 1.46, 16.9 \text{ h}^{-1}$ ;  $k_2 = (1.58\text{--}1.88) \times 10^{-3} \text{ h}^{-1}$  (rainbow trout, Linder et al. 1985)

$k_1 = 87.2 \text{ h}^{-1}$ ;  $k_2 = 0.019 \text{ h}^{-1}$  (4°C, *S. heringianus*, Frank et al. 1986)

$k_1 = 131.1 \text{ mL g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0033 \text{ h}^{-1}$  (4°C, *P. hoyi*, Landrum 1988)

$\log k_2 = .2, -0.01 \text{ d}^{-1}$  (fish, calculated- $K_{\text{OW}}$ , Thomann 1989)

$\log k_2 = -0.96 \text{ d}^{-1}$  (oyster, calculated- $K_{\text{OW}}$ , Thomann 1989)

$k_1 = 1.8\text{--}2.3 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.045 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.58\text{--}1.7 \text{ h}$ , based on photolysis half-life in water (Howard et al. 1991);

half-lives under simulated atmospheric conditions:  $t_{1/2} = 0.20 \text{ h}$  for simulated sunlight,  $t_{1/2} = 0.15 \text{ h}$  for simulated sunlight + ozone with concn of 0.2 ppm,  $t_{1/2} = 1.23 \text{ h}$  for dark reaction ozone with concn of 0.2 ppm (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

calculated atmospheric lifetime of 1.5 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: half-lives for removal from water column at 25°C in midsummer sunlight were,  $t_{1/2} = 10.5 \text{ h}$  for deep, slow, somewhat turbid water;  $t_{1/2} = 21.6 \text{ h}$  for deep, slow, muddy water;  $t_{1/2} = 8.5 \text{ h}$  for deep, slow, clear water;  $t_{1/2} = 3.5 \text{ h}$  for shallow, fast, clear water; and  $t_{1/2} = 1.4 \text{ h}$  for very shallow, fast, clear water (Southworth 1977, Herbes et al. 1980);

computed near-surface  $t_{1/2} = 0.75 \text{ h}$  of a water body and for direct photochemical transformation at latitude 40°N, midday, midsummer and half-lives:  $t_{1/2} = 4.5 \text{ d}$  for no sediment-water partitioning,  $t_{1/2} = 5.2 \text{ d}$  with sediment-water partitioning and for direct photolysis in a 5-m deep inland water body (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.58\text{--}1.7 \text{ h}$ , based on photolysis half-life in water (Howard et al. 1991);

$t_{1/2} = 4.5 \text{ d}$  at 40°N under summer sunlight (Mill & Mabey 1985);

photolysis  $t_{1/2} = 0.50 \text{ h}$  in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

indirect photoreaction  $t_{1/2} = 5.5 \text{ h}$  in surface waters (Mill 1999);

photolysis  $t_{1/2} = 13.3\text{--}13.80$  min at  $15^\circ\text{C}$  in natural water system by UV and sunlight illumination (Yu et al. 1999).

Groundwater:  $t_{1/2} = 2400\text{--}22080$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction  $t_{1/2} = 600$  h for chemical available anthracene and  $t_{1/2} = 77$  h for bioavailable anthracene for amphipod, *P. hoyi* in Lake Michigan sediments at  $4^\circ\text{C}$ . The uptake clearance from sediment was  $(0.024 \pm 0.002)\text{g}$  of dry sediment  $\cdot \text{g}^{-1}$  of organism  $\cdot \text{h}^{-1}$ , and the rate constants to become biologically unavailable were  $(0.009 \pm 0.002)\text{h}^{-1}$  corresponding to  $t_{1/2} = 77$  h (Landrum 1989).

Soil:  $t_{1/2} = 3.3\text{--}175$  d (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 17$  d for 5 mg/kg treatment and  $t_{1/2} = 45$  d for 50 mg/kg treatment (Bulman et al. 1987);

degradation rate constant  $k = 0.0052\text{ d}^{-1}$  with  $t_{1/2} = 134$  d for Kidman sandy loam soil and  $k = 0.138\text{ d}^{-1}$  with  $t_{1/2} = 50$  d for McLauren sandy loam soil (Park et al. 1990);

$t_{1/2} = 1200\text{--}11040$  h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} = 0.5\text{--}26$  wk, 7.9 yr (quoted, Luddington soil, Wild et al. 1991).

Biota:  $t_{1/2} = 17$  h in bluegill sunfish (Spacie et al. 1983);

with depuration  $t_{1/2} = 37.75$  h in *s. heringianus* (Frank et al. 1986);

elimination  $t_{1/2} = 7$  d from rainbow trout,  $t_{1/2} = 1.9$  d from mussel *Mytilus edulis* (quoted, Meador et al. 1995).

TABLE 4.1.1.25.1

Reported aqueous solubilities of anthracene at various temperatures and the reported empirical temperature dependence equations

$$R \cdot \ln x = -[\Delta H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K) \quad (1)$$

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (2)$$

$$\ln x = A - B/(T/K) \quad (3)$$

$$\ln x = A + B/(T/K) + C \cdot \ln (T/K) \quad (4)$$

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_0, T_0 = 298.15 \text{ K} \quad (4a)$$

1.

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
	experimental		smoothed*				
35.4	0.125	0	0.022	8.60	0.0233	5.2	0.0127
35.4	0.122	25	0.075	11.1	0.0244	10.0	0.0175
35.4	0.119	35.4	0.123	12.2	0.0257	14.1	0.0222
39.3	0.152	39.3	0.159	14.0	0.0274	18.3	0.0291
39.3	0.151	44.7	0.214	15.5	0.0296	22.4	0.0372
39.3	0.148	47.5	0.249	19.2	0.0323	24.6	0.0434
44.7	0.208	50	0.286	20.3	0.0396	28.7	0.0557
44.7	0.210	50.1	0.288	23.3	0.0417		
44.7	0.206	54.7	0.372	25.0	0.0410		
47.5	0.279	59.2	0.481	26.2	0.0476	temp dependence eq. 2	
50.1	0.301	64.5	0.66	28.5	0.0579	S	μg/kg
50.1	0.297	65.1	0.68	31.3	0.0695	a	0.0013
50.1	0.302	69.8	0.90			b	-0.0097
54.7	0.391	70.7	0.95			c	0.8861
54.7	0.389	71.9	1.02	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.81$		d	8.21
54.7	0.402	74.7	1.21				
59.2	0.480	75.0	1.23				
59.2	0.488						
59.2	0.525						
64.5	0.72	temp dependence eq. 1					

TABLE 4.1.1.25.1 (Continued)

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
64.5	0.62, 0.64	ln x	mole fraction				
65.1	0.67, 0.64	$\Delta H_{\text{fus}}$	$29.0 \pm 0.29$				
69.8	0.92	$10^2 \cdot b$	$1.81 \pm 0.15$				
70.7	0.90, 0.97	c	$19.3 \pm 0.5$				
70.7	0.96						
71.9	0.91	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 29.0$					
74.7	1.19, 1.13						
74.7	1.26						
<b>2.</b>							
May et al. 1978b		May 1980		May et al. 1983		Velapoldi et al. 1983	
generator column-HPLC		generator column-HPLC		generator column-HPLC		generator column-fluo.	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
25	0.0446	5.2	0.0127	5.20	0.0127	10	0.0177
29	0.0579	10.0	0.0175	10.0	0.0175	15	0.02282
		14.1	0.0222	14.1	0.0222	20	0.03061
temp dependence eq. 2		18.3	0.0281	18.3	0.0291	25	0.04257
S	μg/kg	22.4	0.0372	22.4	0.0372	30	0.06123
a	0.0013	24.6	0.0434	24.6	0.0434		
b	-0.0097	28.7	0.0557	28.7	0.0557		
c	0.8861			9.70	0.0162	eq. 4	x
d	8.21			16.6	0.0251	A	-1078.056
		temp dependence eq. 2		23.2	0.0378	B	41884.5
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 43.76$		S	μg/kg	29.3	0.0572	C	161.175
for temp range 5–30°C		a	0.0013				
		b	-0.0097			$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 51.3$	
		c	0.8886				
		d	8.21				
<b>3.</b>							
Whitehouse 1984		Shaw 1989		Reza et al. 2002		Dohányosová et al. 2003	
generator column-HPLC/UV		IUPAC recommended		generator column-HPLC/fluo		generator column-HPLC/UV	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
4.6	0.00961	0	0.022	8.94	0.0155	0.30	0.00963
8.8	0.0129	10	0.021	11.57	0.0183	5.0	0.0124
12.9	0.0177	20	0.034	13.39	0.0198	10	0.0169
17.0	0.0237	25	0.062*	15.88	0.0246	15	0.0227
21.1	0.0323	30	0.080*	22.54	0.0287	20	0.0320
25.3	0.0442	40	0.16*	24.61	0.0434	25	0.0438
		50	0.29*	27.10	0.0505	30	0.0584
		60	0.51*	28.20	0.0540	35	0.0784
		70	0.91*	29.12	0.0565	40	0.106
				30.53	0.0633	45	0.145

(Continued)

TABLE 4.1.1.25.1 (Continued)

Whitehouse 1984		Shaw 1989		Reza et al. 2002		Dohányosová et al. 2003	
generator column-HPLC/UV		IUPAC recommended		generator column-HPLC/fluor		generator column-HPLC/UV	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
		*tentative		34.87	0.0890	50	0.190
				39.91	0.1157		
				44.90	0.1569	eq. 4a	x
				49.20	0.2123	A	-33.7647
						B	14.5018
				eq. 3	x	C	32.7269
				A	0.050 ± 0.45		
				B	5876 ± 135		
				temp range 282–323 K			
						$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 45.2 \pm 0.3$	
						at 298.15 K.	
						mp/K	489
						$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 29.37$	

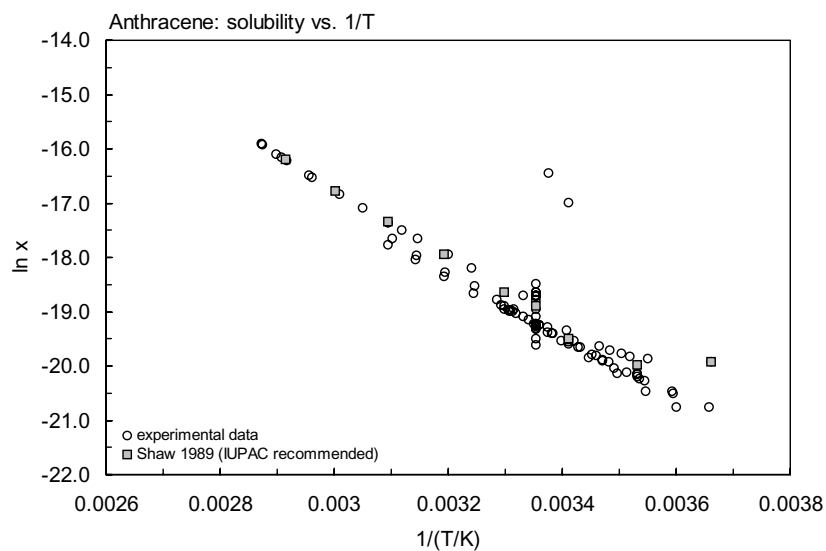
FIGURE 4.1.1.25.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for anthracene.

TABLE 4.1.1.25.2

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

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

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

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

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

1.

Nelson & Senseman 1922		Mortimer & Murphy 1923		Stull 1947		Sears & Hopke 1949	
isoteniscope-Hg manometer		isoteniscope-Hg manometer		summary of literature data		Rodebush gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
220	5680	223.3	6399	145.0	133.3	Data presented by	
225	6599	225.0	7333	173.5	666.6		
230	6306	244.4	11452	187.2	1333	eq. 1	P/mmHg
235	8813	244.6	11532	201.9	2666	A	12.002
240	10133	259.4	16972	217.5	5333	B	5102.0
245	11612	259.8	17105	231.8	7999	measured range 105–125°C	
250	13279	260.3	17359	250.0	13332	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 97.70$	
255	15132	282.0	29277	279.0	26664		
260	17212	282.1	29304	210.2	53329	25	.00103
265	19532	299.0	44050	342.0	101325	extrapolated	
270	22105	300.0	44170				
275	14971	312.8	57715	mp/°C	217.5		
280	28131	313.2	58155				
285	31624	313.4	58262				
290	35450	317.4	76980				
300	44263	327.9	77780				
310	54729	328.0	77860				
320	67048	340.6	98952				
330	81380	340.5	98950				
342	101325						
bp/°C	342	eq. 1	P/mmHg				
		A	7.910				
		B	3093				
		temp range 232–340°C					
		eq. 2	P/mmHg				
		A	10.972				
		B	4584				
		temp range 100–350°C					

2.

Bradley & Cleasby 1953		Kelley & Rice 1964		Malaspina et al. 1973		Power et al. 1977	
effusion		effusion		Knudsen effusion		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
65.7	0.115	data represented by		79.55	0.612	30	0.00937
69.91	0.167			88.25	1.373	30	0.00913
73.35	0.259	eq. 1	P/mmHg	98.05	3.506	50	0.0928

(Continued)

TABLE 4.1.1.25.2 (Continued)

Bradley & Cleasby 1953		Kelley & Rice 1964		Malaspina et al. 1973		Power et al. 1977	
effusion		effusion		Knudsen effusion		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
79.95	0.489	A	12.068	105.95	6.413	70	0.582
67.1	0.140	B	5145	113.75	12.17	70	0.5826
68.75	0.157	measured range 69–86°C		123.75	29.33	100	7.738
71.25	0.208	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 93.91$		135.25	61.06	100	7.771
73.2	0.223	reported extrapolated data		142.35	106.32		
80.4	0.524			149.75	189.31		
				159.15	483.95	eq. 2	P/mmHg
		95	1.667			A	36.40
		100	2.546			B	8634
eq. 1	P/mmHg	105	3.880			C	238.6
A	11.638			eq. 1	P/mmHg		
B	5320			A	12.616		
				B	5277		

## 3.

Macknick & Prausnitz 1979		de Kruif 1980		Grayson & Fosbraey 1982		Sonnefeld et al. 1983	
gas saturation-GC		teorsion-, weighing effusion		gas saturation-GC		gas saturation-HPLC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
85.25	0.892	64.44	0.10	20.0	0.00102	12.3	$1.64 \times 10^{-4}$
90.15	1.36	71.18	0.20	50.1	0.035	12.3	$1.57 \times 10^{-4}$
95.65	2.13	75.20	0.30	60.0	0.0849	12.3	$1.60 \times 10^{-4}$
100.7	3.32	78.12	0.40	70.0	0.267	19.2	$3.76 \times 10^{-4}$
104.7	4.59	80.41	0.50	75.0	0.359	19.2	$3.83 \times 10^{-4}$
111.9	8.04	82.31	0.60	80.5	0.588	19.2	$3.54 \times 10^{-4}$
116.4	11.41	83.93	0.70			19.2	$3.72 \times 10^{-4}$
119.93	14.67	85.35	0.80			25.0	$8.43 \times 10^{-4}$
		86.61	0.90	eq. 1	P/Pa	25.0	$8.17 \times 10^{-4}$
		87.74	1.00	A	30.5	25.0	$8.19 \times 10^{-4}$
eq. 1	P/mmHg			B	10968	25.0	$3.30 \times 10^{-4}$
A	26.805	25.0	0.00875			30.1	$1.46 \times 10^{-3}$
B	111402	extrapolated				30.1	$1.54 \times 10^{-3}$
		$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 100.4$				30.1	$1.51 \times 10^{-3}$
						34.93	$2.59 \times 10^{-3}$
						34.93	$2.63 \times 10^{-3}$
						34.93	$2.69 \times 10^{-3}$
						eq. 1	P/Pa
						A	12.977
						B	4891.87



TABLE 4.1.1.25.2 (Continued)

4.

Bender et al. 1983		Rordorf 1985		Hansen & Eckert 1986		Oja & Suuberg 1998	
gas saturation		gas saturation-GC		gas saturation-IR		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
80.45	0.55	25	0.00106	40	0.0058	27.7	0.00114
82.05	0.67	50	0.023	45	0.0105	39.7	0.00575
85.35	0.864	75	0.322	50	0.0193	47.6	0.0162
90.5	1.418	100	3.17	55	0.039	54.6	0.0355
94.5	2.019	125	23.4	60	0.0675	60.1	0.062
100.8	3.426	150	136.2	65	0.0987	72.7	0.204
105.65	4.99			70	0.1688	74.1	0.258
110.4	7.17	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 98.75$		75	0.3056		
115.35	10.01			80	0.5252	eq. 1a	P/Pa
115.65	10.58	av. selected literature value		85	0.9247	A	33.281
110.857	15.30	25	0.00108	90	1.244	B	12024
125.45	21.30	50	0.0243				
		75	0.344			$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 100.0$	
eq. 1	P/Pa	100	3.38	eq. 1	P/mPa		
A	31.620	125	24.5	A	17.88		
B	1138	150	139.7	B	5359		
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 98.79$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 102.6$			

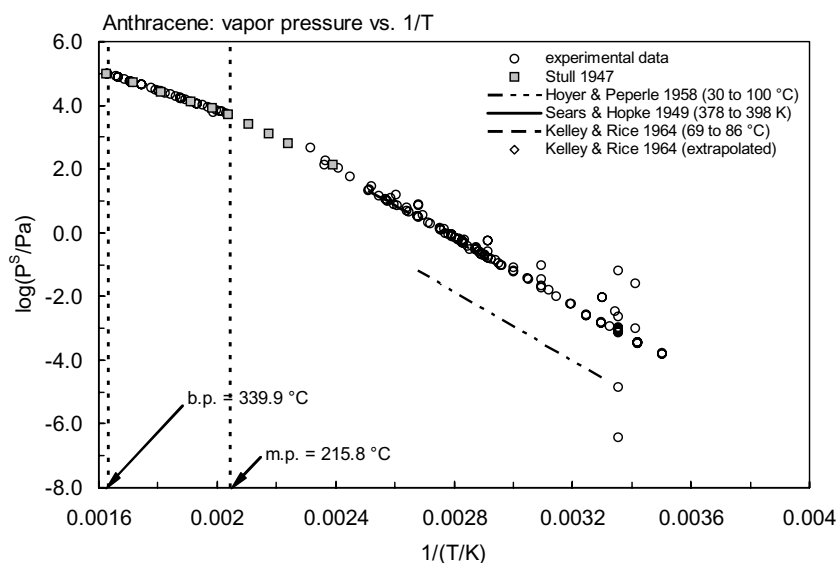
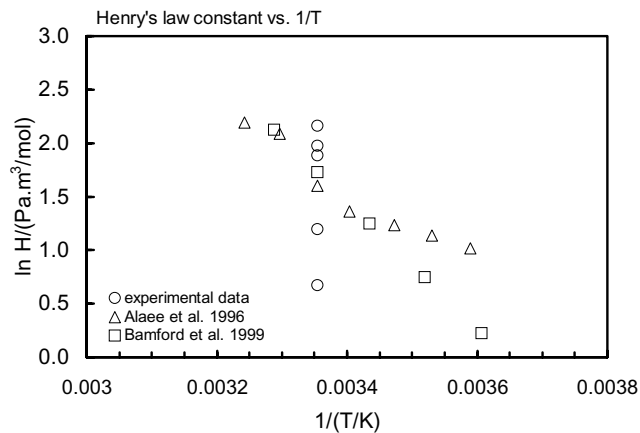


FIGURE 4.1.1.25.2 Logarithm of vapor pressure versus reciprocal temperature for anthracene.

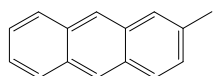
**TABLE 4.1.1.25.3**  
**Reported Henry's law constants of anthracene at various temperatures and temperature dependence equations**

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Alaee et al. 1996			Bamford et al. 1999		
gas stripping-GC			gas stripping-GC/MS		
t/°C	H/(Pa m³/mol)		t/°C	H/(Pa m³/mol)	H/(Pa m³/mol)
					average
5.4	2.76		4.1	1.14, 1.38	1.25
10.1	3.12		11.0	1.99, 2.26	2.12
14.8	3.44		18.0	3.31, 3.70	3.50
20.6	3.91		25.0	5.26, 6.06	5.64
25.0	4.94		31.0	7.60, 9.18	8.36
30.2	8.05				
34.3	8.94		eq. 1	$K_{AW}$	
			A	12.75	
eq. 1	$K_{AW}$		B	5629	
A	4.680				
B	3235.5				
enthalpy of volatilization: $\Delta H_{vol}/(\text{kJ}\cdot\text{mol}^{-1}) = 26.9$			enthalpy, entropy change: $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 46.8 \pm 1.7$ $\Delta S/(\text{J}\cdot\text{K}^{-1} \text{mol}^{-1}) = 106$ at 25°C		



**FIGURE 4.1.1.25.3** Logarithm of Henry's law constant versus reciprocal temperature for anthracene.

## 4.1.1.26 2-Methylantracene



Common Name: 2-Methylantracene

Synonym:

Chemical Name: 2-methylantracene

CAS Registry No: 613-12-7

Molecular Formula:  $C_{15}H_{12}$

Molecular Weight: 192.256

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

209 (Weast 1982–83; Lide 2003)

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

359 (sublimation, Bjørseth 1983)

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

1.80 ( $0^{\circ}C$ , Lide 2003)

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

106 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0157 (mp at  $209^{\circ}C$ )

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

0.039 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0219\* (generator column-HPLC/UV, measured range  $6.3$ – $31.1^{\circ}C$ , May et al. 1978a)

0.0213 (generator column-HPLC/UV, measured range  $5$ – $30^{\circ}C$ , May et al. 1978b)

$S/(\mu g/kg) = 324.0 + 5.413 \cdot (t/^{\circ}) + 0.8059 \cdot (t/^{\circ}C)^2 + 0.0025 \cdot (t/^{\circ}C)^3$ ; temp range  $5$ – $30^{\circ}C$  (generator column-HPLC/UC, May et al. 1978b)

0.0191\* ( $23.1^{\circ}C$ , generator column-HPLC/fluor., temp range  $278.25$ – $302.45$  K, May et al. 1983)

0.031 (average lit. value, Pearlman et al. 1984)

0.0225\* (generator column-HPLC/UV, measured range  $4.6$ – $25.3^{\circ}C$ , Whitehouse 1984)

0.03\* (tentative value, IUPAC Solubility Data Series, Shaw 1989)

$\ln x = -1.841995 - 4616.86/(T/K)$ , temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

0.0262\* (generator column-HPLC/UV, measured range  $0$ – $50^{\circ}C$ , Dohányosová et al. 2003)

$\ln x = -42.7975 + 22.9752/\tau + C \ln \tau$ ,  $\tau = T/298.15$  K; temp range  $0$ – $50^{\circ}C$  (generator column-HPLC/UV, Dohányosová et al. 2003)

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

0.0207 (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -3976/(T/K) + 11.65$ ;  $\Delta H_{vap} = -76.1$  kJ·mol $^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m $^3$ /mol):

Octanol/Water Partition Coefficient,  $\log K_{ow}$  at  $25^{\circ}C$  and reported temperature dependence equations:

5.15 (calculated-fragment const., Yalkowsky & Valvani 1979,1980)

5.00 (shake flask-UV, Alcorn et al. 1993)

5.00 (recommended, Sangster 1993)

4.97; 4.70 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 1.093 + 1154.2/(T/K)$ ; temp range 5–55°C (temperature dependence HPLC- $k'$  correlation, Lei et al. 2000)

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:

Hydrolysis:

Oxidation:

Half-Lives in the Environment:

Biota: elimination  $t_{1/2} = 2$  d from rainbow trout (quoted, Meador et al. 1995).

**TABLE 4.1.1.26.1**

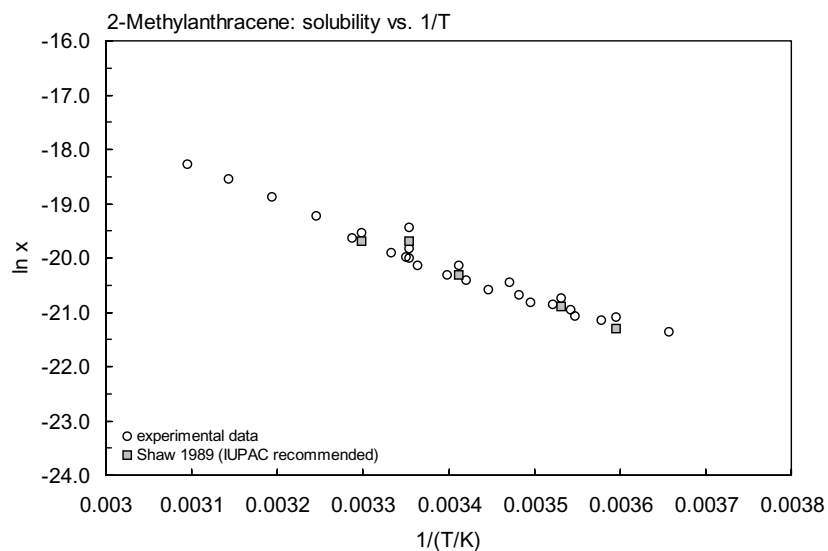
**Reported aqueous solubilities of 2-methylanthracene at various temperature and the empirical temperature dependence equations**

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

$$\ln x = A + B/\tau + C \ln \tau \quad (2)$$

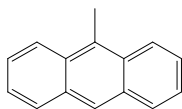
where  $\tau = T/T_0$  and  $T_0 = 298.15$  K

May et al. 1978a, May 1983		Whitehouse 1984		Shaw 1989b		Dohányosová et al. 2003	
generator column-HPLC		generator column-HPLC/UV		IUPAC "tentative" values		generator column-HPLC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
6.3	0.00706	4.6	—	5	0.006	0.30	0.00567
9.1	0.00848	8.8	0.00754	10	0.009	5.0	0.00738
10.8	0.00943	12.9	0.00969	20	0.016	20	0.0106
13.9	0.0111	17.0	0.0123	25	0.03	15	0.0142
18.3	0.0145	21.1	0.0161	30	0.03	20	0.0192
23.1	0.0191	25.3	0.0225			25	0.0262
27.0	0.0242					30	0.0352
31.1	0.0321					35	0.048
						40	0.0674
						45	0.0943
						50	0.125
temp dependence eq. 1						eq. 2	x
S	$\mu\text{g/kg}$					A	−42.7975
a	0.0011					B	22.9752
b	−0.0306					C	41.7206
c	0.8180						
d	2.78						
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 39.08$						$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 46.15 \pm 0.3$	
measured between 5–30°C						0.3	
						at 298.15 K	
						mp/K	479
						$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 24.06$	



**FIGURE 4.1.1.26.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 2-methylanthracene.

## 4.1.1.27 9-Methylantracene



Common Name: 9-Methylantracene

Synonym:

Chemical Name: 9-methylantracene

CAS Registry No: 779-02-2

Molecular Formula:  $C_{15}H_{12}$

Molecular Weight: 192.256

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

81.5 (Weast 1982–83; Lide 2003)

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

196 (12 mm Hg, Weast 1982–83; Lide 2003)

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

1.065 ( $99^{\circ}C$ , Lide 2003)

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

181 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.279 (mp at  $81.5^{\circ}C$ )

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):

0.261 (shake flask-fluorescence, Mackay & Shiu 1977)

0.269 (average lit. value, Pearlman et al. 1984)

0.530 (generator column-HPLC, Vadas et al. 1991)

0.0376\* (generator column-HPLC/UV, measured range  $0$ – $50^{\circ}C$ , Dohányosová et al. 2003)

$\ln x = -76.9798 + 59.8386/\tau + C \ln \tau$ ,  $\tau = T/298.15 K$ , temp range  $0$ – $50^{\circ}C$  (generator column-HPLC/UV, Dohányosová et al. 2003)

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

0.00224 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 11.683 - 5168/(T/K)$ ; temp range  $354$ – $402 K$  (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa  $m^3/mol$ ):

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

5.12 (calculated- $\pi$  const., Southworth et al. 1978)

5.07 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)

5.15 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky & Valvani 1979,1980)

5.14 (average lit. value, Yalkowsky et al. 1983)

5.61 (HPLC-RT correlation; Burkhard et al. 1985)

5.10 (HPLC-RT correlation, Wang et al. 1986)

$5.07 \pm 0.20$  (recommended, Sangster 1989, 1993)

5.07 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

3.66; 3.59 (*Daphnia pulex*; kinetic estimation, Southworth et al. 1978)

3.75	(calculated- $K_{ow}$ , Mackay 1982)
3.94	(calculated-MCI $\chi$ , Sabljic 1987b)
3.683, 3.778	(calculated-MCI $\chi$ , calculated- $K_{ow}$ , Lu et al. 1999)

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

4.81	(natural sediment, average of isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
4.50	(calculated-molecular connectivity indices $\chi$ , Sabljic 1984)
4.81	(calculated-MCI $^1\chi$ , Sabljic et al. 1995)

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

## Volatilization:

## Photolysis:

$t_{1/2}(\text{calc}) = 0.13$  h for direct photochemical transformation near water surface and  $t_{1/2} = 0.78$  d for no sediment-water partitioning; and  $t_{1/2} = 1.2$  d with sediment-water partitioning (Zepp & Schlotzhauer 1979)

$t_{1/2} = 0.79$  d for summer at 40°N latitude under sunlight in surface water (Mill & Mabey 1985)

photodegradation  $k = 0.163 \text{ min}^{-1}$  and  $t_{1/2} = 0.07$  h in methanol-water (2:3, v/v) solution for initial concentration of 5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

the pseudo-first-order direct photolysis  $k(\text{exptl}) = 0.0163 \text{ min}^{-1}$  with calculated  $t_{1/2} = 0.07$  h and the predicted  $k(\text{calc}) = 0.00343 \text{ min}^{-1}$  calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis  $t_{1/2} = 1.85$  h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Oxidation:  $t_{1/2} = 10$  h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

## Hydrolysis:

## Biodegradation:

## Biotransformation:

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

$k_1 = 561 \text{ h}^{-1}$ ;  $k_2 = 0.144 \text{ h}^{-1}$  (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.75 \text{ h}^{-1}$ ;  $\log k_2 = -0.84 \text{ h}^{-1}$  (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

## Half-Lives in the Environment:

Air: direct photolysis  $t_{1/2} = 1.85$  h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Surface water: computed  $t_{1/2} = 0.13$  h at near-surface of a water body, for direct photochemical transformation, and  $t_{1/2} = 0.79$  d for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning,  $t_{1/2} = 1.2$  d with sediment-water partitioning to top cm bottom sediment; and  $t_{1/2} = 10$  h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.79$  d for summer at 40°N latitude under sunlight (Mill & Mabey 1985);

photolysis  $t_{1/2} = 0.07$  h in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

## Groundwater:

## Sediment:

## Soil:

Biota: elimination  $t_{1/2} = 4$  d from rainbow trout (quoted, Meador et al. 1995).

**TABLE 4.1.1.27.1**

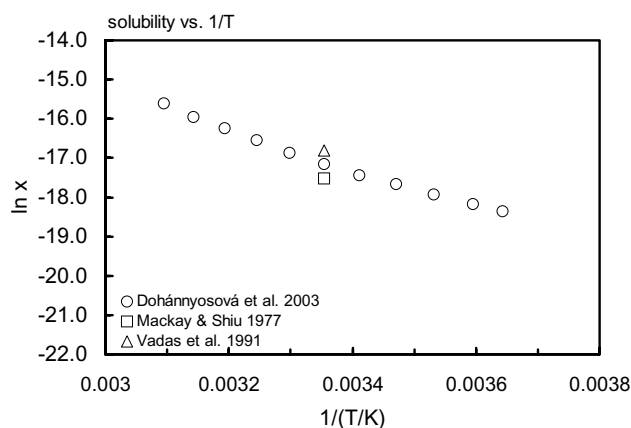
**Reported aqueous solubilities of 9-methylanthracene at various temperature and the empirical temperature dependence equations**

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_0 \text{ and } T_0 = 298.15 \text{ K} \quad (1)$$

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**Generator column-HPLC**

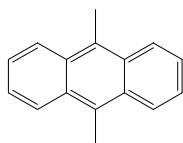
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0.30	0.113
5.0	0.137
20	0.174
15	0.228
20	0.286
25	0.376
30	0.508
35	0.699
40	0.953
45	1.270
50	1.770
eq. 1	mole fraction
A	-76.9798
B	59.8386
C	76.7066
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 41.8 \pm 0.2$	
at 298.15 K	
mp/K	348
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 16.95$	



**FIGURE 4.1.1.27.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 9-methylanthracene.



## 4.1.1.28 9,10-Dimethylantracene



Common Name: 9,10-Dimethylantracene

Synonym:

Chemical Name: 9,10-dimethylantracene

CAS Registry No: 781-43-1

Molecular Formula:  $C_{16}H_{14}$

Molecular Weight: 206.282

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

183.6 (Lide 2003)

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

360 (Lide 2003)

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

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

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0278 (at mp =  $183.6^{\circ}C$ )

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

0.056 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0129\* (generator column-HPLC/UV, measured range  $0-50^{\circ}C$ , Dohányosová et al. 2003)

$\ln x = -73.2594 + 52.6685/\tau + C \ln \tau$ ,  $\tau = T/298.15 K$ ; temp range  $0-50^{\circ}C$  (generator column-HPLC/UV, Dohányosová et al. 2003)

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

$1.53 \times 10^{-4}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.266 - 5391/(T/K)$ ; temp range 381–434 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa  $m^3/mol$ ):

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

5.69 (HPLC-RT correlation, Wang et al. 1986)

5.69 (recommended, Sangster 1989, 1993)

5.69 (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: direct photochemical transformation  $t_{1/2}(\text{calc}) = 0.35$  h, computed near-surface water, latitude  $40^{\circ}N$ , midday, midsummer (Zepp & Schlotzhauer 1979)

photodegradation in methanol-water (2:3, v/v) solution for initial concentration of 5 ppm by high pressure mercury lamp or sunlight with a rate constant  $k = 0.0633 \text{ min}^{-1}$  and  $t_{1/2} = 0.18$  h (Wang et al. 1991)

pseudo-first-order direct photolysis  $k$  (exptl) =  $0.0633 \text{ min}^{-1}$  with the calculated  $t_{1/2} = 0.18 \text{ h}$  and the predicted  $k$  (calc) =  $0.0379 \text{ min}^{-1}$  calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis  $t_{1/2} = 1.17 \text{ h}$  predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Oxidation:  $t_{1/2} = 1.5 \text{ h}$  for photosensitized oxygenation with singlet oxygen at near-surface natural water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979)

Hydrolysis:

Biodegradation:

Biotransformation:

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

#### Half-Lives in the Environment:

Air: direct photolysis  $t_{1/2} = 1.17 \text{ h}$  predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis  $t_{1/2} = 0.35 \text{ h}$  near surface water,  $40^\circ\text{N}$ ; midday, midsummer and photosensitized oxygenation  $t_{1/2} = 1.5 \text{ h}$  at near surface water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979).

photolysis  $t_{1/2} = 0.18 \text{ h}$  in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

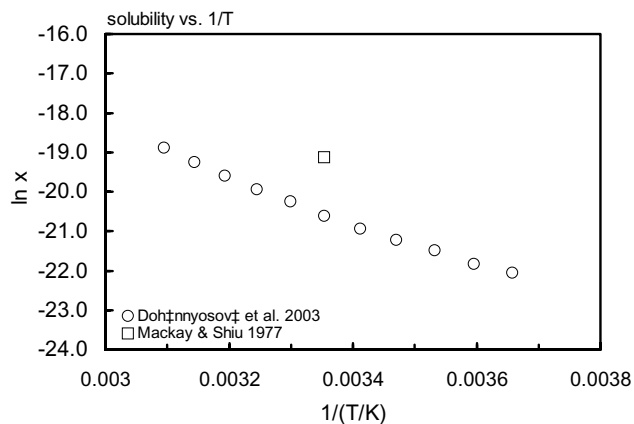
**TABLE 4.1.1.28.1**

**Reported aqueous solubilities of 9,10-dimethylanthracene at various temperature and the empirical temperature dependence equations**

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_0 \text{ and } T_0 = 298.15 \text{ K} \quad (1)$$

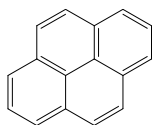
Dohányosová et al. 2003

generator column-HPLC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0.30	0.000391
5.0	0.00382
20	0.00534
15	0.00698
20	0.00932
25	0.0129
30	0.0186
35	0.0252
40	0.0351
45	0.0501
50	0.0728
eq. 1	mole fraction
A	-73.2594
B	52.6685
C	71.9873
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 47.9 \pm 0.3$	
at 298.15 K	
mp/K	455
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.46$	



**FIGURE 4.1.1.28.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 9, 10-dimethylantracene.

## 4.1.1.29 Pyrene



Common Name: Pyrene

Synonym: benzo[*def*]phenanthrene

Chemical Name: pyrene

CAS Registry No: 129-00-0

Molecular Formula: C<sub>16</sub>H<sub>10</sub>

Molecular Weight: 202.250

Melting Point (°C):

150.62 (Lide 2003)

Boiling Point (°C):

404 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.271 (23°C, Weast 1982–83; Lide 2003)

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

159.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

17.11 (Ruelle & Kesselring 1997)

0.29, 17.36; 17.65 (–152.35, 150.65°C; total phase change enthalpy, Chickos et al. 1999)

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

35.98 (Wauchope & Getzen 1972)

40.17 (Casellato et al. 1973)

54.8 (Hinckley et al. 1990)

40.97 (150.65°C, Chickos et al. 1999)

43.36, 43.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0585 (mp at 150.62°C)

0.128 (calculated, ΔS<sub>fus</sub> = 40.3 J/mol K, Passivirta et al. 1999)

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

0.165 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.175 (shake flask-UV, Klevens 1950)

0.148 (Pierotti et al. 1959)

1.56 (shake flask-UV/fluorescence, Barone et al. 1967)

0.105 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)

0.148\* (shake flask-UV, measured range 22.2–74.7°C, Wauchope & Getzen 1972)

$R \cdot \ln x = -3660/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 38.1 + 0.0478 \cdot (T/K)$ ; temp range 22.2–73.4°C (shake flask-UV measurements, Wauchope & Getzen 1972)

0.105, 0.133, 0.107, 0.069 (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

0.171 (shake flask-fluorescence/UV, Schwarz & Wasik 1976)

0.135 (shake flask-fluorescence, Mackay & Shiu 1977)

0.132 (Rossi 1977; Neff 1979)

0.1295\* (shake flask-fluorescence, measured range 12.2–31.3°C, Schwarz 1977)

0.132\* (generator column-HPLC/UV, measured range 5–30°C, May et al. 1978b)

$S/(\mu\text{g/kg}) = 50.2 - 1.051 \cdot (t/^\circ\text{C}) + 0.2007 \cdot (t/^\circ\text{C})^2 - 0.0011 \cdot (t/^\circ\text{C})^3$ ; temp range 5–30°C (generator column-HPLC/UV, May et al. 1978b)

0.032 (shake flask-nephelometry, Hollifield 1979)

0.135 (shake flask-LSC, Means et al. 1979; 1980)

0.130 (shake flask-GC/UV, Rossi & Thomas 1981)

- 0.136\* (25.5°C, generator column-HPLC/UV, measured range 277.85–303.05 K, May et al. 1983)  
 0.129 (average lit. value, Pearlman et al. 1984)  
 0.133 (generator column-HPLC/fluorescence, Walters & Luthy 1984)  
 0.135 (RP-HPLC-RT correlation, Chin et al. 1986)  
 0.118 (generator column-HPLC/UV, Billington et al. 1988)  
 0.132\* (recommended, IUPAC Solubility Data Series, Shaw 1989)  
 0.150 (shake flask-LSC, Eadie et al. 1990)  
 0.107 (generator column-HPLC, Vadas et al. 1991)  
 0.132, 0.050 (solid  $S_s$  at 26°C); 2.61, 1.01 (supercooled liquid  $S_L$  at 4°C) (quoted, Piatt et al. 1996)  
 0.131; 0.077, 0.422 (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)  
 0.150 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)  
 $\log [S_L/(\text{mol/L})] = 0.316 - 895.4/(T/K)$ ; (supercooled liquid, Passivirta et al. 1999)  
 $\ln x = -4.007476 - 4252.03/(T/K)$ , temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)  
 0.1331\* (25.55°C, generator column-HPLC/fluorescence, measured range 0.75–32.08°C, Reza et al. 2002)  
 $\ln x = (-1.30 \pm 0.56) + (-5059 \pm 165)/(T/K)$ ; temp range 281.9–305.23 K (Reza et al. 2002)

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

- 0.00339 (effusion method, Inokuchi et al. 1952)  
 0.000882\* (effusion method, extrapolated from Antoine eq., Bradley & Cleasby 1953)  
 $\log (P/\text{cmHg}) = 10.270 - 4904/(T/K)$ ; temp range 71.75–85.25°C (Antoine eq., Bradley & Cleasby 1953)  
 347\* (200.4°C, temp range 200.4–394.7°C, Tsytkina 1955; quoted, Boublik et al. 1984)  
 0.00033 (effusion method, Hoyer & Peperle 1958; quoted, Mabey et al. 1982; Tsai et al. 1991)  
 $\log (P/\text{mmHg}) = 12.0 - 5248/(T/K)$ , temp range 25–90°C, (Knudsen effusion method, Hoyer & Peperle 1958)  
 0.2118\* (348 K, Knudsen effusion, measured range 348–419 K, Malaspina et al. 1974)  
 12.4\* (125°C, inclined-piston gauge, measured range 125–185°C, Smith et al. 1980)  
 0.00091 (effusion method, Pupp et al. 1974; quoted, Bidleman 1984)  
 0.00027 (lit. average-interpolated, API 1979; quoted, Wasik et al. 1983)  
 0.00088 (extrapolated from Antoine eq., Amidon & Anik 1981)  
 0.00060\* (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)  
 $\log (P/\text{Pa}) = 12.748 - 4760.73/(T/K)$ ; temp range 10–50°C (solid, Antoine eq., Sonnefeld et al. 1983)  
 0.0006 (generator column-HPLC/fluor./UV, Wasik et al. 1983)  
 0.0113, 0.0049 ( $P_{GC}$  by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)  
 0.0158 (supercooled liquid  $P_L$ , converted from literature  $P_S$  with  $\Delta S_{fus}$  Bidleman 1984)  
 $\log (P_L/\text{kPa}) = 4.75092 - 1127.529/(16.02 + t/^\circ\text{C})$ ; temp range 200–394°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 0.00442 (Yamasaki et al. 1984)  
 $\log (P_L/\text{mmHg}) = 5.6184 - 1122.0/(15.2 + t/^\circ\text{C})$ ; temp range 200–395°C (Antoine eq., Dean 1985, 1992)  
 0.00033 (selected, Howard et al. 1986; quoted, Banerjee et al. 1990)  
 0.00055 (interpolated Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_S/\text{kPa}) = 10.75452 - 5072.78/(T/K)$ ; temp range 298–401 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_S/\text{kPa}) = 11.35032 - 5286.784/(T/K)$ ; temp range 360–419 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 5.5106 - 1743.57/(-170.83 + T/K)$ , temp range 513–668 K, (Antoine eq.-III, Stephenson & Malanowski 1987)  
 0.000413, 0.00973 (lit. mean, supercooled liquid value  $P_L$ , Bidleman & Foreman 1987)  
 0.000293\* (pressure gauge, extrapolated-Antoine eq. derived exptl. data, temp 80–140°C, Sasse et al. 1988)  
 $\log (P_S/\text{mmHg}) = 8.654859 - 2967.129/(182.314 + t/^\circ\text{C})$ ; temp range 80.11–139.97°C (solid, Antoine eq., pressure gauge, Sasse et al. 1988)  
 $\log (P_L/\text{mmHg}) = 5.62672 - 1553.755/(112.964 + t/^\circ\text{C})$ ; temp range 139.93–194.16°C (liquid, Antoine eq., pressure gauge, Sasse et al. 1988)

0.010, 0.014 (quoted  $P_L$ , supercooled liquid  $P_L$ , GC-RT correlation, Hinckley 1989)  
 0.0158, 0.0144 (supercooled  $P_L$ , converted from literature  $P_S$  with different  $\Delta S_{fus}$  values, Hinckley et al. 1990)  
 0.0113, 0.00752 ( $P_{GC}$  by GC-RT correlation with different reference standards, Hinckley et al. 1990)  
 $\log(P_L/Pa) = 11.92 - 4104/(T/K)$  (GC-RT correlation, Hinckley et al. 1990)  
 $\log(P/mmHg) = 70.7671 - 6.9413 \times 10^3/(T/K) - 21.79 \cdot \log(T/K) + 6.0727 \times 10^{-3} \cdot (T/K) + 1.5767 \times 10^{-12} \cdot (T/K)^2$ ;  
 temp range 424–926 K (vapor pressure eq., Yaws 1994)  
 0.00446 (supercooled liquid  $P_L$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)  
 0.000334–0.00306; 0.000601; 0.000293 (quoted exptl.: effusion, gas saturation, manometry, Delle Site 1997)  
 0.000173, 0.00088; 0.000247, 0.000572, 0.000713 (quoted lit., calculated; from GC-RT correlation, Delle Site 1997)  
 0.00044\* (Knudsen effusion, extrapolated-Antoine eq. derived from exptl. data, temp range 35–125°C, Oja & Suuberg 1998)  
 $\log(P/Pa) = 33.856 - 12400/(T/K)$ ; temp range 308–398 K (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)  
 $1.51 \times 10^{-2}$ ;  $1.94 \times 10^{-3}$  (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_S$  with fugacity ratio  $F$ , Passivirta et al. 1999)  
 $\log(P_S/Pa) = 11.60 - 4263/(T/K)$  (solid, Passivirta et al. 1999)  
 $\log(P_L/Pa) = 9.49 - 3370/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $0.00073 \pm 0.00033$  (gas saturation-HPLC/fluorescence, de Seze et al. 2000)  
 $\log(P/Pa) = 12.748 - 4760.73/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

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

1.89 (gas stripping, Southworth 1979)  
 1.10 (gas stripping, Mackay & Shiu 1981)  
 1.21 (gas stripping-fluorescence, Shiu & Mackay 1997)  
 2.0, 0.92 (gas stripping-HPLC/fluor., De Maagd et al. 1998)  
 0.496 (wetted wall column-GC, Altschuh et al. 1999)  
 1.71\* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)  
 $\ln K_{AW} = -5159.97/(T/K) + 10.103$ ,  $\Delta H = 42.9 \text{ kJ mol}^{-1}$ , measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)  
 $\log[H/(Pa \text{ m}^3/\text{mol})] = 9.17 - 2475/(T/K)$  (Passivirta et al. 1999)

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

4.90 (calculated- $\pi$  const., Southworth et al. 1978)  
 5.32 (calculated-fragment const., Callahan et al. 1979)  
 4.88 (Hansch & Leo 1979)  
 5.18 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)  
 5.09 (shake flask-LSC, Means et al. 1979, 1980)  
 5.22 (calculated- $f$  const., Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)  
 5.03 (HPLC- $k'$  correlation, Hanai et al. 1981)  
 5.05 (HPLC- $k'$  correlation, McDuffie 1981)  
 5.22 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)  
 4.50 (HPLC- $k'$  correlation, D'Amboise & Hanai 1982)  
 4.88 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 4.88 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)  
 4.96 (HPLC-RT correlation, Rapaport 1984)  
 5.52 (HPLC-RT/MS correlation, Burkhard et al. 1985)  
 4.80 (Hansch & Leo 1985)  
 4.97 (RP-HPLC-RT correlation, Chin et al. 1986)  
 4.95 (Leo 1986)  
 $5.00 \pm 0.20$  (recommended, Sangster 1989, 1993)  
 4.88 (recommended, Hansch et al. 1995)  
 5.08; 5.39 (26°C; 4°C, Piatt et al. 1996)  
 $4.84 \pm 0.19$ ,  $5.14 \pm 0.62$  (HPLC- $k'$  correlation: ODS column; Diol column, Helweg et al. 1997)  
 4.77 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)  
 4.79 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)

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

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

- 8.60 (calculated- $K_{OW}/K_{AW}$ , Wania & Mackay 1996)
- 8.61 (calculated, Finizio et al. 1997)
- 8.80\*; 8.49 (generator column-GC; calculated- $C_O/C_A$ , measured range 0–40°C, Harner & Bidleman 1998)
- $\log K_{OA} = -4.56 + 3985/(T/K)$ ; temp range 0–40°C (generator column-GC, Harner & Bidleman 1998)
- 8.75 (calculated- $S_{oct}$  and vapor pressure  $P$ , Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 3.43 (*Daphnia pulex*, Southworth et al. 1978)
- 4.38 (mixed microbial population, Steen & Karickhoff 1981)
- 4.65 (*P. hoyi*, Eadie et al. 1982)
- 4.56, 4.22, 4.75 (average, *Selenastrum capricornutum*-dosed singly, dosed simultaneously, Casserly et al. 1983)
- 2.66 (goldfish, shake flask-GC, concn. ratio, Ogata et al. 1984)
- 3.43 (*Daphnia pulex*, Mackay & Hughes 1984)
- 3.43 (*Daphnia magna*, Newsted & Giesy 1987)
- 3.65, 3.81, 2.35 (mussel, clam, shrimp, Gobas & Mackay 1989)
- 2.85, 2.70 (*Polychaete*, *Shrimo-hepatopancreas*, Gobas & Mackay 1989)
- 0.716, 1.124 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

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

- 4.92 (natural sediments, sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
- 4.81 (average value of soil and sediment, shake flask-LSC, sorption isotherms, Means et al. 1979)
- 4.92 (Kenaga & Goring 1980)
- 4.80 (average value of 12 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1980)
- 4.78, 4.80 (soil/sediment: calculated- $K_{OW}$ , regress of  $K_p$  versus substrate properties, Means et al. 1980)
- 4.826 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
- 3.11, 3.46 (sediment suspensions, Karickhoff & Morris 1985)
- 5.23; 5.08 (fluorescence quenching interaction with AB humic acid; AB fulvic acid, Gauthier et al. 1986)
- 4.46–4.81; 4.94–5.51; 4.73–5.02 (marine humic acids; soil humic acids; soil fulvic acids, fluorescence quenching technique, Gauthier et al. 1987)
- 5.02 (dissolved humic materials, Aldrich humic acid, fluorescence quenching technique, Gauthier et al. 1987)
- 5.13 (sediment, batch equilibrium-GC, Vowles & Mantoura 1987)
- 4.88 (soil-fine sand 0.2% OC, dynamic soil column studies, Enfield et al. 1989)
- 5.65 (LSC, Eadie et al. 1990)
- 6.51 (sediments average, Kayal & Connell 1990)
- 4.83 (RP-HPLC-RT correlation, Pussemier et al. 1990)
- 4.82, 4.77 (RP-HPLC-RT correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)
- 6.50 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 5.05, 5.00, 4.88; 4.71 (marine porewater organic colloids: Fort Point Channel FPC 7–9 cm, FPC 15–17 cm, FPC 25–29 cm; Spectacle Island 14–16 cm, Chin & Gschwend 1992)
- 5.20, 5.18, 4.99; 5.23 (marine sediments: Fort Point Channel FPC 7–9 cm, FPC 15–17 cm, FPC 25–29 cm; Spectacle Island 14–16 cm, Chin & Gschwend 1992)
- 4.78; 4.78, 4.78 (sediment: concn ratio  $C_{sed}/C_w$ ; concn-based coeff., area-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
- 5.50, 6.61, 6.06 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island, McGroddy & Farrington 1995)
- 5.51, 5.34, 5.31; 7.43 (marine sediments: Fort Point Channel FPC 7–9 cm, FPC 15–17 cm, FPC 25–29 cm; Spectacle Island 14–16 cm, McGroddy & Farrington 1995)
- 4.64 (Aldrich humic acid, Ozretich et al. 1995)
- 4.80, 4.81, 4.72 (RP-HPLC- $k'$  correlation on different stationary phases, Szabo et al. 1995)
- 4.81 (range 4.73–4.66); 4.22 (range 4.20–4.22) (4°C, low organic carbon sediment  $f_{OC} = 0.0002$ , batch equilibrium; column exptl., Piatt et al. 1996)

- 4.62 (range 4.56–4.67); 4.0 (range 3.98–4.00) (26°C, low organic carbon sediment  $f_{oc} = 0.0002$ , batch equilibrium; column exptl., Piatt et al. 1996)
- 4.42–2.56 (5 soils, 20°C, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
- 4.99, 4.98, 4.96, 4.97, 4.97 (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
- 5.14, 5.22, 5.23, 5.12, 5.04, 5.24, 5.45; mean  $4.98 \pm 0.009$  (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
- 3.47, 4.60, 3.53, 4.78, 4.61; mean  $5.18 \pm 0.056$  (HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 4.66, 4.78 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ , average, Delle Site 2001)
- 4.88, 4.90 (sediments: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ , average, Delle Site 2001)
- 5.47–6.68; 4.60–6.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.90; 5.89, 5.60, 5.56 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 4.96; 4.70; 4.46–5.74 (calculated- $K_{ow}$ ; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)
- 4.50 at pH 4, 4.37 at pH 7, 4.33 at pH 10 in 0.001M NaCl; 4.35 at pH 4, 4.20 at pH 7, 4.245 at pH 10 in 0.01M NaCl; 4.35 at pH 4, 4.15 at pH 7, 4.15 at pH 10 in 0.1M NaCl; 4.33 at pH 4, 4.29 at pH 7, 4.15 at pH 10 in 1mM  $Ca^{2+}$  in 0.1M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautman & Morgan 1993a)
- 4.19 at pH 4, 3.89 at pH 7, 3.92 at pH 10 in 0.001M NaCl; 4.15 at pH 4, 3.88 at pH 7, 3.86 at pH 10 in 0.01M NaCl; 4.08 at pH 4, 3.81 at pH 7, 3.785 at pH 10 in 0.1M NaCl; 4.08 at pH 4, 3.90 at pH 7, 4.06 at pH 10 in 1mM  $Ca^{2+}$  in 0.1M total ionic strength solutions (shake flask/fluorescence, fulvic acid; Schlautman & Morgan 1993a)
- 5.52 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)
- 4.66 (Askov soil, a Danish agriculture soil, Sverdrup et al. 2002)
- 5.35–6.33 (field contaminated sediment, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluorescence, ten Hulscher et al. 2003)

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

- Volatilization: sublimation rate constant of  $1.1 \times 10^{-4} s^{-1}$  was measured as loss from glass surface at 24°C at an air flow rate of 3 L/min (Cope & Kalkwarf 1987)
- Photolysis: calculated  $t_{1/2} = 4.2$  d for direct sunlight photolysis in midday of midsummer at 40°N for inland water, and  $t_{1/2} = 5.9$  d for inland water with sediment partitioning (Zepp & Schlotzhauer 1979)
- $k = 1.014 h^{-1}$  (Zepp 1980)
- $t_{1/2} = 0.68$  h atmospheric and aqueous photolysis half-life, based on measured aqueous photolysis quantum yields calculated for midday summer sunlight at 40°N latitude (Zepp & Schlotzhauer 1979; quoted, Harris 1982; Howard et al. 1991) and  $t_{1/2} = 2.04$  h after adjusting for approximate winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
- half-lives:  $t_{1/2} = 21$  h on silica gel,  $t_{1/2} = 31$  h on alumina and  $t_{1/2} = 46$  h on fly ash on different atmospheric particulate substrates (approximate 25  $\mu g/g$  on substrate) (Behymer & Hites 1985);
- $t_{1/2} = 4.2$  d for summer sunlight photolysis in surface water (Mill & Mabey 1995)
- $k < 1.05 \times 10^{-4} m/s$  at 24°C with  $[O_3] = 0.16$  ppm and light intensity of 1.3  $kW/m^2$  on glass surface of (Cope & Kalkwarf 1987)
- photodegradation  $t_{1/2} = 1$  h in summer to days in winter by sunlight for adsorption on airborne particulates (Valerio et al. 1991);
- photolysis  $t_{1/2} = 0.68$  h in water, based on direct photolysis in sunlight at midday, midsummer, latitude 40°N (Zepp 1991)
- $k(exptl) = 0.00362 min^{-1}$  for pseudo-first-order direct photolysis, with  $t_{1/2} = 3.18$  h, and the predicted  $k(calc) = 0.00382 min^{-1}$  by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
- $t_{1/2}(obs.) = 2.63$  h,  $t_{1/2}(calc) = 2.56$  h by QSPR in atmospheric aerosol (Chen et al. 2001);
- $k = (2.08 \pm 0.13) \times 10^{-5} s^{-1}$  and  $t_{1/2} = (9.24 \pm 0.53)h$  in diesel particulate matter, photochemical degradation under atmospheric conditions,  $k = (1.88 \pm 0.16) \times 10^{-5} s^{-1}$  and  $t_{1/2} = (10.22 \pm 0.95)h$  in diesel particulate matter/soil mixture, and  $t_{1/2} = 0.80$  to 1.59 h in various soil components using a 900-W photo-irradiator as light source;  $k = (2.61 \pm 0.53) \times 10^{-7} s^{-1}$  and  $t_{1/2} = (737.55 \pm 124.49)h$  in diesel particulate matter using a 300 W light source (Matsuzawa et al. 2001)



Photodegradation  $k = 3.9 \times 10^{-4} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

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

$k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $2.2 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)

$k = (3.4\text{--}5.3) \times 10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  over pH range 1–7, with  $t_{1/2} = 0.18 \text{ s}$  in presence of  $10^{-4} \text{ M}$  ozone at pH 7 for the reaction with  $\text{O}_3$  in water at  $25^\circ\text{C}$  (Butković et al. 1983)

$k_{\text{OH}} = 5.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $k_{\text{N}_2\text{O}_5} \approx -5.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with  $\text{N}_2\text{O}_5$  at  $296 \pm 2 \text{ K}$  (relative rate method, Atkinson et al. 1990)

photooxidation  $t_{1/2} = 0.802\text{--}8.02 \text{ h}$ , based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: significant degradation within 7 d for a domestic sewage 28-d test for an average of three static-flask screening (Tabak et al. 1981)

$t_{1/2}(\text{aq. aerobic}) = 5040\text{--}45600 \text{ h}$ , based on aerobic soil die-away test data at  $10\text{--}30^\circ\text{C}$  (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991)

$k = 0.29 \text{ h}^{-1}$  in atmosphere (Dragoscu & Friedlander 1989; quoted, Tsai et al. 1991)

$k = 0.0027 \text{ d}^{-1}$  with  $t_{1/2} = 260 \text{ d}$  for Kidman sandy loam and  $k = 0.0035 \text{ d}^{-1}$  with  $t_{1/2} = 199 \text{ d}$  for McLarin sandy loam all at  $-0.33 \text{ bar}$  soil moisture (Park et al. 1990)

$t_{1/2}(\text{anaerobic}) = 20160\text{--}182400 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

$k_1 = 1126 \text{ h}^{-1}$ ;  $k_2 = 0.343 \text{ h}^{-1}$  (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 3.05 \text{ h}^{-1}$ ;  $\log k_2 = -0.46 \text{ h}^{-1}$  (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 113.0 \text{ h}^{-1}$ ;  $k_2 = 0.017 \text{ h}^{-1}$  ( $4^\circ\text{C}$ , *S. heringianus*, Frank et al. 1986)

$k_2 = 0.017 \text{ h}^{-1}$  (*S. heringianus*, Frank et al. 1986)

$k_1 = 199.2 \text{ mL g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0012 \text{ h}^{-1}$  ( $4^\circ\text{C}$ , *P. hoyi*, Landrum 1988)

$k_1 = 3.4\text{--}5.3 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.022 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 0.68\text{--}2.04 \text{ h}$ , based on estimated sunlight photolysis half-life in water (Zepp & Stotzhauer 1979; Lyman et al. 1982; quoted, Howard et al. 1991);

half-lives under simulated atmospheric conditions:  $t_{1/2} = 4.20 \text{ h}$  under simulated sunlight,  $t_{1/2} = 2.75 \text{ h}$  under simulated sunlight + ozone (0.2 ppm),  $t_{1/2} = 15.72 \text{ h}$  under dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 2.5 \text{ h}$  with a steady-state concn of tropospheric ozone of  $2 \times 10^{-9} \text{ M}$  in clean air (Butković et al. 1983); photooxidation  $t_{1/2} = 0.802\text{--}8.02 \text{ h}$ , based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: computed near-surface  $t_{1/2} = 0.58 \text{ h}$  for direct photochemical transformation at latitude  $40^\circ\text{N}$ , midday, midsummer,  $t_{1/2} = 4.2 \text{ h}$  for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning and  $t_{1/2} = 5.9 \text{ d}$  with sediment-water partitioning (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.68\text{--}2.04 \text{ h}$ , based on estimated sunlight photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991);

$t_{1/2} = 1.8 \text{ s}$  in presence of  $10^{-4} \text{ M}$  ozone at pH 7 (Butković et al. 1983);

$t_{1/2} = 4.2 \text{ d}$  for summer at  $40^\circ\text{N}$  latitude under sunlight (Mill & Mabey 1985);

$t_{1/2} = 0.68 \text{ h}$ , based on direct photolysis in sunlight at midday, mid-summer and  $40^\circ\text{N}$  latitude (quoted, Zepp 1991); photolysis  $t_{1/2} = 3.18 \text{ h}$  in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:  $t_{1/2} = 10080\text{--}91200 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction  $t_{1/2} = 547 \text{ h}$  for chemical available pyrene and  $t_{1/2} = 298 \text{ h}$  for bioavailable pyrene for amphipod, *P. hoyi* in Lake Michigan sediments at  $4^\circ\text{C}$ . The uptake clearance from sediment,  $k = (0.019\text{--}0.015) \text{ g of dry sediment} \cdot \text{g}^{-1} \text{ of organism} \cdot \text{h}^{-1}$ , and the rate constants to become biologically unavailable were  $k = 0.0019$

$h^{-1}$  for 10-d aged sediment corresponding to a  $t_{1/2} = 365$  d and  $k = 0.0030$   $h^{-1}$  for nonaged sediment corresponding to a  $t_{1/2} = 231$  h (Landrum 1989).

Soil:  $t_{1/2} = 3\text{--}35$  h (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 58$  d for 5 mg/kg treatment and  $t_{1/2} = 48$  d for 50 mg/kg treatment (Bulman et al. 1987);

$t_{1/2} = 5040\text{--}45600$  h, based on aerobic soil die-away test data at  $10\text{--}30^{\circ}\text{C}$  (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);

$t_{1/2} > 50$  d (Ryan et al. 1988);

degradation rate constant,  $k = 0.0027$   $d^{-1}$  with  $t_{1/2} = 260$  d for Kidman sandy loam soil and  $k = 0.0035$   $d^{-1}$  with  $t_{1/2} = 199$  d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 500$  d in soil (Jury et al. 1990);

$t_{1/2} = 0.4$  to more than 90 wk, 8.5 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: depuration  $t_{1/2} = 40.8$  h in *s. heringianus* (Frank et al. 1986);

elimination  $t_{1/2} = 4.1\text{--}5.5$  d from mussel *Mytilus edulis*;  $t_{1/2} = 10.3$  d from clam *Mya arenaria*,  $t_{1/2} = 14.4$  d from polychaete *Abarenicola pacifica*,  $t_{1/2} = 6.7$  d from Oyster,  $t_{1/2} = 0.80$  d from shrimp,  $t_{1/2} = 3.6$  d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

**TABLE 4.1.1.29.1**

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

1.

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
	experimental		smoothed				
22.2	0.129	0	0.049	12.2	0.055	25	0.132
22.2	0.128	22.2	0.130	15.5	0.069	29	0.162
22.2	0.124	25	0.148	17.4	0.079		
34.5	0.228	34.5	0.235	20.3	0.092	temp dependence eq. 2	
34.5	0.235	44.7	0.399	23.0	0.117	S	µg/kg
44.7	0.397	50	0.532	23.3	0.118	a	−0.0011
44.7	0.395	50.1	0.534	25.0	0.129	b	0.2007
44.7	0.405	55.6	0.730	26.2	0.144	c	−1.051
50.1	0.558	56.0	0.74	26.7	0.145	d	50.2
50.1	0.576	60.7	0.97	28.5	0.164		
50.1	0.556	65.2	1.27	31.3	0.188	ΔH <sub>sol</sub> /(kJ mol <sup>−1</sup> ) = 35.44	
55.6	0.75	71.9	1.90			for temp range 5–30°C	
55.6	0.75	74.7	2.26	ΔH <sub>sol</sub> /(kJ mol <sup>−1</sup> ) = 47.70			
55.6	0.77	75.0	2.31				
56.0	0.74						
60.7	0.96	temp dependence eq. 1					
60.7	0.95	ln x	mole fraction				
60.7	0.90	ΔH <sub>fus</sub>	15.3 ± 0.084				
65.2	1.27	10 <sup>2</sup> ·b	4.78 ± 0.09				
65.2	1.29	c	38.1 ± 0.3				
71.9	1.83						
71.9	1.86						
71.9	1.89						
74.7	2.21						
ΔH <sub>fus</sub> /(kJ mol <sup>−1</sup> ) = 15.3							

Empirical temperature dependence equations:

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

May et al. (1978):  $-S/(\mu\text{g}/\text{kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d$  (2)

TABLE 4.1.1.29.1 (Continued)

2.

May 1980		May et al. 1983		Shaw 1989		Reza et al. 2002	
generator column-HPLC		generator column-HPLC		IUPAC recommended		generator column-HPLC/fluor	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
4.7	0.0492	4.7	0.0492	0	0.050	8.54	0.0474
9.5	0.0585	9.5	0.0586	20	0.090	10.39	0.0566
14.3	0.0720	14.3	0.0721	25	0.132	13.5	0.0635
18.7	0.0933	18.7	0.0934	30	0.175	14.46	0.0694
21.2	0.109	21.2	0.1091	40	0.30	15.7	0.0804
25.5	0.136	25.5	0.1361	50	0.50	18.05	0.0871
29.9	0.170	29.9	0.1701	60	0.90	21.53	0.1087
				70	1.70	25.55	0.1331
				75	2.30	27.36	0.1505
temp dependence eq. 2						29.66	0.1686
S	μg/kg					21.28	0.1931
a	-0.0011						
b	0.2007						
c	-1.051						
d	50.2						
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 35.44$						$\ln x = A - B/T(\text{K})$	
for temp range 5–30°C						A	-1.30
						B	5059
						temp range 282–305 K	

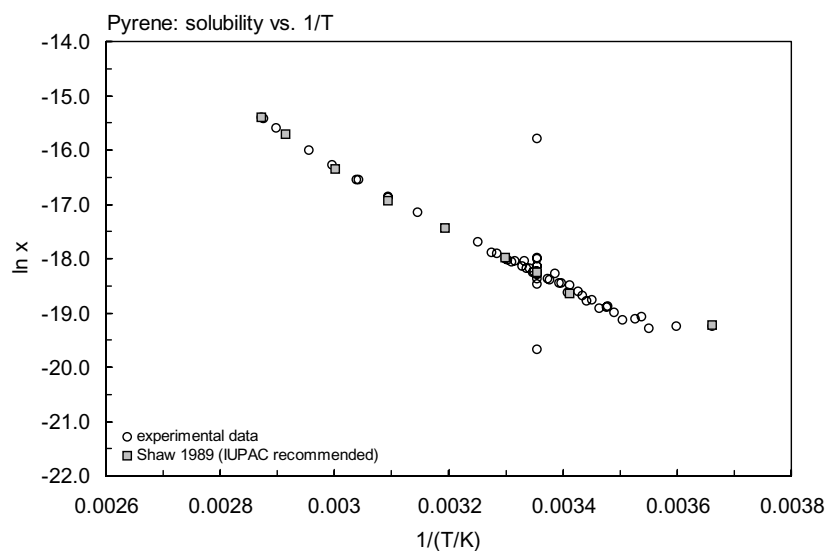
FIGURE 4.1.1.29.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for pyrene.

TABLE 4.1.1.29.2

Reported vapor pressures of pyrene 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.

Bradley & Cleasby 1953		TsyPKina 1955		Hoyer & Peperle 1958		Malaspina et al. 1974	
effusion		in Boublik et al. 1984		effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
68.9	0.1147	200.4	347	data presented by		348	0.2118
74.15	0.1880	220.8	920	eq. 1	P/mmHg	361	0.508
78.1	0.263	242.7	2440	A	12.00	364	0.717
78.1	0.274	256.4	4373	B	5348	369	1.034
81.7	0.2746	270.0	6493	temp range 25–90°C		377	2.016
82.65	0.3893	277.0	7999	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 100.5$		384	3.871
85.0	0.4093	288.7	10866			393	7.934
71.75	0.1440	293.0	12599			402	15.20
75.85	0.2226	306.0	17932			411	31.01
82.7	0.2880	316.0	22665			419	55.42
82.25	0.4053	394.7	101324				
85.0	0.5066			for solid pyrene:			
		bp/°C	394.707			eq. 1	P/atm
eq. 1	P/mmHg					A	8.848
A	10.270					B	5091
B	4904						
						$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 101.04$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 93.90$						at 298.15 K	

2.

Smith et al. 1980		Sonnefeld et al. 1983		Sasse et al. 1988		Oja & Suuberg 1998	
inclined-piston gauge		gas saturation-HPLC		electronic manometry		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
solid				solid			
125	12.4	10.5	$9.20 \times 10^{-5}$	80.11	0.30	46.95	0.00863
130	17.5	10.5	$9.21 \times 10^{-5}$	90.10	0.764	56.99	0.0243
135	24.7	10.5	$9.53 \times 10^{-5}$	100.11	1.853	37.98	0.0209
140	34.7	20.9	$3.35 \times 10^{-4}$	110.14	4.360	68.03	0.0852
145	48.0	20.9	$3.35 \times 10^{-4}$	120.08	9.213	72.99	0.164
149	62.1	20.9	$3.39 \times 10^{-4}$	120.10	9.40	83.99	0.428
150	66.1	30.0	$1.10 \times 10^{-4}$	129.99	19.20	93.02	0.945
liquid		30.0	$1.09 \times 10^{-4}$	134.98	26.80		
125	17.1*	30.0	$1.03 \times 10^{-4}$	139.97	37.07	eq. 1a	P/Pa
130	22.5*	39.34	$3.31 \times 10^{-3}$	liquid		A	33.856
135	29.9*	39.34	$3.47 \times 10^{-3}$	139.93	40.80	B	12400
140	39.5*	39.34	$3.25 \times 10^{-3}$	144.90	53.06		
145	51.3*	39.45	$3.41 \times 10^{-3}$	149.82	68.66	$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 103.10$	

TABLE 4.1.1.29.2 (Continued)

2.

Smith et al. 1980		Sonnefeld et al. 1983		Sasse et al. 1988		Oja & Suuberg 1998	
inclined-piston gauge		gas saturation-HPLC		electronic manometry		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
149	63.3*	39.45	$3.20 \times 10^{-3}$	159.75	112.5		
150	66.7*	25.0	$6.0 \times 10^{-4}$	169.61	178.8		
152	78.3			179.45	279.4		
155	86.5	eq. 2	P/Pa	189.25	405.7		
160	110.7	A	12.748	194.16	490.1		
165	141.6	B	4760.73				
170	178.9	temp range 10–50°C		for solid			
175	224.6			eq. 2	P/mmHg		
180	280.4	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 91.20$		A	8.654859		
185	345.3	B		2967.129			
				C	182,314		
				temp range: 80.1–139.97°C			
				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 97.70$			
*supercooled liquid values							
reported vapor pressure eq.							
see foot note		eq. 2		P/mmHg			
				A	5.62672		
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 103.9$		B		1553.755			
				C	112.964		
				temp range: 139.97–194°C			

note:  $\ln(P_L/P_S) = 268.6187 - 699.31/(T/K) - 45.6846 \ln(T/K) + 0.057217(T/K)$ ; in which  $P_L$  and  $P_S$  are the vapor pressure of supercooled liquid and crystal phase, respectively, at temperature T.

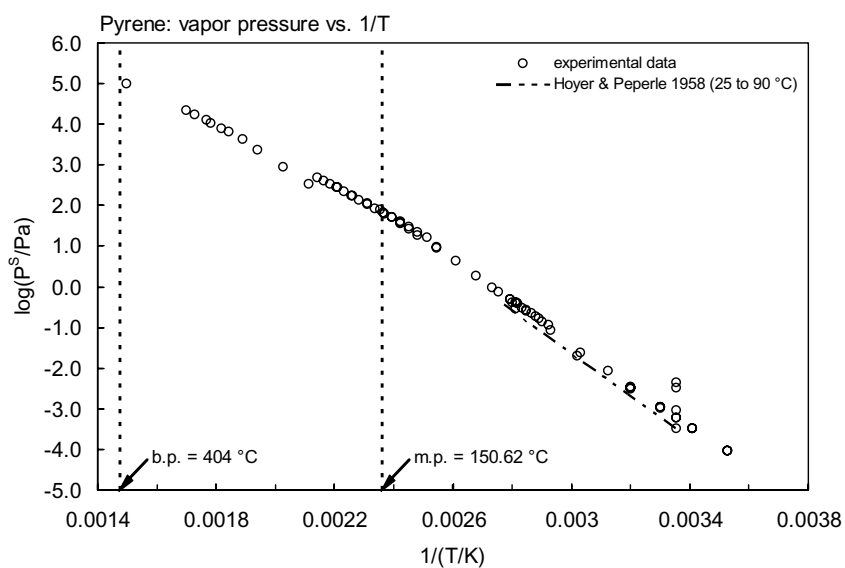


FIGURE 4.1.1.29.2 Logarithm of vapor pressure versus reciprocal temperature for pyrene.

TABLE 4.1.1.29.3

Reported Henry's law constants and octanol-air partition coefficients of pyrene at various temperatures and temperature dependence equations

Henry's law constant			log K <sub>OA</sub>	
Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)	t/°C	log K <sub>OA</sub>
		average		
4.1	0.37, 0.49	0.43	0	9.966
11.0	0.63, 0.76	0.69	10	9.528
18.0	1.02, 1.19	1.10	20	9.155
25.0	1.54, 1.89	1.71	30	8.647
31.0	2.15, 2.80	2.45	40	8.121
			25(exptl)	8.80
			25(calc)	8.49
ln K <sub>AW</sub> = A - B/(T/K)			log K <sub>OA</sub> = A + B/(T/K)	
A	10.1034		A	-4.56
B	5160		B	3985
enthalpy, entropy change:			enthalpy of phase change	
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 42.9 \pm 2.3$			$\Delta H_{\text{OA}}/(\text{kJ}\cdot\text{mol}^{-1}) = 76.3$	
$\Delta S/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = 84$				
at 25°C				

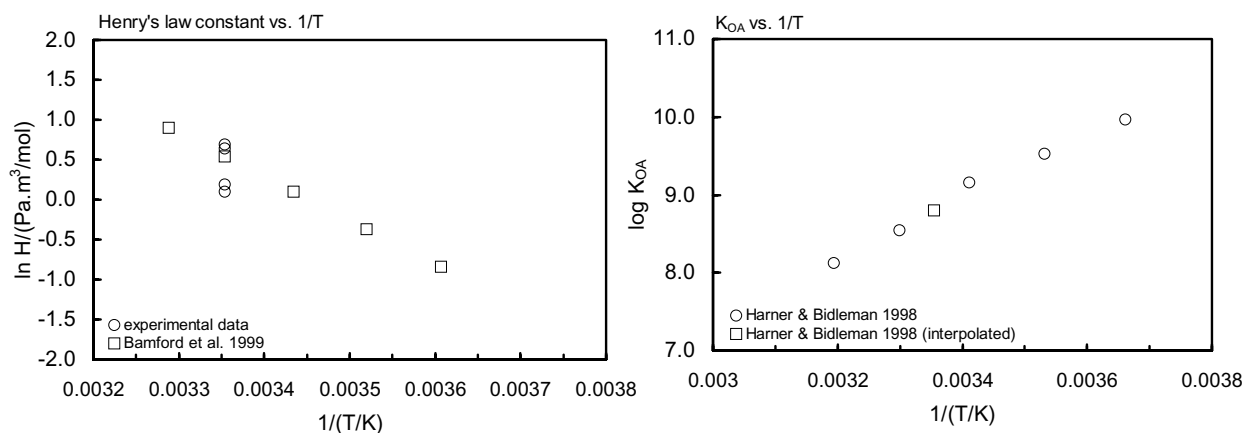
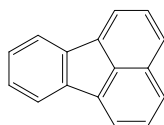


FIGURE 4.1.1.29.3 Logarithm of Henry's law constant and  $K_{\text{OA}}$  versus reciprocal temperature for pyrene.

## 4.1.1.30 Fluoranthene



Common Name: Fluoranthene

Synonym: idryl, 1,2-benzacenaphthene, benzo[*j,k*]fluorene, benz[*a*]acenaphthylene, fluoranthrene

Chemical Name: 1,2-benzacenaphthene

CAS Registry No: 206-44-0

Molecular Formula: C<sub>16</sub>H<sub>10</sub>

Molecular Weight: 202.250

Melting Point (°C):

110.19 (Lide 2003)

Boiling Point (°C):

384 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.252 (0°C, Weast 1982–83, Dean 1985; Lide 2003)

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

162 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

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

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

18.87 (Ruelle & Kesselring 1997)

18.74 (exptl., Chickos et al. 1999)

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

49.37 (Casellato et al. 1973; quoted, Yalkowsky 1981)

47.70 (differential scanning calorimetry, Hinckley et al. 1990)

48.89, 36.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

49.6 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming  $\Delta S_{\text{fus}} = 56$  J/mol K), F: 0.146 (mp at 110.19°C)

0.191 (calculated,  $\Delta S_{\text{fus}} = 49.6$  J/mol K, Passivirta et al. 1999)

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

0.240 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.265 (shake flask-UV, Klevens 1950)

0.240 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)

0.236 (fluorescence/UV, Schwarz & Wasik 1976)

0.260 (shake flask-fluorescence, Mackay & Shiu 1977)

0.206 (Rossi 1977; Neff 1979)

0.206\* (generator column-HPLC/UV, measured range 8.1–29.9°C, May et al. 1978a,b)

$S/(\mu\text{g/kg}) = 50.4 + 4.322 \cdot (t/^\circ\text{C}) - 0.1047 \cdot (t/^\circ\text{C})^2 + 0.0072 \cdot (t/^\circ\text{C})^3$ ; temp range 5–30°C (generator column-HPLC/UC, May et al. 1978b)

0.120 (shake flask-nephelometry, Hollifield 1979)

0.218 (OECD 1979/1980; quoted, He et al. 1995)

0.275, 0.373 (15, 25°C, generator column/elution method, average values of 6–7 laboratories, OECD 1981)

0.200 (20°C, quoted, Schmidt-Bleek et al. 1982)

0.190 (20°C, generator column-fluorescence, Hashimoto et al. 1982)

0.203\* (24.6°C, generator column-HPLC, measured range 281.25–303.05 K, May et al. 1983)

0.243 (average lit. value, Pearlman et al. 1984)

0.199 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

1.43 (RP-HPLC-RT correlation, Chin et al. 1986)

0.283 (vapor saturation-UV, Akiyoshi et al. 1987)

0.240 (recommended, Shaw 1989)

0.222 (generator column-HPLC/fluorescence, Kishi & Hashimoto 1989)

0.373 (average value of Japan, OECD tests, Kishi & Hashimoto 1989)  
 0.166 (shake flask-fluorescence, Kishi & Hashimoto 1989)  
 0.265 (shake flask-HPLC/UV/fluorescence, Pinal et al. 1991)  
 0.177 (generator column-HPLC, Vadas et al. 1991)  
 0.248 (generator column-HPLC/UV, Yu & Xu 1993)  
 0.207 (generator column-HPLC/fluorescence, De Maagd et al. 1998)  
 $0.2289 \pm 0.0008$  (shake flask-SPME (solid-phase micro-extraction)-GC, Paschke et al. 1999)  
 $\log [S_L/(\text{mol/L})] = 0.779 - 987.5/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $\ln x = -1.796327 - 4772.17/(T/K)$ ; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

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

653\* (197.0°C, temp range 197.0–384.2°C, Tsytkina 1955; quoted, Boublik et al. 1984)  
 $6.67 \times 10^{-4}$  (effusion method, Hoyer & Peperle 1958)  
 $\log (P/\text{mmHg}) = 12.67 - 5357/(T/K)$ ; temp range 25–85°C (Knudsen effusion method, Hoyer & Peperle 1958)  
 0.00123\* (gas saturation-HPLC/fluor. or UV, Sonnefeld et al. 1983)  
 $\log (P/\text{Pa}) = 11.901 - 4416.56/(T/K)$ ; temp range 10–50°C (Antoine eq., gas saturation, Sonnefeld et al. 1983)  
 0.00124 (generator column-HPLC/fluor., Wasik et al. 1983)  
 1.79 (supercooled liquid  $P_L$ , extrapolated from Antoine eq., Boublik et al. 1984)  
 0.0154, 0.0067 ( $P_{GC}$  by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)  
 0.00861 (supercooled liquid  $P_L$ , converted from literature  $P_S$  with  $\Delta S_{fus}$  Bidleman 1984)  
 0.000125 (extrapolated-Antoine eq., Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 5.45017 - 1717.489/(114.025 + t/^\circ\text{C})$ ; temp range 197–384.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $1.65 \times 10^{-4}$  (extrapolated, Antoine eq., Dean 1985, 1992)  
 $\log (P/\text{mmHg}) = 6.373 - 1756/(118 + t/^\circ\text{C})$ ; temp range 197–384°C (Antoine eq., Dean 1985, 1992)  
 0.00105 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_S/\text{kPa}) = 11.96071 - 5348.06/(T/K)$ ; temp range 298–383 K (Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.67549 - 2957.01/(-24.15 + T/K)$ ; temp range 503–658 K (Antoine eq.-II, Stephenson & Malanowski 1987)  
 0.00068, 0.0056 (lit. solid  $P_S$ , supercooled liquid  $P_L$ , Bidleman & Foreman 1987)  
 0.992 (WERL Treatability database, quoted, Ryan et al. 1988)  
 0.00861, 0.00635 (supercooled  $P_L$ , converted from literature  $P_S$  with different  $\Delta S_{fus}$  values, Hinckley et al. 1990)  
 0.0155, 0.00955 ( $P_{GC}$  by GC-RT correlation with different reference standards, Hinckley et al. 1990)  
 $\log (P_L/\text{Pa}) = 11.35 - 4040/(T/K)$  (GC-RT correlation, Hinckley et al. 1990)  
 $\log (P/\text{mmHg}) = 70.6802 - 6.484 \times 10^3/(T/K) - 22.241 \cdot \log (T/K) + 7.2184 \times 10^{-3} \cdot (T/K) - 6.3035 \times 10^{-13} \cdot (T/K)^2$ ;  
 temp range 383–905 K (vapor pressure eq., Yaws 1994)  
 0.00692 (supercooled liquid  $P_L$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)  
 0.00168, 0.000672; 0.00124 (quoted exptl. values, effusion; gas saturation, Delle Site 1997)  
 0.00218, 0.000939, 0.000889 (quoted lit. values, from GC-RT correlation, Delle Site 1997)  
 $7.48 \times 10^{-3}$ ;  $1.43 \times 10^{-3}$  (supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_S$  with fugacity ratio  $F$ , Passivirta et al. 1999)  
 $\log (P_S/\text{Pa}) = 11.62 - 4310/(T/K)$  (solid, Passivirta et al. 1999)  
 $\log (P_L/\text{Pa}) = 9.03 - 3323/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $\log (P/\text{Pa}) = 11.901 - 4415.56/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)  
 0.00598 (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)  
 $\log (P_L/\text{Pa}) = -4141/(T/K) + 11.66$ ;  $\Delta H_{vap.} = -79.3 \text{ kJ} \cdot \text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

0.65\* (gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)  
 1.10 (gas stripping-HPLC/fluorescence, De Maagd et al. 1998)  
 1.96\* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)  
 $\ln K_{AW} = -4654.8/(T/K) + 8.42$ ,  $\Delta H = 38.7 \text{ kJ} \cdot \text{mol}^{-1}$ ; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)  
 $\log [H/(\text{Pa m}^3/\text{mol})] = 8.23 - 2336/(T/K)$  (Passivirta et al. 1999)



- 1.96 (quoted from Bamford et al. 1999; Dachs & Eisenreich 2000)  
 0.602 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 6.175 - 2868/(T/K)$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 5.22 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)  
 4.47 (HPLC- $k'$  correlation, Harnisch et al. 1983)  
 4.84 (RP-HPLC-RT correlation, Chin et al. 1986)  
 4.85 (HPLC-RT correlation, Wang et al. 1986)  
 5.16 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 5.20 (recommended, Sangster 1989, 1993)  
 5.17 (TLC-RT correlation, De Voogt et al. 1990)  
 $5.148 \pm 0.077$ ,  $5.155 \pm 0.015$  (shake flask/slow stirring-GC/HPLC, interlaboratory studies, Brooke et al. 1990)  
 5.00 (shake flask-UV spec., Alcorn et al. 1993)  
 5.16 (recommended, Hansch et al. 1995)  
 5.23 (5.12–5.31) (shake flask/slow stirring-HPLC/fluorescence., De Maagd et al. 1998)  
 5.16 (shake flask-SPME solid-phase micro-extraction; Paschke et al. 1999)  
 0.602 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)  
 $\log K_{AW} = 5.485 - 2682/(T/K)$ , (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 8.60 (calculated- $K_{OW}/K_{AW}$ , Wania & Mackay 1996)  
 8.60 (calculated, Finizio et al. 1997)  
 8.80\*; 8.60 (generator column-GC; calculated- $C_O/C_A$ , measured range 0–40°C, Harner & Bidleman 1998)  
 $\log K_{OA} = -5.94 + 4417/(T/K)$ ; temp range 20–40°C (generator column-GC, Harner & Bidleman 1998)  
 8.61 (calculated- $S_{oct}$  and vapor pressure  $P$ , Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 3.18 (calculated as per Kenaga & Goring 1979, Eadie et al. 1982)  
 4.90 (*P. hoyi*, Eadie et al. 1982)  
 4.08 (microorganisms-water, calculated from  $K_{OW}$ , Mabey et al. 1982)  
 3.24 (*Daphnia magna*, Newsted & Giesy 1987)  
 0.756, 1.079 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

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

- 6.38 (sediments average, Kayal & Connell 1990)  
 4.74, 4.62 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)  
 6.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)  
 4.816; 4.81, 4.82 (sediment: concn ratio  $C_{sed}/C_W$ ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)  
 4.51, 5.05, 4.16 (sediments from Brown's Lake, Hamlet City Lake, WES reference soil, shake flask-LSC, Brannon et al. 1995)  
 6.56, 6.66, 6.08 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island, McGroddy & Farrington 1995)  
 4.62 (calculated-MCI  $\chi$ , Sabljic et al. 1995)  
 5.25 (10°C), 5.22, 5.12 (20°C), 5.05 (35°C), 4.89, 4.96 (45°C) ( $\log K_{DOC}$  - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)  
 5.40 (20°C,  $\log K_{POC}$  - particulate organic material from lake, Lüers & ten Hulscher 1996)  
 4.81, 4.65, 4.80, 4.82; 4.813; 4.727 (4 soils with different organic carbon content  $f_{OC}$ , adsorption equilibrium-shake flask-HPLC; calculated- $K_{OW}$ ; calculated- $S$ , He et al. 1996)  
 5.32 (5.29–5.35), 4.89 (4.89–4.90) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)  
 4.62, 4.03; 3.40, 4.49, 3.55, 4.53, 4.56 (quoted lit., calculated- $K_{OW}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)

- 5.32–6.59; 4.60–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)  
 5.83; 6.79, 5.53, 5.52 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)  
 4.91, 4.65 (average values for sediments, soils, organic carbon OC  $\geq 0.5\%$ , Delle Site 2001)  
 4.62 (Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)  
 5.21–6.60 (field contaminated sediment, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluorescence, ten Hulscher et al. 2003)

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

##### Volatilization:

Photolysis: direct photochemical transformation  $t_{1/2}(\text{calc}) = 21$  h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis  $t_{1/2} = 160$  d and 200 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)  
 $t_{1/2} = 21$  h, atmospheric and aqueous photolysis half life, based on measured sunlight photolysis rate constant in water adjusted for midday summer sunlight at 40°N latitude and  $t_{1/2} = 63$  h after adjusting for approximate winter sunlight intensity (Howard et al. 1991);  
 $t_{1/2} = 160$  d under summer sunlight in surface water (Mill & Mabey 1985);  
 half-lives on different atmospheric particulate substrates (appr. 25  $\mu\text{g/g}$  on substrate):  $t_{1/2} = 74$  h on silica gel,  $t_{1/2} = 23$  h on alumina and  $t_{1/2} = 44$  h on fly ash (Behymer & Hites 1985);  
 direct photolysis  $t_{1/2}(\text{obs.}) = 3.61$  h,  $t_{1/2}(\text{calc}) = 4.78$  h, by QSPR in atmospheric aerosol (Chen et al. 2001);  
 $k = (1.76 \pm 0.13) \times 10^{-5} \text{ s}^{-1}$  and  $t_{1/2} = (10.93 \pm 0.75) \text{ h}$  in diesel particulate matter, photochemical degradation under atmospheric conditions,  $k = (2.97 \pm 0.40) \times 10^{-5} \text{ s}^{-1}$  and  $t_{1/2} = (6.48 \pm 1.03) \text{ h}$  in diesel particulate matter/soil mixture, and  $t_{1/2} = 1.6$  to 4.15 h in various soil components using a 900-W photo-irradiator as light source;  $k = (8.69 \pm 0.29) \times 10^{-6} \text{ s}^{-1}$  and  $t_{1/2} = (22.16 \pm 0.77) \text{ h}$  in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation  $k = 5.0 \times 10^{-6} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

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

$k(\text{calc}) < 3600 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $< 360 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)

$k_{\text{OH}} = 5.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $k_{\text{N}_2\text{O}_5} \approx 1.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for reaction with  $\text{N}_2\text{O}_5$  at 296  $\pm$  2 K (relative rate method, Atkinson et al. 1990)

photooxidation half-life of 2.02–20.2 h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{\text{OH}}^* = 11 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K, measured range 306–366 K with a calculated atmospheric lifetime of 26 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aquatic  $k = 2.2 \times 10^{-3} \mu\text{mol h}^{-1} \text{ mg}^{-1}$  with bacterial protein (Barnsley 1975; quoted, Callahan et al. 1979)

significant with gradual degradation for a domestic sewer test for an average three static-flask screening (Tabak et al. 1981)

$t_{1/2}(\text{aerobic}) = 3360\text{--}10560$  h, based on aerobic soil die-away test data at 10–30°C (Coover & Sims 1987; quoted, Howard et al. 1991)

$k = 0.19 \text{ h}^{-1}$  in atmosphere (Dragoescu & Friedlander 1989)

$k = 0.0018 \text{ d}^{-1}$  with  $t_{1/2} = 377$  d for Kidman sandy loam and  $k = 0.0026 \text{ d}^{-1}$  with  $t_{1/2} = 268$  d for McLarin sandy loam all at  $-0.33$  bar soil moisture (Park et al. 1990)

$t_{1/2}(\text{anaerobic}) = 13440\text{--}42240$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

first order  $k = 0.132$  to  $0.162 \text{ L mg}^{-1} \text{ d}^{-1}$  for a marine PAH-degrading enrichment without sediment, the degradation rate was 2.1 to 5.3 times faster with sediment present (Poeton et al. 1999)

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

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

$k_1 = 4.1\text{--}6.1 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.026 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

$k_2 = 0.15 \text{ h}^{-1}$  in water with corresponding  $t_{1/2} = 4.7 \text{ h}$  and  $k_2 = 0.14 \text{ h}^{-1}$  in sediment with corresponding  $t_{1/2} = 4.9 \text{ h}$  for copepods *S. knabeni* in 24-h experiments (Lotufo 1998)

$k_2 = 0.17 \text{ h}^{-1}$  in sediment with corresponding  $t_{1/2} = 4.2 \text{ h}$  and  $k_2 = 0.09 \text{ h}^{-1}$  in sediment with corresponding  $t_{1/2} = 7.4 \text{ h}$  for copepods *Coullana* sp. in 24-h experiments (Lotufo 1998)

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 2.02\text{--}20.2 \text{ h}$ , based on estimated sunlight photolysis half-life in water (Howard et al. 1991); calculated atmospheric lifetime of 26 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: computed near-surface  $t_{1/2} = 21 \text{ h}$  for photochemical transformation of a water body (latitude  $40^\circ\text{N}$ , midday, midsummer),  $t_{1/2} = 160 \text{ d}$  for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning and  $t_{1/2} = 200 \text{ d}$  with sediment-water partitioning (Zepp & Schlotzhauer 1979);

$t_{1/2} = 21\text{--}63 \text{ h}$ , based on photolysis half-life in water (Howard et al. 1991);

$t_{1/2} = 160 \text{ d}$  for summer sunlight at  $40^\circ\text{N}$  latitude (Mill & Mabey 1985).

Groundwater:  $t_{1/2} = 6720\text{--}21120 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption  $t_{1/2} = 8.3 \text{ d}$  from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil:  $t_{1/2} = 44\text{--}182 \text{ d}$  (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 39 \text{ d}$  for 5 mg/kg treatment and 34 d for 50 mg/kg treatment (Bulman et al. 1987);

biodegradation rate constant  $k = 0.0018 \text{ d}^{-1}$  with  $t_{1/2} = 377 \text{ d}$  for Kidman sandy loam soil, and  $k = 0.0026 \text{ d}^{-1}$  with  $t_{1/2} = 268 \text{ d}$  for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 3360\text{--}10560 \text{ h}$ , based on aerobic soil die-away test data at  $10\text{--}30^\circ\text{C}$  (Howard et al. 1991);

$t_{1/2} > 50 \text{ d}$  (Ryan et al. 1988);

$t_{1/2} = 17.961 \text{ wk}$ , 7.8 yr (Luddington soil, Wild et al. 1991).

Biota:  $t_{1/2} = 5 \text{ d}$  depuration half life by oysters (Lee et al. 1978);

elimination  $t_{1/2} = 6 \text{ d}$  from rainbow trout,  $t_{1/2} = 2.0\text{--}29.8 \text{ d}$  from mussel *Mytilus edulis*;  $t_{1/2} = 8.4 \text{ d}$  from clam *Mya arenaria*,  $t_{1/2} = 5.8 \text{ d}$  from polychaete *Abarenicola pacifica*,  $t_{1/2} = 5.9 \text{ d}$  from Oyster,  $t_{1/2} = 0.8 \text{ d}$  from shrimp (Meador et al. 1995)

depuration  $t_{1/2} \sim 4.8 \text{ h}$  in sediment and water for copepod *S. knabeni*,  $t_{1/2} = 4.2 \text{ h}$  in sediment and  $t_{1/2} = 7.4 \text{ h}$  in water for copepod *Coullana* sp. (Lotufo 1998)

**TABLE 4.1.1.30.1**  
**Reported aqueous solubilities of fluoranthene at various temperatures**  
**and reported temperature dependence equation**

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

May 1980, 1983		May et al. 1978b	
generator column-HPLC		generator column-HPLC/fluo.	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
8.1	0.082	25	0.206
13.2	0.107	29	0.264
19.7	0.1483		
24.6	0.2027	temp dependence eq. 1	
29.9	0.2793	S	$\mu\text{g/kg}$
		a	0.0072
temp dependence eq. 1		b	-0.1047
given in May et al. 1980		c	4.322
S	$\mu\text{g/kg}$	d	50.4
a	0.0072		
b	-0.1047	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 39.83$	
c	4.322	measured between $5\text{--}30^\circ\text{C}$	
d	50.4		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 39.83$			
measured between $5\text{--}30^\circ\text{C}$			

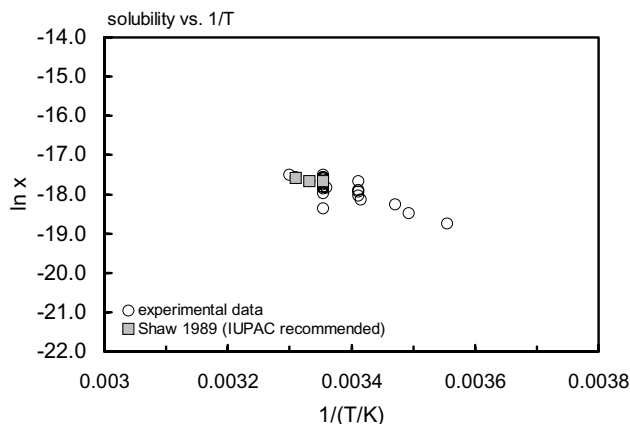


FIGURE 4.1.1.30.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for fluoranthene.

TABLE 4.1.1.30.2

Reported vapor pressures of fluoranthene 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)		

Tsyapkina 1955		Hoyer & Peperle 1958		Sonnefeld et al. 1983	
		effusion		generator column-HPLC	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
197.0	653	data presented in eq. 1		10.88	$2.17 \times 10^{-4}$
209.0	1053	A	P/mmHg	10.88	$2.05 \times 10^{-4}$
228.5	2586	B	12.67	10.88	$2.15 \times 10^{-4}$
238.1	3786	for temp range 25–85 $^{\circ}\text{C}$		10.88	$2.57 \times 10^{-4}$
247.7	5386	$\Delta H_{\text{sub}}(\text{kJ/mol}) = 100$		20.25	$7.07 \times 10^{-4}$
255.0	6586			20.25	$7.39 \times 10^{-4}$
261.3	7919			20.25	$7.25 \times 10^{-4}$
270.9	10319			20.25	$7.63 \times 10^{-4}$
281.5	13386			29.79	$2.03 \times 10^{-3}$
305.0	20318			29.79	$1.99 \times 10^{-3}$
314.5	27384			29.80	$2.17 \times 10^{-3}$
382.9	99058			29.80	$2.20 \times 10^{-3}$
384.2	101325			38.9	$5.81 \times 10^{-3}$
				38.9	$5.67 \times 10^{-3}$
				38.9	$5.58 \times 10^{-3}$
				38.9	$5.77 \times 10^{-3}$
				38.9	$5.46 \times 10^{-3}$
				38.9	$5.45 \times 10^{-3}$
				25.0	$1.23 \times 10^{-3}$
				eq. 2	P/Pa
				A	11.901
				B	4415.56
				temp range 10–50 $^{\circ}\text{C}$	

ref. Tsyapkina, O.YA. Zh. Prikl. Khim 28, 185 (1955).

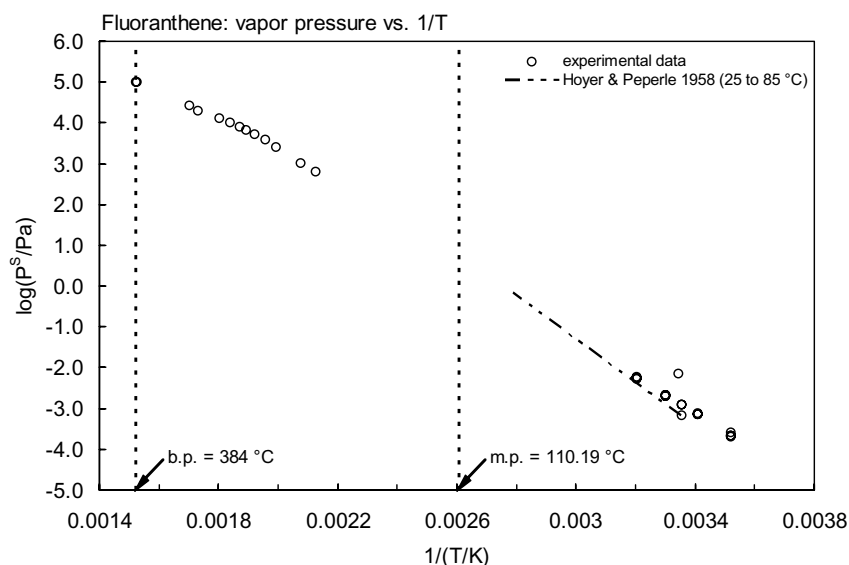
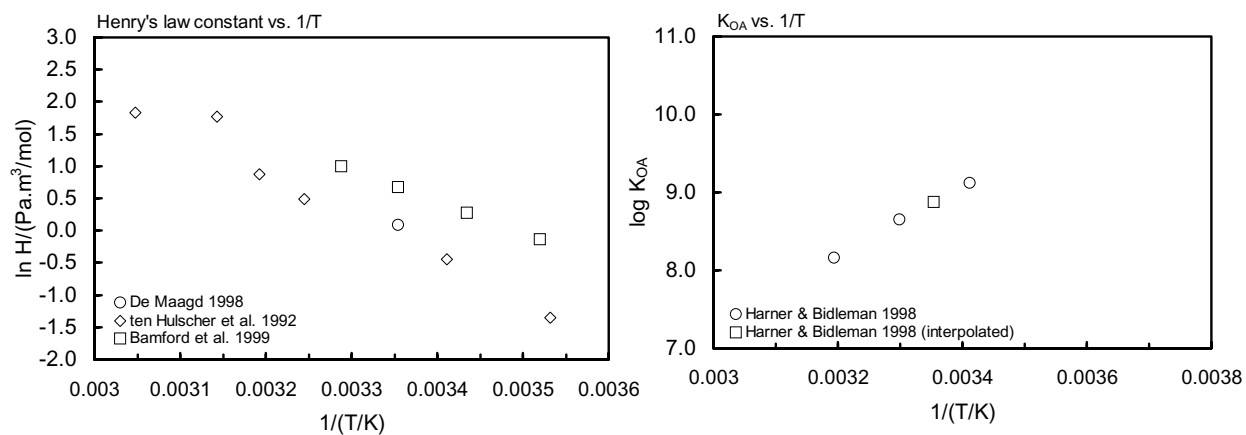


FIGURE 4.1.1.30.2 Logarithm of vapor pressure versus reciprocal temperature for fluoranthene.

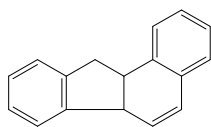
TABLE 4.1.1.30.3

Reported Henry's law constants and octanol-air partition coefficients of fluoranthene at various temperatures and temperature dependence equations

Henry's law constant					log $K_{OA}$	
ten Hulscher et al. 1992		Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-HPLC/fluo.		gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)	t/°C	log $K_{OA}$
				average		
10.0	0.26	4.1	0.37, 0.49	0.56	0	-
20.0	0.64	11.0	0.79, 0.95	0.87	10	-
35.0	1.63	18.0	1.21, 1.43	1.32	20	11.124
40.1	2.38	25.0	1.76, 2.18	1.96	30	8.652
45.0	5.84	31.0	2.36, 3.14	2.72	40	8.161
55.0	6.23				25(exptl)	8.88
					25(calc)	8.60
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\ln K_{AW} = A - B/(T/K)$			$\log K_{OA} = A + B/(T/K)$	
$R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$		A			A	
$\Delta S/R$		B			B	
$\Delta H/R$		enthalpy, entropy change:			enthalpy of phase change	
		$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 38.7 \pm 2.5$			$\Delta H_{OA}/(\text{kJ mol}^{-1}) =$	
		$\Delta S/(\text{J} \cdot \text{K}^{-1} \text{ mol}^{-1}) = 70$				
		at 25°C				
enthalpy of volatilization:						
$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 57 \pm 5$						
entropy of volatilization, $\Delta S$						
$T\Delta S/(\text{kJ} \cdot \text{K}^{-1} \text{ mol}^{-1}) = 54 \pm 5$						
at 20°C						



**FIGURE 4.1.1.30.3** Logarithm of Henry's law constant and  $K_{OA}$  versus reciprocal temperature for fluoranthene.

4.1.1.31 Benzo[*a*]fluorene

Common Name: Benzo[*a*]fluorene

Synonym: 1,2-benzofluorene, 11*H*-benzo[*a*]fluorene, chrysofluorene

Chemical Name: benzo[*a*]fluorene, 1,2-benzofluorene

CAS Registry No: 238-84-6

Molecular Formula: C<sub>17</sub>H<sub>12</sub>

Molecular Weight: 216.227

Melting Point (°C):

189.5 (Lide 2003)

Boiling Point (°C):

405 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

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

200.9 (Ruelle & Kesselring 1997)

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

Enthalpy of Fusion, Δ*H*<sub>fus</sub> (kJ/mol):

3.8, 18.4; 22.2 (126.75, 189.65°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, Δ*S*<sub>fus</sub> (J/mol K):

39.76 (exptl., Chickos et al. 1999)

49.26, 50.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming Δ*S*<sub>fus</sub> = 56 J/mol K), *F*: 0.0243 (mp at 189.5°C)

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

0.045 (shake flask-fluorescence, Mackay & Shiu 1977)

0.045 (average lit. value, Pearlman et al. 1984)

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

0.00136 (supercooled liquid *P*<sub>L</sub>, calibrated GC-RT correlation, Lei et al. 2002)

log (*P*<sub>L</sub>/Pa) = -4373/(*T*/K) + 11.80; Δ*H*<sub>vap</sub> = -83.7 kJ·mol<sup>-1</sup> (GC-RT correlation, Lei et al. 2002)

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

2.70\* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)

ln *K*<sub>AW</sub> = -4113.54/(*T*/K) + 6.976, Δ*H* = 34.2 kJ mol<sup>-1</sup>, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, log *K*<sub>OW</sub>:

5.68 (HPLC-RT correlation, Wang et al. 1986)

5.40 (recommended, Sangster 1989, 1993)

6.5387 (calculated-UNIFAC group contribution, Chen et al. 1993)

5.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log *K*<sub>OA</sub>:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log *K*<sub>OC</sub>:

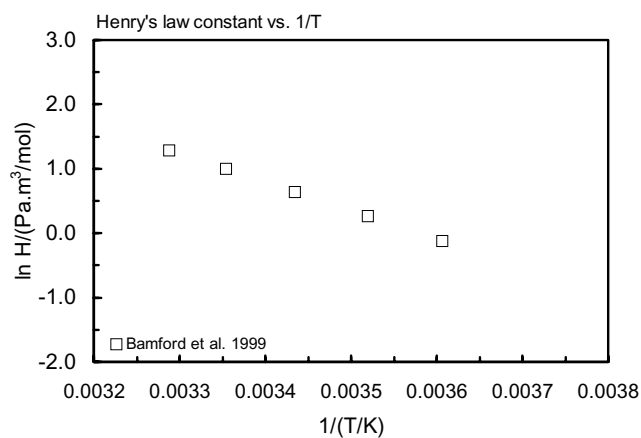
Environmental Fate Rate Constants, *k*, or Half-Lives, *t*<sub>1/2</sub>:

## Half-Lives in the Environment:

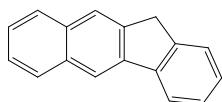
Biota: elimination  $t_{1/2} = 10.5$  d from Oyster,  $t_{1/2} = 4.2$  d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

**TABLE 4.1.1.31.1****Reported Henry's law constants of benzo[a]fluorene at various temperatures**

Bamford et al. 1999		
gas stripping-GC/MS		
$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	$H/(\text{Pa m}^3/\text{mol})$
		average
4.1	0.67, 1.16	0.88
11.0	1.08, 1.57	1.30
18.0	1.61., 2.23	1.89
25.0	2.19, 3.33	2.70
31.0	2.74, 4.78	3.62
$\ln K_{\text{AW}} = A - B/(T/\text{K})$		
A	6.9762	
B	4113.5	
enthalpy, entropy change:		
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 34.2 \pm 4.9$		
$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 58$		
at 25°C		

**FIGURE 4.1.1.31.1** Logarithm of Henry's law constant versus reciprocal temperature for benzo[a]fluorene.



4.1.1.32 Benzo[*b*]fluorene

Common Name: Benzo[*b*]fluorene

Synonym: 2,3-benzofluorene, 11H-benzo[*b*]fluorene, isonaphthofluorene

Chemical Name: benzo[*b*]fluorene

CAS Registry No: 243-17-4

Molecular Formula: C<sub>17</sub>H<sub>12</sub>

Molecular Weight: 216.227

Melting Point (°C):

212 (Lide 2003)

Boiling Point (°C):

401 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

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

200.9 (Ruelle & Kesselring 1997)

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

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

23.4 (exptl., Chickos et al. 1999)

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

47.78, 50.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0146 (mp at 212°C)

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

0.0020 (shake flask-fluorescence, Mackay & Shiu 1977)

0.002 (average lit. value, Pearlman et al. 1984)

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):

7.37 × 10<sup>-6</sup>\* (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 71–125°C, Oja & Suuberg 1998)

log (P/Pa) = 36.325 – 14354/(T/K); temp range 344–398 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

0.00107 (supercooled liquid P<sub>L</sub>, calibrated GC-RT correlation, Lei et al. 2002)

log (P<sub>L</sub>/Pa) = –4423/(T/K) + 11.86; ΔH<sub>vap</sub> = –84.7 kJ·mol<sup>-1</sup> (GC-RT correlation, Lei et al. 2002)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

5.77 (HPLC-RT correlation, Wang et al. 1986)

5.75 (recommended, Sangster 1989, 1994)

5.77 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K<sub>OC</sub>:

Environmental Fate Rate Constants, k or Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

Biota: elimination t<sub>1/2</sub> = 10.5 d from Oyster, t<sub>1/2</sub> = 4.3 d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.32.1

Reported vapor pressures of benzo[b]fluorene at various temperatures and the coefficients for the vapor pressure equations

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

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

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

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

Oja & Suuberg 1998

Knudsen effusion

t/°C	P/Pa
70.92	0.00454
83.14	0.0188
97.55	0.0936
124.4	1.230
mp/K	484–486
eq. 1a	P/Pa
A	36.325
B	14354
for temp range 344–398 K	
$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 119.3$	

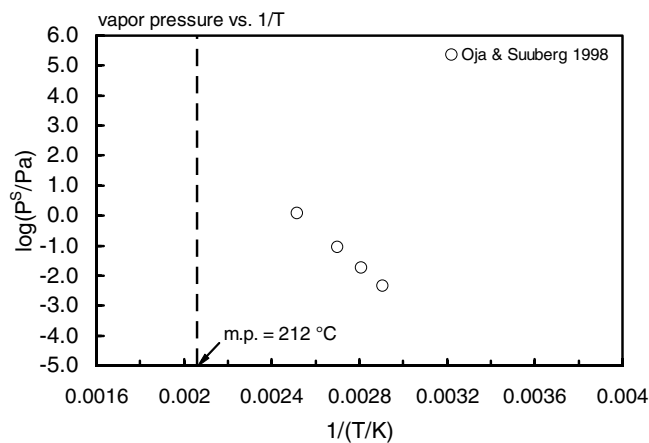
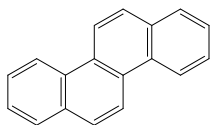


FIGURE 4.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for benzo[b]fluorene.

## 4.1.1.33 Chrysene



Common Name: Chrysene

Synonym: 1,2-benzophenanthrene, benzo(*a*)phenanthrene, 1,2,5,6-dibenzonaphthalene

Chemical Name: chrysene

CAS Registry No: 218-01-9

Molecular Formula:  $C_{18}H_{12}$

Molecular Weight: 228.288

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

255.5 (Lide 2003)

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

448 (Weast 1975; Lide 2003)

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

1.274 (Weast 1982–83; Lide 2003)

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

179.2 ( $20^{\circ}C$ , calculated-density)

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

Enthalpy of Fusion,  $\Delta H_{fus}$  cal/mol:

26.153 (Ruelle & Kesselring 1997)

3.22, 26.15; 29.37 (239.05, 28.25 $^{\circ}C$ , total phase change enthalpy, Chickos et al. 1999)

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

49.37 (Casellato et al. 1973)

62.34 (Ubbelohde 1978)

49.21 (Chickos et al. 1999)

55.5, 44.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.00548 (mp at  $255.5^{\circ}C$ )

0.00976 (calculated, Passivirta et al. 1999)

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

0.0015 ( $27^{\circ}C$ , shake flask-nephelometry, Davis et al. 1942)

0.006 (shake flask-UV, Klevens 1950)

0.0015 (Weimer & Prausnitz 1965)

0.0041, 0.0014 (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

0.002 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0018 (Rossi 1977; Neff 1979; quoted, Eadie et al. 1982)

0.0018\* (generator column-HPLC/UV, measured range  $6.5$ – $29^{\circ}C$  May et al. 1978a,b)

$S/(\mu g/kg) = 0.609 + 0.0144 \cdot (t/^{\circ}C) + 0.0024 \cdot (t/^{\circ}C)^2$ ; temp range  $5$ – $30^{\circ}C$  (generator column-HPLC/UV, May et al. 1978)

0.017 (shake flask-nephelometry, Hollifield 1979)

0.00189\* ( $25.3^{\circ}C$ , generator column-HPLC, measured range  $279.65$ – $301.85$  K, May et al. 1983)

0.0018\* (average lit. value, Pearlman et al. 1984)

0.00327 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.00102, 0.0012 (generator column-HPLC/UV, Billington et al. 1988)

0.0019 (recommended, Shaw 1989)

0.0016 (generator column-HPLC, Vadas et al. 1991)

0.0015 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

$\log [S_L/(mol/L)] = -0.323 - 1369/(T/K)$  (supercooled liquid, Passivirta et al. 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):

- $5.7 \times 10^{-7}$ \* (effusion method, extrapolated, De Kruif 1980)
- $8.4 \times 10^{-7}$  (effusion method, Hoyer & Peperle 1958; quoted, Mabey et al. 1982)
- $\log(P/\text{mmHg}) = 13.07 - 6340/(T/K)$ ; temp range 80–145°C (Knudsen effusion method, Hoyer & Peperle 1958)
- $6.08 \times 10^{-7}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_s/\text{kPa}) = 11.445 - 6160/(T/K)$ ; temp range 358–463 K (Antoine eq., Stephenson & Malanowski 1987)
- $\log(P/\text{mmHg}) = -50.1566 - 3.4381 \times 10^3/(T/K) + 25.178 \cdot \log(T/K) - 2.462 \times 10^{-2} \cdot (T/K) + 7.1044 \times 10^{-6} \cdot (T/K)^2$ ;  
temp range 531–979 K (vapor pressure eq., Yaws 1994)
- $2.29 \times 10^{-4}$  (supercooled liquid  $P_L$ , calculated from Yamasaki et al. 1984, quoted, Finizio et al. 1997)
- $5.70 \times 10^{-7}$ ;  $5.84 \times 10^{-5}$  (quoted solid  $P_s$  from Mackay et al. 1992; converted to supercooled liquid  $P_L$  with fugacity ratio  $F$ , Passivirta et al. 1999)
- $\log(P_s/\text{Pa}) = 12.24 - 5507/(T/K)$  (solid, Passivirta et al. 1999)
- $\log(P_L/\text{Pa}) = 9.66 - 4139/(T/K)$  (supercooled liquid, Passivirta et al. 1999)
- $\log(P/\text{Pa}) = 14.848 - 6189/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- $1.70 \times 10^{-4}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)
- $\log(P_L/\text{Pa}) = -4679/(T/K) + 11.92$ ;  $\Delta H_{\text{vap}} = -89.6 \text{ kJ} \cdot \text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)
- $2.11 \times 10^{-6}$  (solid  $P_s$ , gas saturation-GC/MS, Mader & Pankow 2003)
- $4.03 \times 10^{-4}$  (supercooled liquid  $P_L$ , calculated from  $P_s$  assuming  $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$ , Mader & Pankow 2003)

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

- 0.107 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
- 0.53\* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)
- $\ln K_{\text{AW}} = -12136.2/(T/K) + 32.235$ ,  $\Delta H = 100.9 \text{ kJ} \cdot \text{mol}^{-1}$ , measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
- $\log(H/(\text{Pa m}^3/\text{mol})) = 9.98 - 2770/(T/K)$  (Passivirta et al. 1999)
- 0.53 (quoted, Dachs & Eisenreich 2000)

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

- 5.79 (HPLC- $k'$  correlation, Hanai et al. 1981)
- 5.91 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)
- 5.73 (HPLC-RT correlation, Wang et al. 1986)
- $5.61 \pm 0.40$  (recommended, Sangster 1989)
- 5.84 (TLC retention time correlation, De Voogt et al. 1990)
- 5.50 (shake flask-UV, Alcorn et al. 1993)
- 5.86 (recommended, Sangster 1993)
- 5.73 (recommended, Hansch et al. 1995)
- 5.81 (range 6.63–5.94) (shake flask/slow stirring-HPLC/fluor., De Maagd et al. 1998)
- 5.78 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

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

- 10.40 (calculated- $K_{\text{OW}}/K_{\text{AW}}$ , Wania & Mackay 1996)
- 10.44 (calculated, Finizio et al. 1997)

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

- 4.31 (*P. hoyi*, Eadie et al. 1982)
- 4.72 (microorganisms-water, calculated from  $K_{\text{OW}}$ , Mabey et al. 1982)
- 3.785 (*Daphnia magna*, Newsted & Giesy 1987)
- 1.17, 0.792 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

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

- 6.27 (sediments average, Kayal & Connell 1990)
- 6.9 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 4.0 (predicted dissolved  $\log K_{\text{OC}}$ , Broman et al. 1991)

- 5.79 (5.74–5.83), 5.40 (5.35–5.50) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 5.52–7.38; 4.90–7.80 (for chrysene + triphenylene, range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.92; 6.12, 5.77, 6.14 (for chrysene + triphenylene, 20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

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

##### Volatilization:

Photolysis: calculated  $t_{1/2}$  = 4.4 h of direct sunlight photolysis for 50% conversion at 40°N latitude of midday in midsummer: 4.4 h in near-surface water; (Herbes et al. 1980)

direct photochemical transformation  $t_{1/2}(\text{calc})$  = 4.4 h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis  $t_{1/2}$  = 13 d and 68 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)

$t_{1/2}$  = 13 d in 5-m deep inland water and  $t_{1/2}$  = 68 d in inland water with sediment partitioning (Zepp & Schlotzhauer 1979)

half-lives on different atmospheric particulate substrates (appr. 25 µg/g on substrate):  $t_{1/2}$  = 100 h on silica gel,  $t_{1/2}$  = 78 h on alumina and  $t_{1/2}$  = 38 h on fly ash (Behymer & Hites 1985)

first order daytime decay constants:  $k$  = 0.0056 min<sup>-1</sup> for soot particles loading of 1000–2000 ng/mg and  $k$  = 0.0090 min<sup>-1</sup> with 30–350 ng/mg loading (Kamens et al. 1988)

photodegradation  $k$  =  $7.07 \times 10^{-3}$  min with  $t_{1/2}$  = 1.63 h in ethanol-water (1:1, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

$k(\text{exptl})$  = 0.00707 min<sup>-1</sup> with the calculated  $t_{1/2}$  = 1.63 h and the predicted  $k$  = 0.0114 min<sup>-1</sup> calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

$k$  = 1.01–1.30 min<sup>-1</sup> in natural water system by UV and sunlight (Yu et al. 1999)

$t_{1/2}(\text{obs})$  = 1.58 h,  $t_{1/2}(\text{calc})$  = 1.34 h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

photochemical degradation  $k$  =  $(1.60 \pm 0.08) \times 10^{-5}$  s<sup>-1</sup> and  $t_{1/2}$  =  $(11.99 \pm 0.53)$ h in diesel particulate matter under atmospheric conditions;  $k$  =  $(2.29 \pm 0.22) \times 10^{-5}$  s<sup>-1</sup> and  $t_{1/2}$  =  $(8.41 \pm 0.91)$ h in diesel particulate matter/soil mixture, and  $t_{1/2}$  = 1.69 – 8.82 h in various soil components using a 900-W photo-irradiator as light source;  $k$  =  $(4.76 \pm 0.40) \times 10^{-7}$  s<sup>-1</sup> and  $t_{1/2}$  =  $(405.26 \pm 37.27)$ h in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation  $k$  =  $9.0 \times 10^{-5}$  s<sup>-1</sup> in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation:  $t_{1/2}$  = 2.6 h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

$k > 1 \times 10^6$  M<sup>-1</sup> h<sup>-1</sup> for singlet oxygen and  $k = 1 \times 10^3$  M<sup>-1</sup> h<sup>-1</sup> for peroxy radical (Mabey et al. 1982);

photooxidation  $t_{1/2}$  = 0.802–8.02 h in air, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: significant degradation with gradual adaptation within 7 d for a domestic sewer 28 d test for an average of three static-flask screening (Tabak et al. 1981)

aerobic  $t_{1/2}$  = 8904–24000 h, based on aerobic soil dieaway test data (Howard et al. 1991)

rate constants  $k$  = 0.0019 d<sup>-1</sup> with  $t_{1/2}$  = 371 d for Kidman sandy loam and  $k$  = 0.0018 d<sup>-1</sup> with  $t_{1/2}$  = 387 d for McLarin sandy loam all at –0.33 bar soil moisture (Park et al. 1990)

anaerobic  $t_{1/2}$  = 35616–96000 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

$k_1$  = 0.35–0.71 mg g<sup>-1</sup> h<sup>-1</sup>;  $k_2$  = 0.15 h<sup>-1</sup> (freshwater oligochaete from sediment, Van Hoof et al. 2001)

#### Half-Lives in the Environment:

Air:  $t_{1/2}$  = 0.802–8.02 h, based on estimated photooxidation half-life in air (Howard et al. 1987);

$t_{1/2} = 1.3$  h for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated rate constant  $k = 0.0092 \text{ min}^{-1}$  at  $1 \text{ cal cm}^{-2} \text{ min}^{-1}$ ,  $10 \text{ g/m}^3 \text{ H}_2\text{O}$  and  $20^\circ\text{C}$  (Kamens et al. 1988).

Surface water: photolysis  $t_{1/2} = 4.4$  h near surface water,  $t_{1/2} = 13$  d and 68 d in 5-m deep water body without and with sediment-water partitioning in full summer day,  $40^\circ\text{N}$ ; photosensitized oxygenation  $t_{1/2} = 2.6$  h at near surface water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979)

$t_{1/2} \sim 4.4\text{--}13$  h, based on photolysis half-life in water (Howard et al. 1991);

photolysis  $t_{1/2} = 1.63$  h in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996);

photolysis  $t_{1/2} = 533\text{--}693$  min at  $18^\circ\text{C}$  in natural water system by UV and sunlight illumination (Yu et al. 1999).

Groundwater:  $t_{1/2} = 17808\text{--}48000$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption  $t_{1/2} = 31.9$  d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil:  $t_{1/2} > 5.5$  d (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 328$  d for 5 mg/kg treatment and  $t_{1/2} = 224$  d for 50 mg/kg treatment (Bulman et al. 1987);

biodegradation rate constant  $l = 0.0019 \text{ d}^{-1}$  with  $t_{1/2} = 371$  d for Kidman sandy loam soil, and  $k = 0.0018 \text{ h}^{-1}$  with  $t_{1/2} = 387$  d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 8904\text{--}24000$  h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} > 50$  d (Ryan et al. 1988).

Biota: elimination  $t_{1/2} = 5.0\text{--}14.2$  d from mussel *Mytilus edulis*;  $t_{1/2} = 15.1$  d from Oyster,  $t_{1/2} = 4.3$  d from clam *Mercenaria mercenaria*,  $t_{1/2} = 3.3$  d from clam *Macoma balthica* (quoted, Meador et al. 1995).

**TABLE 4.1.1.33.1**

**Reported aqueous solubilities of chrysene at various temperatures and reported temperature dependence equations**

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

May et al. 1978b		May 1980, May et al. 1983	
generator column-HPLC		generator column-HPLC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
25	0.0018	6.5	0.00071
29	0.0022	11.0	0.00080
		20.4	0.0014
		24.0	0.00168
		25.3	0.00189
		28.7	0.00221
temp dependence eq. 1		temp dependence eq. 1 given in May 1980	
S	$\mu\text{g/kg}$		
a	0	S	$\mu\text{g/kg}$
b	0.0024	a	0
c	-0.0144	b	0.0024
d	0.69	c	-0.0144
		d	0.69
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 41.25$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 41.25$	
measured between $5\text{--}30^\circ\text{C}$		measured between $5\text{--}30^\circ\text{C}$	

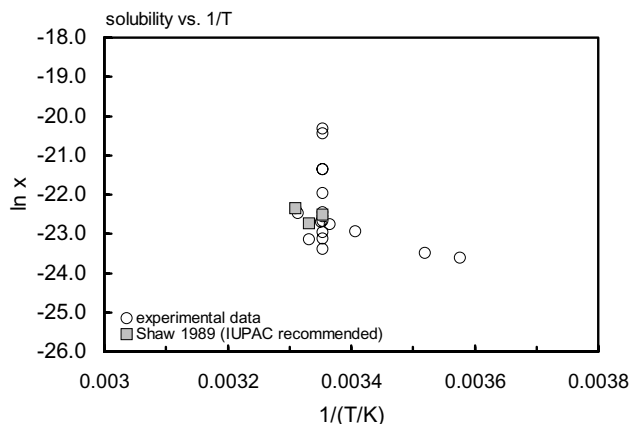
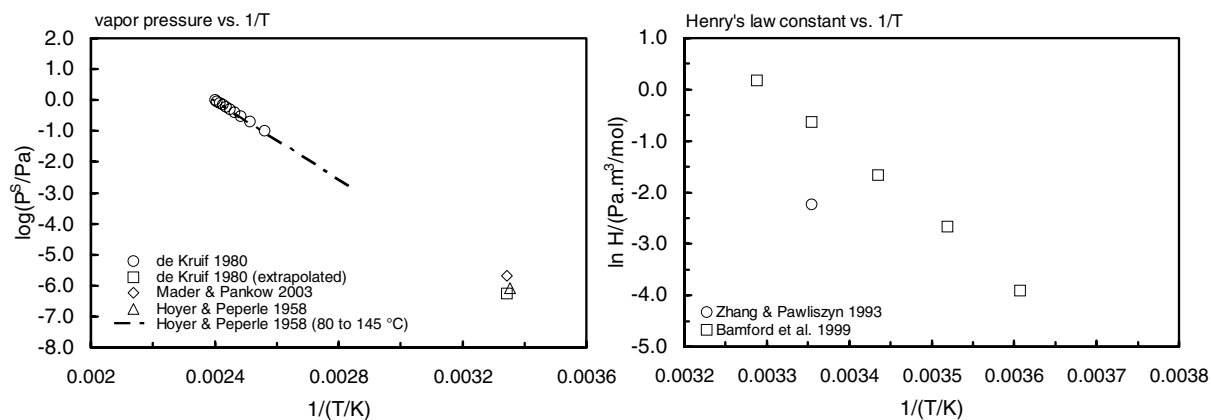


FIGURE 4.1.1.33.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for chrysene.

TABLE 4.1.1.33.2

Reported vapor pressures and Henry's law constants of chrysene at various temperatures and temperature dependence equations

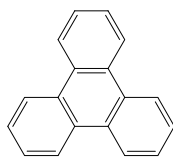
Vapor pressure		Henry's law constant				
Hoyer & Peperle 1958		de Kruif 1980		Bamford et al. 1999		
effusion		torsion-, weighing effusion		gas stripping-GC/MS		
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)	H/(Pa m³/mol)
				average		
data presented by equation		117.31	0.1	4.1	0.01, 0.03	0.02
log P/mmHg = A – B/(T/K)		124.84	0.2	11.0	0.05, 0.09	0.07
A	13.07	129.38	0.3	18.0	0.15, 0.25	0.19
B	6340	132.67	0.4	25.0	0.38, 0.73	0.53
temp range 80–145°C		135.26	0.5	31.0	0.78, 1.86	1.20
		137.39	0.6			
ΔH <sub>subl</sub> /(kJ/mol) = 118.8		139.22	0.7	ln K <sub>AW</sub> = A – B/(T/K)		
		140.81	0.8	A	32.235	
		142.23	0.9	B	12136	
		143.51	1.0			
		25.0	5.7 × 10 <sup>-7</sup>	enthalpy, entropy change:		
		extrapolated)		ΔH/(kJ·mol <sup>-1</sup> ) = 100.9 ± 7.7		
ΔH <sub>subl</sub> /(kJ/mol) = 118.5				ΔS/(J·K <sup>-1</sup> mol <sup>-1</sup> ) = 268		
				at 25°C		



**FIGURE 4.1.1.33.2** Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for chrysene.



## 4.1.1.34 Triphenylene



Common Name: Triphenylene

Synonym: 9,10-benzophenanthrene, isochrysene, 1,2,3,4-dibenznaphthalene

Chemical Name: triphenylene

CAS Registry No: 217-59-4

Molecular Formula:  $C_{18}H_{12}$

Molecular Weight: 228.288

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

197.8 (Lide 2003)

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

425 (Weast 1982–83; Dean 1985; Pearlman et al. 1984; Budavari 1989; Lide 2003)

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

1.302 (Dean 1985; Budavari 1989)

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

211.8 (Ruelle & Kesselring 1997)

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

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

24.74 (exptl., Chickos et al. 1999)

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

52.53, 44.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0202 (mp at  $197.8^{\circ}C$ )

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

0.0388 ( $27^{\circ}C$ , nephelometry, Davis et al. 1942)

0.043 (shake flask-UV, Klevens 1950)

0.043 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0049\* ( $20.5^{\circ}C$ , generator column-HPLC, measured range 281.15–301.35 K, May et al. 1983)

0.041 (lit. mean, Pearlman et al. 1984)

0.0307 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.041 (vapor saturation-UV, Akiyoshi et al. 1987)

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):

$\log(P/mmHg) = 12.89 - 6154/(T/K)$ ; temp range:  $65-125^{\circ}C$  (Knudsen effusion method, Hoyer & Peperle 1958)

$2.30 \times 10^{-6}$ \* (effusion, De Kruif 1980)

$3.85 \times 10^{-7}$  (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 9.435 - 5620/(T/K)$ ; temp range: 363–468 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$1.17 \times 10^{-2}$  (extrapolated-Antoine eq.-II, supercooled liquid  $P_L$ , Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.8974 - 3527/(T/K)$ ; temp range: 600–720 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$2.39 \times 10^{-4}$  (supercooled liquid  $P_L$ , GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -4624/(T/K) + 11.89$ ;  $\Delta H_{vap} = -88.5 kJ \cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ( $Pa m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$  at  $25^{\circ}C$  and the reported temperature dependence equations:

5.45 (shake flask-UV, Karickhoff et al. 1979)

5.49 (HPLC-RT correlation, Wang et al. 1986)

5.84 (TLC retention time correlation, De Voogt et al. 1990)

- 5.49 (recommended, Sangster 1993)  
 5.49 (recommended, Hansch et al. 1995)  
 5.15; 4.83 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)  
 $\log K_{OW} = 1.313 + 1138.55/(T/K)$ ; temp range 5–55°C (temperature dependence HPLC-k' correlation, Lei et al. 2000)  
 6.27 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

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

Bioconcentration Factor,  $\log BCF$ :

- 3.96 (*Daphnia magna*, Newsted & Giesy 1987)

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

- 6.90 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)  
 4.0 (predicted dissolved  $\log K_{OC}$ , Broman et al. 1991)  
 5.52–7.38; 4.90–7.80 (for chrysene + triphenylene, range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)  
 5.92; 6.12, 5.77, 6.14 (for chrysene + triphenylene, 20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

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

Half-Lives in the Environment:

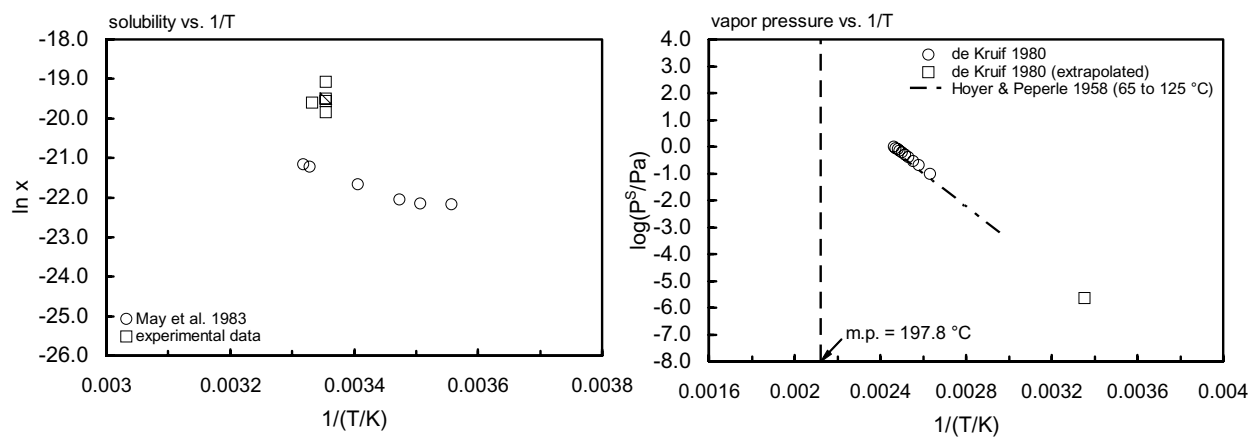
- Biota: elimination  $t_{1/2} = 2$  d from rainbow trout,  $t_{1/2} = 4.4$  d from clam *Mya arenaria*,  $t_{1/2} = 8.0$  d from mussel *Mytilus edulis*,  $t_{1/2} = 14.4$  d from polychaete *Abarenicola pacifica*,  $t_{1/2} = 21.7$  d from Oyster,  $t_{1/2} = 2.4$  d from shrimp (quoted, Meador et al. 1995).

TABLE 4.1.1.34.1

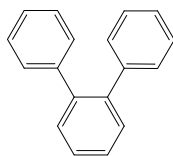
Reported aqueous solubilities and vapor pressures of triphenylene at various temperatures and reported temperature dependence equation

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

Aqueous solubility		Vapor pressure					
May 1980, May et al. 1983		Hoyer & Peperle 1958		de Kruif 1980			
generator column-HPLC		effusion		torsion, weighing effusion			
t/°C	S/g·m <sup>-3</sup>	t/°C	P/Pa	t/°C	P/Pa		
8.0	0.00299	data presented by		107.02	0.1		
12.0	0.00393	log P/mmHg = A – B/(T/K)		114.36	0.2		
14.8	0.00339	A	12.89	118.39	0.3		
20.5	0.00489	B	6154	134.52	0.4		
27.3	0.00765	temp range 65–125°C		122.0	0.5		
28.2	0.00811	ΔH <sub>subl</sub> /(kJ mol <sup>-1</sup> ) = 114.6		126.61	0.6		
temp dependence eq. 1 given in May 1980				128.38	0.7		
				129.94	0.8		
				131.32	0.9		
				132.56	1.0		
S	μg/kg			25.0	2.3 × 10 <sup>-6</sup>		
a	–0.0002			extrapolated			
b	0.0250						
c	–0.4250						
d	4.89			ΔH <sub>subl</sub> /(kJ mol <sup>-1</sup> ) = 115.2			
ΔH <sub>sol</sub> /(kJ mol <sup>-1</sup> ) = 41.25 measured between 5–30°C							



**FIGURE 4.1.1.34.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for triphenylene.

4.1.1.35 *o*-Terphenyl

Common Name: *o*-Terphenyl

Synonym: 1,2-diphenyl benzene

Chemical Name:

CAS Registry No: 84-15-1

Molecular Formula:  $C_{18}H_{14}$ , 1,2- $(C_6H_5)_2C_6H_4$

Molecular Weight: 230.304

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

56.2 (Lide 2003)

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

332 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$ ):

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

225.4 ( $93^{\circ}C$ , Stephenson & Malanowski 1987)

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

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

17.2 (Chickos et al. 1999)

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

52.3, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ),  $F$ : 0.494 (mp at  $56.2^{\circ}C$ )

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

1.24 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

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

$\log(P/kPa) = 6.29308 - [2160.24/(-106.38 + (T/K))]$ ; temp range 462–650 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -8.0641 - 4.0928 \times 10^3/(T/K) + 9.1076 \cdot \log(T/K) - 1.6326 \times 10^{-2} \cdot (T/K) + 6.0467 \times 10^{-6} \cdot (T/K)^2$ ; temp range 329–891 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,  $\log BCF$  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:

Air:

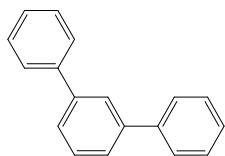
Surface water: a first order reduction process in river water with an estimated  $t_{1/2} = 0.6$  d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

Ground water:

Sediment:

Soil:

Biota:

4.1.1.36 *m*-Terphenyl

Common Name: *m*-Terphenyl

Synonym: 1,3-diphenyl benzene

Chemical Name:

CAS Registry No: 92-06-8

Molecular Formula:  $C_{18}H_{14}$ , 1,3- $(C_6H_5)_2C_6H_4$

Molecular Weight: 230.304

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

87 (Lide 2003)

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

363 (Lide 2003)

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

1.199 (Lide 2003)

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

227 ( $93^{\circ}C$ , Stephenson & Malanowski 1987)

192.1 ( $20^{\circ}C$ , calculated-density)

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

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

22.59 (Chickos et al. 1999)

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

62.76, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.246 (mp at  $87^{\circ}C$ )

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):

1.51 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

0.0305\* ( $24.99^{\circ}C$ , generator column-HPLC/fluorescence, Reza et al. 2002)

$\ln x = (-2.62 \pm 0.91) + (-5134 \pm 271)/(T/K)$ ; temp range 278–323.13 K (Reza et al. 2002)

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

$\log (P/kPa) = 6.48808 - [2445.98/(-102.76 + (T/K))]$ ; temp range 462–691 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

$\log (P/mmHg) = -14.7175 - 4.3577 \times 10^3/(T/K) + 11.935 \cdot \log (T/K) - 1.8441 \times 10^{-2} \cdot (T/K) + 6.437 \times 10^{-6} \cdot (T/K)^2$ ; temp range 360–925 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,  $\log BCF$  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:

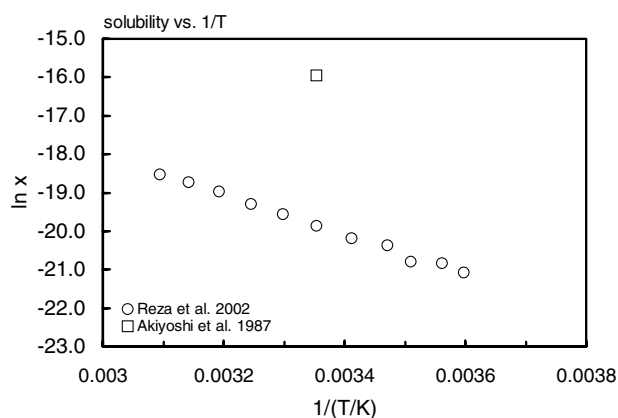
Air:

Surface water: a first order reduction process in river water with an estimated  $t_{1/2} = 0.6$  d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

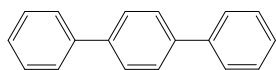
Ground water:  
Sediment:  
Soil:  
Biota:

**TABLE 4.1.1.36.1**  
**Reported aqueous solubilities of *m*-terphenyl at various temperatures**

Reza et al. 2002			
generator column-HPLC			
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
4.85	0.009	40.07	0.0741
7.64	0.0115	45.07	0.095
11.8	0.012	49.98	0.1159
14.98	0.0183	$\ln x = A - B/(T/\text{K})$	
19.95	0.0219	A	-2.62
24.99	0.0305	B	5134
30.0	0.0409	for temp range 287–323 K	
35.0	0.0535		



**FIGURE 4.1.1.36.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *m*-terphenyl.

4.1.1.37 *p*-Terphenyl

Common Name: *p*-Terphenyl

Synonym: 1,4-diphenyl benzene

Chemical Name: *p*-terphenyl

CAS Registry No: 92-94-4

Molecular Formula:  $C_{18}H_{14}$ , 1,4- $(C_6H_5)_2C_6H_4$

Molecular Weight: 230.304

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

213.9 (Lide 2003)

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

376 (Lide 2003)

Density ( $g/cm^3$ ):

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

262.0 (315.6 $^{\circ}C$ , Stephenson & Malanowski 1987)

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

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

0.3, 35.3; 35.6 (−79.55, 213.85 $^{\circ}C$ ; total phase change enthalpy, Chickos et al. 1999)

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

74.1, 73.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25 $^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.014 (mp at 213.9 $^{\circ}C$ )

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

1.80 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

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

$4.86 \times 10^{-6}$  (extrapolated from solid, Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.515 - 6210/(T/K)$ ; temp range 338–431 K (Antoine eq.-I, solid phase, Stephenson & Malanowski 1987)

$1.78 \times 10^{-5}$  ( $P_L$  extrapolated from liquid state, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.16107 - [2125.84/(-145.29 + (T/K))]$ ; temp range 499–700 K (Antoine eq.-II, liquid phase, Stephenson & Malanowski 1987)

$\log (P/mmHg) = -39.6342 - 3.2661 \times 10^3/(T/K) + 21.08 \cdot \log (T/K) - 2.2574 \times 10^{-2} \cdot (T/K) + 6.902 \times 10^{-6} \cdot (T/K)^2$ ; temp range 485–926 K (vapor pressure eq., Yaws 1994)

$5.40 \times 10^{-4}$  (supercooled liquid  $P_L$ , GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -4135/(T/K) + 10.60$ ;  $\Delta H_{vap.} = -79.2$  kJ $\cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa $\cdot m^3/mol$ ):

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

6.03, 5.88 (HPLC-RV correlation, Garst 1984)

$6.03 \pm 0.50$  (recommended, Sangster 1989)

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:

Air:

Surface water: a first order reduction process in river water with an estimated  $t_{1/2} = 0.6$  d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

Ground water:

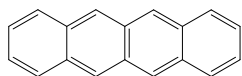
Sediment:

Soil:

Biota:



## 4.1.1.38 Naphthacene



Common Name: Naphthacene

Synonym: benz[*b*]anthracene, 2,3-benzanthracene, tetracene

Chemical Name: benz[*b*]anthracene

CAS Registry No: 92-24-0

Molecular Formula: C<sub>18</sub>H<sub>12</sub>

Molecular Weight: 228.288

Melting Point (°C):

357 (Lide 2003)

Boiling Point (°C):

450 (sublimation, Bjørseth 1983; Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

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

211.8 (Ruelle & Kesselring 1997)

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

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

38.64 (Ruelle & Kesselring 1997)

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

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.000553 (mp at 357°C)

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C or as indicated):

0.0010 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.0015 (approximate, shake flask-UV, Klevens 1950)

0.0036 (shake flask-UV, Eisenbrand & Baumann 1970)

0.00057 (shake flask-fluorescence, Mackay & Shiu 1977)

0.044 (shake flask-nephelometry, Hollifield 1979)

0.00103 (lit. mean, Pearlman et al. 1984)

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):

$7.30 \times 10^{-9}$ \* (effusion method, De Kruif 1980)

$3.70 \times 10^{-8}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 11.505 - 6540/(T/\text{K})$ ; temp range 376–489 K (Antoine eq., Stephenson & Malanowski 1987)

$2.31 \times 10^{-8}$ \* (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 113–199°C, Oja & Suuberg 1998)

$\log(P/\text{Pa}) = 33.594 - 15151/(T/\text{K})$ ; temp range 368–472 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

5.90 (shake flask-UV, concn. ratio, Karickhoff et al., 1979)

6.02 (HPLC-*k'* correlation, McDuffie 1981)

5.76 (HPLC-RT correlation, Wang et al. 1986)

5.76. (recommended, Sangster 1989, 1993)

5.84 (TLC retention time correlation, De Voogt et al. 1990)

5.90 (shake flask-HPLC, De Voogt et al. 1990)

5.90 (recommended, Hansch et al 1995)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

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

5.81 (sediment, batch equilibrium-sorption isotherms by GC/UV, Karickhoff et al. 1979)

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

Volatilization:

Photolysis: direct photochemical transformation  $t_{1/2} = 0.034$  h, computed near-surface water, latitude  $40^\circ\text{N}$ , midday, midsummer and photolysis  $t_{1/2} = 0.20$  d and  $0.95$  d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day,  $40^\circ\text{N}$  (Zepp & Schlotzhauer 1979)

photodegradation  $k = 0.051 \text{ min}^{-1}$  and  $t_{1/2} = 0.23$  h in ethanol-water (1:1, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

pseudo-first-order direct photolysis  $k(\text{exptl}) = 0.051 \text{ min}^{-1}$  with the calculated  $k = 0.051 \text{ min}^{-1}$  and  $t_{1/2} = 0.23$  h and the predicted  $k(\text{calc}) = 0.0355 \text{ min}^{-1}$  calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis  $t_{1/2} = 0.92$  h predicted by QSPR in atmospheric aerosol (Chen et al. 2001).

Oxidation:  $t_{1/2} = 2.6$  h for photosensitized oxygenation with singlet oxygen at near-surface natural water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: direct photolysis  $t_{1/2} = 0.92$  h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis  $t_{1/2} = 0.034$  h near surface water,  $t_{1/2} = 0.20$  d and  $0.95$  d in 5-m deep water body without and with sediment-water partitioning in full summer day,  $40^\circ\text{N}$ ; photosensitized oxygenation  $t_{1/2} = 2.6$  h at near surface water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979).

photolysis  $t_{1/2} = 0.23$  h in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996).

**TABLE 4.1.1.38.1**

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

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<b>de Kruif 1980</b>		<b>Oja &amp; Suuberg 1998</b>	
<b>torsion-, weighing effusion</b>		<b>Knudsen effusion</b>	
<b>t/^{\circ}C</b>	<b>P/Pa</b>	<b>t/^{\circ}C</b>	<b>P/Pa</b>
147.35	0.1	113.4	0.00344
155.46	0.2	128.78	0.0199
160.35	0.3	139.56	0.0535
163.89	0.4	145.44	0.0496
166.67	0.5	160.69	0.322
168.97	0.6	172.88	0.584
170.94	0.7	198.99	4.81
172.65	0.8		
173.98	0.9	mp/K	630
175.65	1.0		

TABLE 4.1.1.38.1 (Continued)

de Kruif 1980		Oja & Suuberg 1998	
torsion-, weighing effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
25.0	$9.7 \times 10^{-9}$	eq. 1a	P/Pa
	extrapolated	A	35.594
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 155.0$		for temp range 386–472 K	
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 126.1$	

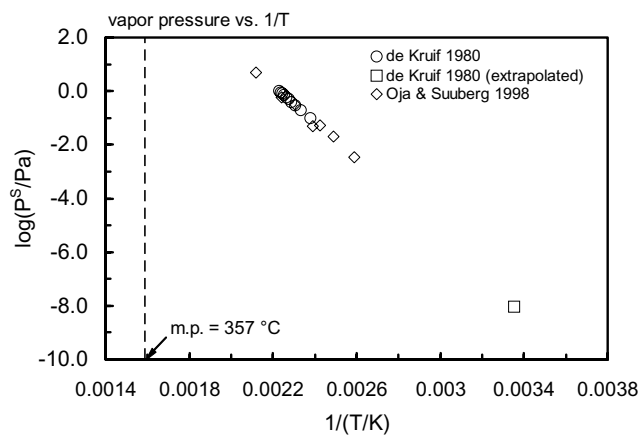
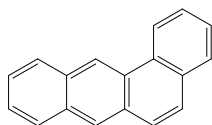


FIGURE 4.1.1.38.1 Logarithm of vapor pressure versus reciprocal temperature for naphthalene.

## 4.1.1.39 Benz[a]anthracene



Common Name: Benz[a]anthracene

Synonym: 1,2-benzanthracene, 2,3-benzophenanthrene, naphthanthracene, BaA, B(a) a, tetraphene

Chemical Name: 1,2-benzanthracene

CAS Registry No: 56-55-3

Molecular Formula: C<sub>18</sub>H<sub>12</sub>

Molecular Weight: 228.288

Melting Point (°C):

160.5 (Lide 2003)

Boiling Point (°C):

438 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

1.2544 (Mailhot & Peters 1988)

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

211.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

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

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

49.23, 44.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

49.2 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0468 (mp at 160.5°C)

0.040 (calculated, assuming ΔS<sub>fus</sub> = 56 J/mol K, Mackay et al. 1980)

0.0661 (calculated, ΔS<sub>fus</sub> = 49.2 J/mol K, Passivirta et al. 1999)

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

0.011 (27°C, shake flask-nephelometry, Davis & Parker 1942)

0.010 (shake flask-UV, Klevens 1950)

0.014 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0094, 0.0122 (25, 29°C, generator column-HPLC/UV, May et al. 1978b)

S/(μg/kg) = 1.74 + 0.1897·(t/°C) + 0.0031·(t/°C)<sup>2</sup> + 0.0003·(t/°C)<sup>3</sup>, temp range 5–30°C (generator column-HPLC/UV, May et al. 1978b, May 1980)

0.044 (shake flask-nephelometry, Hollifield 1979)

0.00837\* (generator column-HPLC, measured range 6.9–29.7°C, May 1980)

0.0086\* (generator column-HPLC, measured range 6.9–29.7°C, May et al. 1983)

0.00935\* (generator column-fluo., measured range 10–30°C, Velapoldi et al. 1983)

0.011 (average lit. value, Pearlman et al. 1984)

0.0168 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.00854 (generator column-HPLC/UV, measured range 3.7–25.0°C, Whitehouse 1984)

0.011 (recommended, IUPAC Solubility Data Series, Shaw 1989)

0.0146 (shake flask-HPLC, Haines & Sandler 1995)

0.0130 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

log [S<sub>L</sub>/(mol/L)] = −0.326 − 1119/(T/K) (supercooled liquid, Passivirta et al. 1999)

ln x = −3.060466 − 5354.51/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

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

2.93 × 10<sup>−6</sup> (20°C, Hoyer & Peperle 1958)

log (P/mmHg) = 13.68 − 6250/(T/K); temp range 60–120°C (Knudsen effusion method, Hoyer & Peperle 1958)

$2.17 \times 10^{-5}$  (solid, extrapolated from Antoine eq., Kelley & Rice 1964; quoted, Bidleman 1984)  
 $\log (P/\text{mmHg}) = 11.528 - 5461/(T/K)$ ; temp range: 104–127°C (effusion method, Kelley & Rice 1964)  
 $3.87 \times 10^{-7}$  (effusion method, Wakayama & Inokuchi 1967)  
 $1.47 \times 10^{-5}$  (solid, effusion method, extrapolated-Antoine eq., Murray et al. 1974)  
 $\log (P/\text{mmHg}) = 10.045 - 5929/(T/K)$ ; temp range: 330–390 K (effusion method, Murray et al. 1974)  
 $6.67 \times 10^{-7}$  (20°C, effusion, Pupp et al. 1974)  
 $7.30 \times 10^{-6*}$  (effusion method, De Kruif 1980)  
 $2.71 \times 10^{-5*}$  (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)  
 $\log (P/\text{Pa}) = 9.684 - 4246.51/(T/K)$ ; temp range 10–50°C (solid, Antoine eq., Sonnefeld et al. 1983)  
0.00107, 0.0003 ( $P_{GC}$  by GC-RT correlation, different GC columns, Bidleman 1984)  
0.000543 (supercooled liquid  $P_L$ , converted from literature  $P_S$  with  $\Delta S_{fus}$  Bidleman 1984)  
 $2.49 \times 10^{-4}$  (Yamasaki et al. 1984)  
 $4.10 \times 10^{-6}$  (selected, Howard et al. 1986)  
 $1.51 \times 10^{-5}$ ,  $2.17 \times 10^{-5}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_S/\text{kPa}) = 12.0507 - 5925/(T/K)$ ; temp range 330–390 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_S/\text{kPa}) = 10.653 - 5461/(T/K)$ ; temp range 377–400 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)  
 $5.43 \times 10^{-4}$  (supercooled  $P_L$ , converted from literature  $P_S$ , Hinckley et al. 1990)  
0.00107,  $3.23 \times 10^{-4}$  ( $P_{GC}$  by GC-RT correlation with different reference standards, Hinckley et al. 1990)  
 $\log P_L/\text{Pa} = 12.63 - 4742/(T/K)$  (GC-RT correlation, Hinckley et al. 1990)  
 $2.51 \times 10^{-4}$  (supercooled liquid  $P_L$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)  
 $(4.11\text{--}281) \times 10^{-7}$ ;  $2.76 \times 10^{-5}$  ( $P_S$ , quoted exptl., effusion; gas saturation, Delle Site 1997)  
 $3.39 \times 10^{-5}$ ;  $5.29 \times 10^{-5}$ ,  $1.48 \times 10^{-5}$ ,  $2.57 \times 10^{-5}$  ( $P_S$ , quoted lit., calculated; GC-RT correlation, Delle Site 1997)  
 $5.47 \times 10^{-4}$ ;  $3.59 \times 10^{-5}$  (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_S$  with fugacity ratio  $F$ , Passivirta et al. 1999)  
 $\log (P_S/\text{Pa}) = 11.91 - 4858/(T/K)$  (solid, Passivirta et al. 1999)  
 $\log (P_L/\text{Pa}) = 9.34 - 3760/(T/K)$  (supercooled liquid, Passivirta et al. 1999)  
 $\log (P/\text{Pa}) = 9.683 - 4246.51/(T/K)$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

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

0.813 (gas stripping-GC, Southworth 1979)  
0.102 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)  
1.22\* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)  
 $\ln K_{AW} = -7986.53/(T/K) + 19.124$ ,  $\Delta H = 66.4 \text{ kJ mol}^{-1}$ , measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)  
 $\log (H/(\text{Pa m}^3/\text{mol})) = 9.67 - 2641/(T/K)$  (Passivirta et al. 1999)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C and the reported temperature dependence equations:

5.61 (Radding et al. 1976)  
5.66 (Leo 1986; quoted, Schüürmann & Klein 1988)  
5.79 (HPLC-RT correlation, Wang et al. 1986)  
5.91 (recommended, Sangster 1989, 1993)  
5.84 (TLC retention time correlation, De Voogt et al. 1990)  
5.79 (recommended, Hansch et al. 1995)  
 $5.54 \pm 0.19$ ,  $5.50 \pm 0.64$  (HPLC- $k'$  correlation: ODS column; Diol column, Helweg et al. 1997)  
5.91 (range 5.74–6.04) (shake flask/slow stirring-HPLC/fluorescence, De Maagd et al. 1998)  
5.75 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)  
5.33; 4.98 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)  
 $\log K_{OW} = 1.238 + 1216.89/(T/K)$ ; temp range 5–55°C (temperature dependence HPLC- $k'$  correlation, Lei et al. 2000)

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

9.50 (calculated- $K_{OW}/K_{AW}$ , Wania & Mackay 1996)  
9.54 (calculated, Finizio et al. 1997)

## Bioconcentration Factor, log BCF:

- 4.56 (Smith et al. 1978; Steen & Karickhoff 1981)
- 4.0 (*Daphnia pulex*, Southworth et al. 1978)
- 4.0 (fathead minnow, Veith et al. 1979)
- 4.56, 5.0 (bacteria, Baughman & Paris 1981)
- 4.39 (activated sludge, Freitag et al. 1984)
- 4.0 (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Howell & Connell 1986)
- 4.39, 3.50, 2.54 (activated sludge, algae, fish, Freitag et al. 1985)
- 4.01 (*Daphnia magna*, Newsted & Giesy 1987)
- 4.303, 4266 (calculated-molecular connectivity indices, calculated- $K_{ow}$ , Lu et al. 1999)

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

- 4.52 (22°C, suspended particulates, Herbes et al. 1980)
- 6.30 (sediments average, Kayal & Connell 1990)
- 7.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 5.62 (humic acid, HPLC- $k'$  correlation; Nielsen et al. 1997)
- 5.77 (5.73–5.80), 5.47 (5.44–5.50) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 5.20 (soil, calculated-universal solvation model; Winget et al. 2000)
- 5.63–7.53; 4.50–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.11; 6.33, 5.84, 6.18 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

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

- Volatilization: aquatic fate rate  $k = 8 \times 10^3 \text{ h}^{-1}$  with  $t_{1/2} \sim 90 \text{ h}$  (Callahan et al. 1979);
  - half-lives predicted by one compartment model:  $t_{1/2} > 1000 \text{ h}$  in stream, eutrophic pond or lake and oligotrophic lake (Smith et al. 1978);
  - calculated  $t_{1/2} = 500 \text{ h}$  for a river of 1-m deep with water velocity of 0.5 m/s and wind velocity of 1 m/s (Southworth 1979; quoted, Herbes et al. 1980; Hallett & Brecher 1984).
- Photolysis: aquatic fate rate  $k \sim 6 \times 10^{-5} \text{ s}^{-1}$  with  $t_{1/2} = 10\text{--}50 \text{ h}$  (Callahan et al. 1979)
  - $t_{1/2} = 20 \text{ h}$  in stream,  $t_{1/2} = 50 \text{ h}$  in eutrophic pond or lake and  $t_{1/2} = 10 \text{ h}$  in oligotrophic lake, predicated by one compartment model (Smith et al. 1978)
- direct photochemical transformation  $t_{1/2}(\text{calc}) = 0.59 \text{ h}$ , computed near-surface water, latitude 40°N, midday, midsummer and photolysis  $t_{1/2} = 3.7 \text{ d}$  and  $9.2 \text{ d}$  in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)
  - $t_{1/2} = 0.58 \text{ h}$  in aquatics (quoted of EPA Report 600/7-78-074, Haque et al. 1980)
  - $t_{1/2} = 0.2 \text{ d}$  for early day in March (Mill et al. 1981);
  - $k = 1.93 \text{ h}^{-1}$  (Zepp 1980; quoted, Mill & Mabey 1985)
  - $k = 13.4 \times 10^{-5} \text{ s}^{-1}$  in early March with  $t_{1/2} = 5 \text{ h}$  in pure water at 366 nm, in sunlight at 23–28°C and  $k = 2.28 \times 10^{-5} \text{ s}^{-1}$  at 313 nm with 1% acetonitrile in filter-sterilized natural water (Mill et al. 1981);
  - $k = 1.39 \text{ h}^{-1}$  for summer midday at 40°N latitude (quoted, Mabey et al. 1982)
  - $t_{1/2} = 1\text{--}3 \text{ h}$ , atmospheric and aqueous photolysis half-life, based on measured photolysis rate constant for midday March sunlight on a cloudy day (Smith et al. 1978; quoted, Harris 1982; Howard et al. 1991) and adjusted for approximate summer and winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
  - half-lives on different atmospheric particulate substrates (approx. 25 µg/g on substrate):  $t_{1/2} = 4.0 \text{ h}$  on silica gel,  $t_{1/2} = 2.0 \text{ h}$  on alumina and  $t_{1/2} = 38 \text{ h}$  on fly ash (Behymer & Hites 1985)
  - first order daytime decay  $k = 0.0125 \text{ min}^{-1}$  for soot particles loading of 1000–2000 ng/mg and  $k = 0.0250 \text{ min}^{-1}$  for soot particles loading of 30–350 ng/mg (Kamens et al. 1988)
  - photodegradation  $k = 0.0251 \text{ min}^{-1}$  with  $t_{1/2} = 0.46 \text{ h}$  in ethanol-water (2:3, v/v) solution for initial concentration of 12.5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
  - pseudo-first-order direct photolysis  $k(\text{exptl}) = 0.0251 \text{ min}^{-1}$  with the calculated  $t_{1/2} = 0.46 \text{ h}$  and the predicted  $k = 0.0245 \text{ min}^{-1}$  calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis  $t_{1/2}(\text{obs}) = 0.94 \text{ h}$ ,  $t_{1/2}(\text{calc}) = 0.89 \text{ h}$  predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)

Photodegradation  $k = 5.0 \times 10^{-4} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: half-lives predicted by one compartment model:  $t_{1/2} = 38 \text{ h}$  in stream, eutrophic pond or lake and oligotrophic lake based on peroxy radical concentration of  $10^{-9} \text{ M}$  (Smith et al. 1978)

aquatic fate rate  $k = 5 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 38 \text{ h}$  (Callahan et al. 1979);

$t_{1/2} = 6400 \text{ h}$  for photosensitized oxygenation with singlet oxygen at near-surface natural water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979)

$k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $2 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)

$k = 3.3 \times 10^{-4} \text{ h}^{-1}$  with  $t_{1/2} = 0.6 \text{ h}$  under natural sunlight conditions;  $k(\text{aq.}) = 5.0 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$  with  $t_{1/2} = 1.6 \text{ d}$  for free-radical oxidation in air-saturated water (NRCC 1983)

photooxidation  $t_{1/2} = 0.801\text{--}8.01 \text{ h}$ , based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);

photooxidation  $t_{1/2} = 77\text{--}3850 \text{ h}$  in water, based on measured rate constant for reaction with hydroxyl radical in water (Howard et al. 1991)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: not observed during enrichment procedures (Smith et al. 1978)

no significant degradation in 7 d for an average of three static-flask screening test (Tabak et al. 1981)

$k = 3.3 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 208 \text{ h}$  for mixed bacterial populations in stream sediment (NRCC 1983)

$k = 1.0 \times 10^{-4} \text{ h}^{-1}$  with  $t_{1/2} = 288 \text{ d}$ ;  $k = 4.0 \times 10^{-6} \text{ h}^{-1}$  with  $t_{1/2} = 20 \text{ yr}$  for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)

$k = 0.0026 \text{ d}^{-1}$  with  $t_{1/2} = 261 \text{ d}$  for Kidman sandy loam and  $k = 0.0043 \text{ d}^{-1}$  with  $t_{1/2} = 162 \text{ d}$  for McLarin sandy loam all at  $-0.33 \text{ bar}$  soil moisture (Park et al. 1990)

$t_{1/2}(\text{aq. aerobic}) = 2448\text{--}16320 \text{ h}$ , based on aerobic soil dieaway test data at  $10\text{--}30^\circ\text{C}$  (Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 9792\text{--}65280 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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

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

$k_1 = 669 \text{ h}^{-1}$ ;  $k_2 = 0.144 \text{ h}^{-1}$  (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.83 \text{ h}^{-1}$ ;  $\log k_2 = -0.84 \text{ h}^{-1}$  (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 138.6 \text{ mL g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0022 \text{ h}^{-1}$  ( $4^\circ\text{C}$ , *P. hoyi*, Landrum 1988)

$k_1 = 0.72\text{--}1.4 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0096 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 1\text{--}3 \text{ h}$ , based on estimated photolysis half-life in air (Howard et al. 1991);

$t_{1/2} = 4.20 \text{ h}$  under simulated sunlight,  $t_{1/2} = 1.35 \text{ h}$  in simulated sunlight + ozone (0.2 ppm),  $t_{1/2} = 2.88 \text{ h}$  in dark reaction ozone (0.2 ppm), under simulated atmospheric conditions (Katz et al. 1979)

$t_{1/2} = 0.4 \text{ h}$  for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant  $k = 0.0265 \text{ min}^{-1}$  at  $1 \text{ cal cm}^{-2} \text{ min}^{-1}$ ,  $10 \text{ g/m}^3 \text{ H}_2\text{O}$  and  $20^\circ\text{C}$  (Kamens et al. 1988).

Surface water: photolysis  $t_{1/2} = 0.59 \text{ h}$  near surface water,  $t_{1/2} = 3.7 \text{ d}$  and  $9.2 \text{ d}$  in 5-m deep water body without and with sediment-water partitioning in full summer day,  $40^\circ\text{N}$ ; photosensitized oxygenation  $t_{1/2} = 2.6 \text{ h}$  at near surface water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979)

$t_{1/2} = 0.20 \text{ d}$  under summer sunlight (Mill & Mabey 1985);

$t_{1/2} = 1\text{--}3 \text{ h}$ , based on estimated photolysis half-life in water, Howard et al. 1991);

photolysis  $t_{1/2} = 0.46 \text{ h}$  (reported in units of minutes) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:  $t_{1/2} = 4896\text{--}32640 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: The uptake clearance from sediment was  $k = (0.005 \pm 0.001) \text{ g of dry sediment} \cdot \text{g}^{-1} \text{ of organism} \cdot \text{h}^{-1}$ , and the elimination rate constants  $k = (0.0014 \pm 0.0006) \text{ h}^{-1}$  for amphipod, *P. hoyi* in Lake Michigan sediments at  $4^\circ\text{C}$  (Landrum 1989);

desorption  $t_{1/2} = 11.1 \text{ d}$  from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil:  $t_{1/2} = 4\text{--}6250 \text{ d}$  (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 240$  d for 5 mg/kg treatment and 130 d for 50 mg/kg treatment (Bulman et al. 1987);  
 biodegradation  $k = 0.0026$  d<sup>-1</sup> with  $t_{1/2} = 261$  d for Kidman sandy loam soil, and  $k = 0.0043$  d<sup>-1</sup> with  $t_{1/2} = 162$  d for McLaurin sandy loam soil (Park et al. 1990);  
 $t_{1/2} \sim 2448$ – $16320$  h, based on aerobic die-away test data at 10–30°C (Howard et al. 1991);  
 $t_{1/2} > 50$  d (Ryan et al. 1988).

Biota: depuration  $t_{1/2} = 9$  d by oysters (Lee et al. 1978);

elimination  $t_{1/2} = 4.3$ – $17.8$  d from mussel *Mytilus edulis*;  $t_{1/2} = 7$ – $15.4$  d from Oyster,  $t_{1/2} = 8.0$  d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

**TABLE 4.1.1.39.1**

**Reported aqueous solubilities of benz[a]anthracene at various temperatures and reported temperature dependence equation**

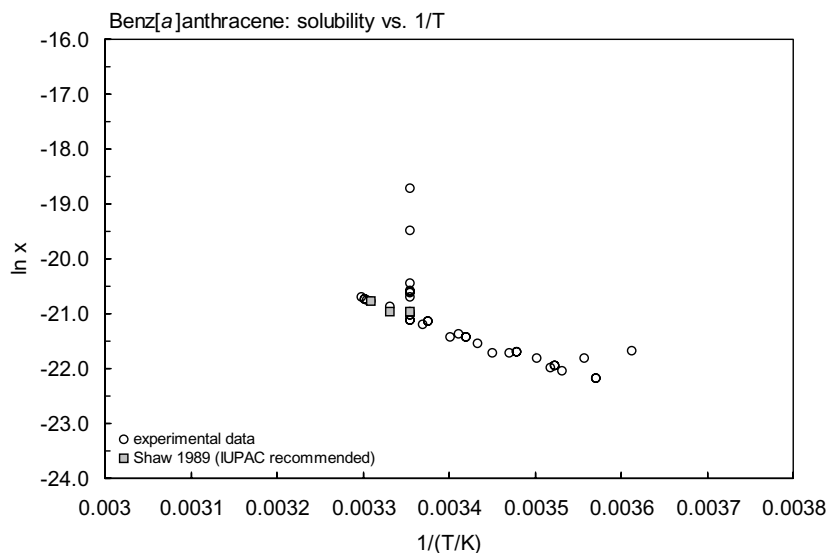
$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

$$\ln x = A + B/(T/K) + C \cdot \ln(T/K) \quad (2)$$

May 1980		May et al. 1978b		May et al. 1983		Velapoldi et al. 1983	
generator column-HPLC		generator column-HPLC		generator column-HPLC		generator column-fluo.	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
6.9	0.00299	25	0.0094	6.9	0.00299	10	0.00342
10.7	0.00378	29	0.0122	10.7	0.00378	15	0.00475
14.3	0.00479			11.0	0.00361	20	0.00669
19.3	0.00633			14.7	0.00558	25	0.00935
23.1	0.00837	temp dependence eq. 1		18.1	0.00634	30	0.01297
29.7	0.0127	S	μg/kg	19.3	0.00801		
		a	0.0003	23.6	0.00838		
temp dependence eq. 1		b	-0.0031	25.0	0.00862	eq. 2	mole fraction
S	μg/kg	c	0.1897	29.5	0.0124	A	-83.75982
a	0.0003	d	1.74	29.7	0.0127	B	41884.5
b	-0.0031					C	161.175
c	0.1897	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 44.81$					
d	1.74	measured between 5–30°C				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 49.0$	
						at 25°C	

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 44.81$   
 measured between 5–30°C





**FIGURE 4.1.1.39.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for benz[a]anthracene.

**TABLE 4.1.1.39.2**

**Reported vapor pressures of benz[a]anthracene at various temperatures and the coefficients for the vapor pressure equations**

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

Kelley & Rice 1964		Murray et al. 1972		de Kruif 1980		Sonnefeld et al. 1983	
effusion-electrobalance		Knudsen effusion		torsion-, effusion method		generator column-HPLC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
data represented by		data presented by graph and		98.07	0.1	13.81	$8.05 \times 10^{-5}$
		eq. 2		105.21	0.2	13.81	$6.06 \times 10^{-5}$
eq. 1	P/mmHg	A	10.045	109.51	0.3	13.81	$1.13 \times 10^{-5}$
A	11.528	B	5925	112.62	0.4	25.1	$2.66 \times 10^{-5}$
B	5461	temp range 330–390 K		115.06	0.5	25.1	$2.56 \times 10^{-5}$
measured range 104–127°C				117.09	0.6	25.1	$2.81 \times 10^{-5}$
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 104.56$				118.82	0.7	40.12	$1.39 \times 10^{-4}$
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 113.5$		120.32	0.8	40.12	$1.41 \times 10^{-4}$
mp/°C	160–161.5			121.66	0.9	40.12	$1.36 \times 10^{-4}$
				122.87	1.0	40.75	$1.31 \times 10^{-4}$
				25.0	$7.3 \times 10^{-6}$	40.85	$1.17 \times 10^{-4}$
				$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 113$		extrapolated	$1.27 \times 10^{-4}$
						40.85	$1.21 \times 10^{-4}$
						40.85	$1.21 \times 10^{-4}$
						49.56	$3.87 \times 10^{-4}$
						49.56	$3.85 \times 10^{-4}$
Hoyer & Peperle 1958						49.56	$3.88 \times 10^{-4}$
effusion method						34.93	$2.69 \times 10^{-4}$
t/°C	P/Pa					25.0	$2.80 \times 10^{-5}$
data presented by equation.							

(Continued)

TABLE 4.1.1.39.2 (Continued)

Kelley & Rice 1964		Murray et al. 1972		de Kruif 1980		Sonnefeld et al. 1983	
effusion-electrobalance		Knudsen effusion		torsion-, effusion method		generator column-HPLC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
eq. 1	P/mmHg					eq. 1	P/Pa
A	13.68					A	9.684
B	6250					B	4246.51
for temp range 60–120°C						$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 51.83$	
						for temp range 10–50°C	

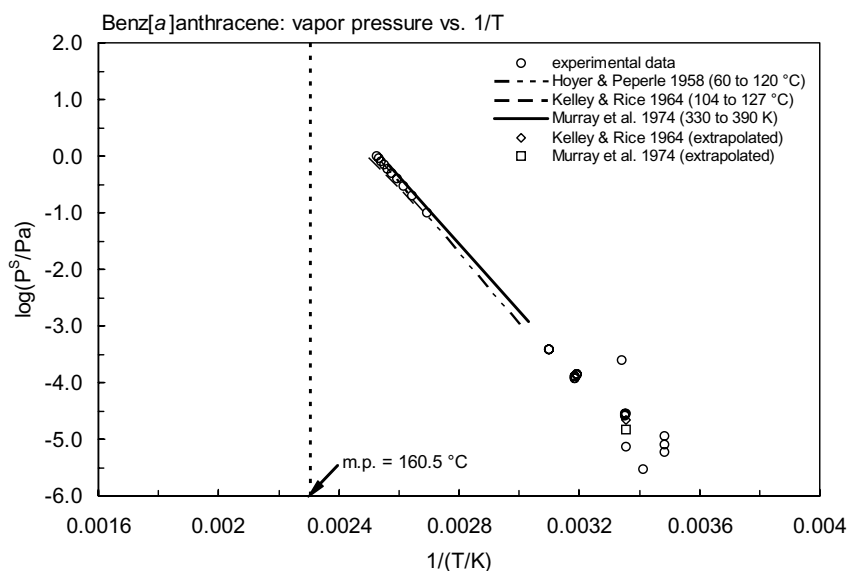


FIGURE 4.1.1.39.2 Logarithm of vapor pressure versus reciprocal temperature for benz[a]anthracene.

TABLE 4.1.1.39.3

Reported Henry's law constants of benz[a]anthracene at various temperatures and temperature dependence equations

$\ln K_{\text{AW}} = A - B/(T/K)$	(1)	$\log K_{\text{AW}} = A - B/(T/K)$	(1a)
$\ln (1/K_{\text{AW}}) = A - B/(T/K)$	(2)	$\log (1/K_{\text{AW}}) = A - B/(T/K)$	(2a)
$\ln (k_{\text{H}}/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{\text{AW}} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Bamford et al. 1999

gas stripping-GC/MS

t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)
		average
4.1	0.10, 0.22	0.15
11.0	0.24, 0.41	0.31
18.0	0.50, 0.79	0.63
25.0	0.91, 1.64	1.22
31.0	1.43, 3.13	2.11

 $\ln K_{\text{AW}} = A - B/(T/K)$

TABLE 4.1.1.39.3 (Continued)

Bamford et al. 1999		
gas stripping-GC/MS		
t/°C	H/(Pa m <sup>3</sup> /mol)	H/(Pa m <sup>3</sup> /mol)
A	19.124	
B	7986.5	
enthalpy, entropy change:		
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 66.4 \pm 6.9$		
$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 159$		
at 25°C		

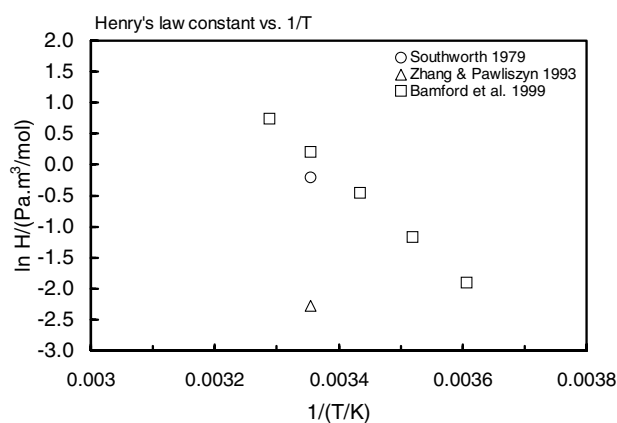
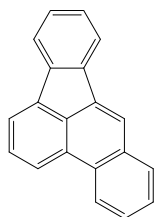


FIGURE 4.1.1.39.3 Logarithm of Henry's law constant versus reciprocal temperature for benz[a]anthracene.

4.1.1.40 Benzo[*b*]fluoranthene

Common Name: Benzo[*b*]fluoranthene

Synonym: 2,3-benzofluoranthene, 3,4-benzofluoranthene, benz[*e*]acephenanthrylene, B[*b*]F

Chemical Name: 2,3-benzofluoranthene

CAS Registry No: 205-99-2

Molecular Formula: C<sub>20</sub>H<sub>12</sub>

Molecular Weight: 252.309

Melting Point (°C):

168 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)

Boiling Point (°C):

481 (Bjørseth 1983)

Density (g/cm<sup>3</sup> at 20°C):

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

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

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

56.5 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0395 (mp at 168°C)

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C or as indicated and reported temperature dependence equations):

0.0015 (generator column-HPLC/fluorescence, Wise et al. 1981)

0.0015 (average lit. value, Pearlman et al. 1984)

0.00109 (generator column-HPLC/fluor., De Maagd et al. 1998)

log [S<sub>L</sub>/(mol/L)] = -0.351 - 1303/(T/K) (supercooled liquid, Passivirta et al. 1999)

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

6.67 × 10<sup>-5</sup> (20°C, estimated, Callahan et al. 1979)

2.12 × 10<sup>-5</sup> (Yamasaki et al. 1984)

5.0 × 10<sup>-8</sup>; 1.30 × 10<sup>-6</sup> (quoted solid P<sub>s</sub> from Mackay et al. 1992; converted to supercooled liquid P<sub>L</sub> with fugacity ratio F, Passivirta et al. 1999)

log (P<sub>s</sub>/Pa) = 12.43 - 5880/(T/K) (solid, Passivirta et al. 1999)

log (P<sub>L</sub>/Pa) = 9.48 - 4578/(T/K) (supercooled liquid, Passivirta et al. 1999)

7.55 × 10<sup>-6</sup> (supercooled liquid P<sub>L</sub>, calibrated GC-RT correlation, Lei et al. 2002)

log (P<sub>L</sub>/Pa) = -4682/(T/K) + 10.58, ΔH<sub>vap</sub> = -89.7 kJ·mol<sup>-1</sup> (GC-RT correlation, Lei et al. 2002)

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

0.051 (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)

log [H/(Pa m<sup>3</sup>/mol)] = 9.83 - 3274/(T/K) (Passivirta et al. 1999)

0.0485 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

log K<sub>AW</sub> = 2.955 - 2245/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

5.78 (HPLC-RT correlation, Wang et al. 1986)

5.78 (recommended, Sangster 1989, 1993)

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

Bioconcentration Factor,  $\log BCF$ :

5.15	(microorganisms-water, Mabey et al. 1982)
4.00	( <i>Daphnia magna</i> , Newsted & Giesy 1987)
0.959, 0.230	( <i>Polychaete sp.</i> , <i>Capitella capitata</i> , Bayona et al. 1991)

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

6.182; 6.00, 6.18	(sediment: concn ratio $C_{sed}/C_w$ ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
5.45	( $\log K_{DOC}$ - Aldrich humic acid, RP-HPLC, Ozretich et al. 1995)
6.57	(10°C), 6.55, 6.61 (20°C), 6.26 (35°C), 6.44, 6.45 (45°C) ( $\log K_{DOC}$ , dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
6.20	(20°C, $\log K_{DOC}$ , particulate organic material from lake, Lüers & ten Hulscher 1996)
6.15–8.02; 5.70–7.50	(range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001, for benzo[b + j + k]fluoranthenes)
5.91; 6.50, 6.26, 6.68	(20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001, for benzo[b + j + k]fluoranthenes)

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

Volatilization:

Photolysis: atmospheric and aqueous  $t_{1/2} = 8.7$ –720 h, based on measured rate of photolysis in heptane irradiated with light  $> 290$  nm (Howard et al. 1991);

first order daytime decay rate constants:  $k = 0.0065 \text{ min}^{-1}$  for 1000–2000 ng/mg soot particles loading and  $k = 0.0090 \text{ min}^{-1}$  with 30–350 ng/mg loading (Kamens et al. 1988);

$t_{1/2}(\text{obs.}) = 4.31 \text{ h}$ ,  $t_{1/2}(\text{calc}) = 1.49 \text{ h}$  predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Photodegradation  $k = 3 \times 10^{-5} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002).

Oxidation: rate constant  $k = 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 5 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982);

photooxidation  $t_{1/2} = 1.43$ –14.3 h, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).

Hydrolysis: not hydrolyzable (Mabey et al. 1982; no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

aerobic  $t_{1/2} = 8640$ –14640 h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$k = 0.0024 \text{ d}^{-1}$  with  $t_{1/2} = 294 \text{ d}$  for Kidman sandy loam and  $k = 0.0033 \text{ d}^{-1}$  with  $t_{1/2} = 211 \text{ d}$  for McLarin sandy loam all at  $-0.33$  bar soil moisture (Park et al. 1990);

$t_{1/2}(\text{aq. anaerobic}) = 34560$ –58560 h, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991).

Biotransformation: estimated to be  $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

$k_1 = 0.11$ –0.38  $\text{mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0029 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Sorption-Desorption Rate constants: desorption rate constant  $k = 0.016 \text{ d}^{-1}$  with  $t_{1/2} = 42.4 \text{ d}$  from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Half-Lives in the Environment:

Air:  $t_{1/2} = 1.43$ –14.3 h, based on estimated photooxidation half-life in air (Howard et al. 1991)

half-lives under simulated atmospheric conditions: simulated sunlight  $-t_{1/2} = 8.70 \text{ h}$ , simulated sunlight + ozone (0.2 ppm)  $t_{1/2} = 4.20 \text{ h}$ , dark reaction ozone (0.2 ppm)  $t_{1/2} = 52.70 \text{ h}$  (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 1.3 \text{ h}$  for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant  $k = 0.0091 \text{ min}^{-1}$  at  $1 \text{ cal cm}^{-2} \text{ min}^{-1}$ ,  $10 \text{ g/m}^3 \text{ H}_2\text{O}$  and  $20^\circ\text{C}$  (Kamens et al. 1988).

Surface water:  $t_{1/2} = 8.7$ –720 h, based on estimated aqueous photolysis half-life (Lane & Katz 1977; Muel & Saguem 1985; quoted, Howard et al. 1991).

Groundwater:  $t_{1/2} = 17280\text{--}29280$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

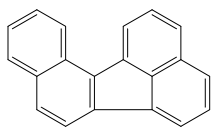
Sediment: desorption  $t_{1/2} = 42.4$  d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: biodegradation rate constant  $k = 0.0024\text{ d}^{-1}$  with  $t_{1/2} = 294$  d for Kidman sandy loam soil, and  $k = 0.0033\text{ d}^{-1}$  with  $t_{1/2} = 211$  d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 8640\text{--}14640$  h, based on aerobic die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$t_{1/2} = 42$  wk, 9.0 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: elimination  $t_{1/2} = 5.7\text{--}16.9$  d from mussel *Mytilus edulis*;  $t_{1/2} = 7.7$  d from Oyster (isomer unspecified),  $t_{1/2} = 3.9$  d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).

4.1.1.41 Benzo[*j*]fluoranthene

Common Name: Benzo[*j*]fluoranthene

Synonym: 7,8-benzofluoranthene, 10,11-fluoranthene

Chemical Name: benzo[*j*]fluoranthene

CAS Registry No: 205-82-3

Molecular Formula: C<sub>20</sub>H<sub>12</sub>

Molecular Weight: 252.309

Melting Point (°C):

166 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)

Boiling Point (°C):

480 (Bjørseth 1983)

Density (g/cm<sup>3</sup> at 20°C):

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

222.8 (Ruelle & Kesselring 1997)

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

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

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

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0414 (mp at 166°C)

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

0.0025 (generator column-HPLC/fluorescence, Wise et al. 1981)

0.0025 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C):

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

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

6.44 (calculated-MCI χ as per Rekker & De Kort 1979, Ruepert et al. 1985)

6.40 (Bayona et al. 1991)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

0.914; -0.222 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, log K<sub>OC</sub>:

6.15–8.02; 5.70–7.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001, for benzo[*b + j + k*]fluoranthenes)

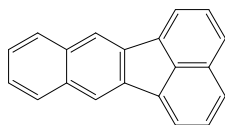
5.91; 6.50, 6.26, 6.68 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001, for benzo[*b + j + k*]fluoranthenes)

Environmental Fate Rate Constants, k or Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

Biota: elimination t<sub>1/2</sub> = 7.7 d from Oyster (isomer unspecified), t<sub>1/2</sub> = 3.9 d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).

## 4.1.1.42 Benzo[k]fluoranthene



Common Name: Benzo[k]fluoranthene

Synonym: 8,9-benzofluoranthene, 11,12-benzofluoranthene, B[k]F

Chemical Name: 8,9-benzofluoranthene

CAS Registry No: 207-08-9

Molecular Formula:  $C_{20}H_{12}$

Molecular Weight: 252.309

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

217 (Weast 1977; Bjørseth 1983; Stephenson & Malanowski 1987; Lide 2003)

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

480 (Stephenson & Malanowski 1987; Lide 2003)

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

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

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

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

56.6 (Passivirta et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0131 (mp at  $217^{\circ}C$ )

0.0126 (calculated, Passivirta et al. 1999)

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

0.0008 (generator column-HPLC/UV, Wise et al. 1981)

0.00081 (average lit. value, Pearlman et al. 1984)

0.00109 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

$\log [S_L/(mol/L)] = -0.351 - 1448/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

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

$1.28 \times 10^{-8}$  ( $20^{\circ}C$ , Radding et al. 1976)

$6.70 \times 10^{-5}$  ( $20^{\circ}C$ , Mabey et al. 1982)

$2.07 \times 10^{-5}$  (Yamasaki et al. 1984)

$5.20 \times 10^{-8}$ ,  $4.93 \times 10^{-6}$  ( $20^{\circ}C$ , lit. mean solid  $P_s$ , supercooled liquid value  $P_L$ , Bidleman & Foreman 1987)

$1.29 \times 10^{-7}$  (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.8907 - 6792/(T/K)$ ; temp range 363–430 K (Antoine eq., Stephenson & Malanowski 1987)

$2.09 \times 10^{-5}$  (supercooled liquid  $P_L$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)

$5.20 \times 10^{-8}$ ;  $4.14 \times 10^{-6}$  (quoted solid  $P_s$  from Mackay et al. 1992; converted to supercooled liquid  $P_L$  with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.43 - 5874/(T/K)$  (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.48 - 4427/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$8.96 \times 10^{-6}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -4623/(T/K) + 10.46$ ;  $\Delta H_{vap} = -88.5$  kJ·mol $^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

0.111 ( $15^{\circ}C$ , calculated, Baker & Eisenreich 1990)

0.043\* ( $20^{\circ}C$ , gas stripping-HPLC/fluorescence, measured range 10–55 $^{\circ}C$ , ten Hulscher et al. 1992)

$\log (H/(Pa\ m^3/mol)) = 9.83 - 2979/(T/K)$  (Passivirta et al. 1999)

0.0422 ( $20^{\circ}C$ , selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 3.498 - 2421/(T/K)$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)



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

6.84	(calculated-fragment const., Callahan et al. 1979)
6.06	(calculated-f const., Mabey et al. 1982)
6.44	(calculated-MCI $\chi$ as per Rekker & De Kort 1979)
6.40	(Bayona et al. 1991)
6.50	(calculated-S and mp, Capel et al. 1991)
7.20	(calculated- $K_{OC}$ , Broman et al. 1991)
6.00	(selected, Mackay et al. 1992; quoted, Finizio et al. 1997)
6.30	(computed-expert system SPARC, Kolliig 1995)
6.50–6.85; 6.73	(quoted lit. range; lit. mean, Meador et al. 1995)
6.11	(range 5.86–6.28) (shake flask/slow stirring-HPLC/fluor., De Maagd et al. 1998)
5.94; 6.16	(quoted lit.; calculated, Passivirta et al. 1999)

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

11.19	(calculated, Finizio et al. 1997)
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Bioconcentration Factor,  $\log BCF$ :

5.15	(microorganisms-water, calculated from $K_{ow}$ , Mabey et al. 1982)
4.12	( <i>Daphnia magna</i> , Newsted & Giesy 1987)

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

5.99	(sediments average, Kayal & Connell 1990)
7.00	(Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
6.80 (10°C), 6.74, 6.89 (20°C), 6.46 (35°C), 6.44, 6.45 (45°C)	( $\log K_{DOC}$ - dissolved organic material from lake, gas-purge technique- HPLC/fluorescence, Lüers & ten Hulscher 1996)
6.30	(20°C, $\log K_{POC}$ - particulate organic material from lake, Lüers & ten Hulscher 1996)
6.04 (5.93–6.12), 5.47 (5.39–5.54)	(sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
6.15–8.02; 5.70–7.50	(range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001, for benzo[ <i>b</i> + <i>j</i> + <i>k</i> ]fluoranthenes)
5.91; 6.50, 6.26, 6.68 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1, 2, 3-solvophobic approach, Krauss & Wilcke 2001, for benzo[ <i>b</i> + <i>j</i> + <i>k</i> ]fluoranthenes)	

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

## Volatilization:

Photolysis: atmospheric and aqueous photolysis  $t_{1/2} = 3.8$ –499 h, based on measured rate of photolysis in heptane under November sunlight and adjusted by ratio of sunlight photolysis half-lives in water versus heptane (Howard et al. 1991);

first-order daytime decay constants:  $k = 0.0047 \text{ min}^{-1}$  for soot particles loading of 1000–2000 ng/mg and  $k = 0.0013 \text{ min}^{-1}$  with 30–350 ng/mg loading (Kamens et al. 1988);

direct photolysis  $t_{1/2}(\text{obs}) = 0.88 \text{ h}$ ,  $t_{1/2}(\text{calc}) = 0.80 \text{ h}$  predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Photodegradation  $k = 3 \times 10^{-5} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant  $k = 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 5 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982);

photooxidation  $t_{1/2} = 1.1$ –11 h, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).

Hydrolysis: not hydrolyzable (Mabey et al. 1982);

no hydrolyzable groups (Howard et al. 1991).

## Biodegradation:

aerobic  $t_{1/2} = 21840$ –51360 h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 87360$ –205440 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated to be  $3 \times 10^{-12}$  mL cell<sup>-1</sup> h<sup>-1</sup> for bacteria (Mabey et al. 1982).

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 1.1\text{--}11$  h, based on estimated photooxidation half-life in air (Howard et al. 1991);

$t_{1/2} = 14.10$  h in simulated sunlight:  $t_{1/2} = 3.90$  h in simulated sunlight + ozone (0.2 ppm),  $t_{1/2} = 34.90$  h in dark reaction ozone (0.2 ppm) u) under simulated atmospheric conditions (Katz et al. 1979);

$t_{1/2} = 0.8$  h for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant  $k = 0.0138$  min<sup>-1</sup> at 1 cal cm<sup>-2</sup> min<sup>-1</sup> and 10 g/m<sup>3</sup> H<sub>2</sub>O at 20°C (Kamens et al. 1988).

Surface water:  $t_{1/2} = 3.8\text{--}499$  h, based on photolysis half-life in water (Howard et al. 1991).

Groundwater:  $t_{1/2} = 42680\text{--}102720$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption  $t_{1/2} = 23.2$  d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil:  $t_{1/2} = 21840\text{--}51360$  h, based on aerobic soil die-away test data Howard et al. 1991);

$t_{1/2} > 50$  d (Ryan et al. 1988);

mean  $t_{1/2} = 8.7$  yr for Luddington soil (Wild et al. 1991).

Biota: elimination  $t_{1/2} = 11.9$  d from mussel *Mytilus edulis*;  $t_{1/2} = 7.7$  d from Oyster (isomer unspecified),  $t_{1/2} = 3.9$  d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).

**TABLE 4.1.1.42.1**

**Reported Henry's law constants of benzo[k]fluoranthene at various temperatures and temperature dependence equations**

$$\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_p/\text{atm}) = A - B/(T/K) \quad (3)$$

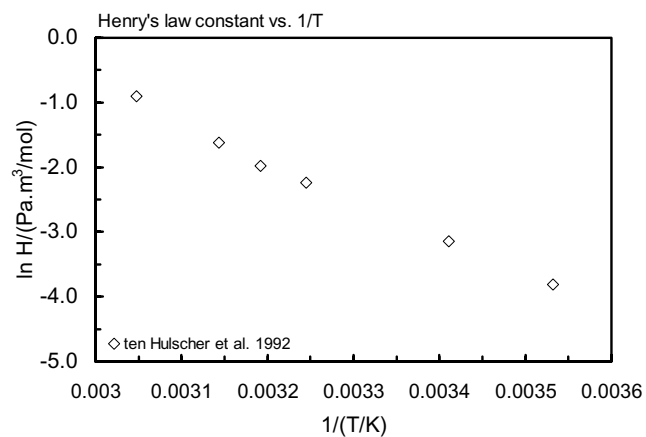
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4) \quad \ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

**ten Hulscher et al. 1992**

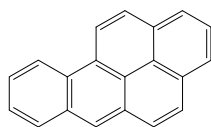
#### gas stripping-HPLC/fluorescence

t/°C	H/(Pa m <sup>3</sup> /mol)
10.0	0.022
20.0	0.043
35.0	0.107
40.1	0.138
45.0	0.198
55.0	0.403
$\ln K_{AW} = -\Delta H_{vol}/RT + \Delta S_{vol}/R$ $R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$ $\Delta S_{vol} = 16.41$ $\Delta H_{vol} = 5893.7$ enthalpy of volatilization: $\Delta H_{vol}/(\text{kJ} \cdot \text{mol}^{-1}) = 49 \pm 1.9$ entropy of volatilization, $\Delta S$ $T\Delta S_{vol}/(\text{kJ} \cdot \text{mol}^{-1}) = 40 \pm 4$ at 20°C	



**FIGURE 4.1.1.42.1** Logarithm of Henry's law constant versus reciprocal temperature for benzo[k]fluoranthrene.

## 4.1.1.43 Benzo[a]pyrene



Common Name: Benzo[a]pyrene

Synonym: BaP, B(a)P, 3,4-benzopyrene

Chemical Name: benzo[a]pyrene

CAS Registry No: 50-32-8

Molecular Formula:  $C_{20}H_{12}$

Molecular Weight: 252.309

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

181.1 (Lide 2003)

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

495 (Stephenson & Malanowski 1987; Dean 1992)

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

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

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

17.324 (Ruelle & Kesselring 1997)

8.49, 17.32; 25.61 (117.05, 181.05 $^{\circ}C$ ; total phase change enthalpy, Chickos et al. 1999)

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

38.5 (differential scanning calorimetry, Hinckley et al. 1990)

21.77, 38.13 (117.05, 181.05 $^{\circ}C$ , Chickos et al. 1999)

42.35, 43.7 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

38.2 (Passivirta et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0294 (mp at 181.1 $^{\circ}C$ )

0.0903 (calculated, Passivirta et al. 1999)

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

0.004 (27 $^{\circ}C$ , nephelometry, Davis et al. 1942)

0.0043 (shake flask-UV/fluorescence, Barone et al. 1967)

0.0061 (average, Barone et al. 1967)

0.0005 (20 $^{\circ}C$ , shake flask-UV, Eisenbrand & Baumann 1970)

0.000038, 0.0000606, 0.000038, 0.0000505 (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

0.00121 (Haque & Schmedding 1975)

0.0038 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0002 (Rossi 1977; Neff 1979)

0.0012 (generator column-HPLC, Wise et al. 1981)

0.00162\* (generator column-HPLC, measured range 10–30 $^{\circ}C$ , May et al. 1983)

0.00158\* (generator column-spectrofluorimetry, measured range 10–30 $^{\circ}C$ , Velapoldi et al. 1983)

0.0038 (selected value, Pearlman et al. 1984)

0.00154\* (generator column-HPLC/UV, measured 8.0–25.0 $^{\circ}C$ , Whitehouse 1984)

0.0016 (generator column-HPLC/UV, Billington et al. 1988)

0.000504 (shake flask-LSC, Eadie et al. 1990)

0.00472 (shake flask-fluorescence, Haines & Sandler 1995)

0.00182 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

0.00622  $\pm$  0.00023; 0.0038, 0.0018  $\pm$  0.0003 (shake flask-SPME (solid-phase micro-extraction)-GC; quoted lit. values; Paschke et al. 1999)

$\log S_L$  (mol/L) =  $-1.310 - 906.6/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$\ln x = -2.59638 - 6046.87/(T/K)$ ; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

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

$7.32 \times 10^{-7}$  (effusion method, extrapolated, Murray et al. 1974)

$\log (P/\text{mmHg}) = 9.601 - 6181/(T/K)$ ; temp range 358–431 K (Knudsen effusion method, Murray et al. 1974)

$1.12 \times 10^{-4}$ ,  $1.50 \times 10^{-5}$  ( $P_{GC}$ , GC-RT correlation with different GC columns, Bidleman 1984)

$2.35 \times 10^{-5}$  (supercooled liquid  $P_L$ , converted from literature  $P_S$  with  $\Delta S_{fus}$  Bidleman 1984)

$1.22 \times 10^{-5}$  (Yamasaki et al. 1984)

$3.2 \times 10^{-7}$ ,  $1.23 \times 10^{-5}$  (lit. mean, supercooled liq. value, Bidleman & Foreman 1987)

$7.51 \times 10^{-7}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 11.6067 - 6181/(T/K)$ ; temp range 358–431 K (Antoine eq., Stephenson & Malanowski 1987)

$1.12 \times 10^{-4}$ ,  $7.24 \times 10^{-5}$  ( $P_{GC}$ , GC-RT correlation with different reference standards, Hinckley et al. 1990)

$2.35 \times 10^{-5}$ ,  $7.28 \times 10^{-6}$  (supercooled liquid  $P_L$ , converted from literature  $P_S$  with different  $\Delta S_{fus}$  Hinckley et al. 1990)

$\log (P_L/\text{Pa}) = 11.59 - 4989/(T/K)$  (liquid phase, GC-RT correlation, Clausius-Clapeyron eq., Hinckley et al. 1990)

$1.17 \times 10^{-5}$  (supercooled liquid  $P_L$ , calculated from Yamasaki et al 1984, Finizio et al. 1997)

$7.51 \times 10^{-7}$ ,  $7.45 \times 10^{-7}$  (quoted exptl., effusion, Delle Site 1997)

$7.01 \times 10^{-7}$ ;  $3.51 \times 10^{-6}$ ,  $4.73 \times 10^{-7}$ ,  $2.25 \times 10^{-7}$  (quoted lit., calculated-UNIFAC; GC-RT correlation, Delle Site 1997)

$1.54 \times 10^{-5}$ ;  $1.39 \times 10^{-6}$  (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_S$  with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/\text{Pa}) = 12.17 - 5371/(T/K)$  (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 10.71 - 4465/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$5.90 \times 10^{-6}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/\text{Pa}) = -4755/(T/K) + 10.72$ ;  $\Delta H_{vap.} = -91.0 \text{ kJ}\cdot\text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

0.009 (15°C, calculated, Baker & Eisenreich 1990)

0.0079 (10°C, estimated, McLachlan et al. 1990)

0.034\* (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)

0.074 (wetted wall column-GC, Altschuh et al. 1999)

$\log [H/(\text{Pa m}^3/\text{mol})] = 12.02 - 3558/(T/K)$  (Passivirta et al. 1999)

0.035 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 1.732 - 1927/(T/K)$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

6.04 (Radding et al. 1976)

6.31 (Smith et al. 1978)

5.99, 5.78 (calculated-fragment const., Hansch & Leo 1979)

6.34 (Steen & Karickhoff 1981)

6.50 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)

6.20 (shake flask-GC, Hanai et al. 1982)

5.85–5.12; 5.88–6.04; 5.99,  $6.00 \pm 0.1$  (23°C, shake flask- concentration ratio/UV spec.; shake flask-HPLC/UV; exptl. mean value, recommended value; Mallon & Harris 1984)

6.74, 7.77, 7.99 (HPLC-RT correlation, Sarna et al. 1984)

6.42 (HPLC-RT correlation, Rapaport et al. 1984)

5.97 (Hansch & Leo 1985)

6.78 (HPLC-RT correlation, Webster et al. 1985)

6.04 (HPLC-RT correlation, Wang et al. 1986)

6.44 (TLC retention time correlation, De Voogt et al. 1990)

6.35 (recommended, Sangster 1993)

5.97 (recommended, Hansch et al. 1995)

- 6.02 ± 0.19, 6.14 ± 0.71 (HPLC- $k'$  correlation: ODS column; Diol column, Helweg et al. 1997)  
 6.13 (5.91–6.28) (slow stirring-HPLC/fluorescence, De Maagd et al. 1998)  
 6.27 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)

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

- 10.80 (calculated- $K_{OW}/K_{AW}$ , Wania & Mackay 1996)  
 10.77 (calculated, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.09; 2.22; 3.45 (steady-state, bluegills; midge larva; periphyton, Leversee et al. 1981)  
 4.74 (*P. hoyi*, Eadie et al. 1982)  
 3.90 (*Daphnia magna*, McCarthy 1983)  
 3.69, 4.45 (*Lepomis macrochirus*, bluegill sunfish, Spacie et al., 1983)  
 4.00 (activated sludge, Freitag et al. 1984)  
 3.42 (bluegills, McCarthy & Jimenez 1985)  
 2.35, 2.45 (bluegills-with dissolved humic material, McCarthy & Jimenez 1985)  
 2.68, 3.52, 4.0 (fish, algae, activated sludge, Freitag et al. 1985)  
 3.51 (worms, Frank et al. 1986)  
 6.95, 6.51 (*P. hoyi* of Lake Michigan interstitial waters, Landrum et al. 1985)  
 3.34 (*P. hoyi* of Government Pond of Grand Haven in Michigan, Landrum et al. 1985)  
 2.69 (Gobas et al. 1987)  
 4.11 (*Daphnia magna*, Newsted & Giesy 1987)  
 3.77 (10–20°C, *H. limbata*, Landrum & Poore 1988)  
 4.61, 3.86, 3.87 (4°C, *P. hoyi*, *S. heringianus*, *Mysis relicta*, Landrum & Poore 1988)  
 4.69, 3.93 (calculated for amphipods and mysids, Evans & Landrum 1989)  
 3.22–3.59; 2.96–3.32 (*Daphnia magna* in natural waters with humic substances, measured range; predicted range, Kokkonen et al. 1989)  
 1.140, –0.155 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)  
 6.22, 6.04; 3.68, 5.01, 4.90, 5.15 (oligochaetes; chironomid larvae, Bott & Standley 2000)

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

- 5.95 (Aldrich humic acid, RP-HPLC separation, Landrum et al. 1984)  
 4.59, 4.72, 4.26 (humic materials in natural water: Huron River 6.1% OC winter, Grand River 10.7% DOC spring, Lake Michigan 5.5% DOC spring, RP-HPLC separation method, Landrum et al. 1984)  
 6.66 (LSC, Eadie et al. 1990)  
 6.26 (sediments average, Kayal & Connell 1990)  
 8.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)  
 7.0 (Rotterdam Harbor sediment 4.6% OC, batch sorption equilibrium, Hegeman et al. 1995)  
 6.00, 6.28, 6.17; 5.81 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island; quoted lit., McGroddy & Farrington 1995)  
 5.93 (Aldrich humic acid, Ozretich et al. 1995)  
 6.54 (10°C), 6.46, 6.60 (20°C), 6.14 (35°C), 6.07, 6.09 (45°C) (log  $K_{DOC}$  - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)  
 6.30 (20°C, log  $K_{POC}$  - particulate organic material from lake, Lüers & ten Hulscher 1996)  
 6.27; 6.30 (humic acid, HPLC- $k'$  correlation; quoted lit., Nielsen et al. 1997)  
 5.72, 5.89, 5.51 (pH 5, 6.5, 8, humic acid from sediments of River Arno, De Paolis & Kukkonen 1997)  
 4.81, 4.87, 4.49 (pH 5, 6.5, 8, fulvic acid from sediments of River Arno, De Paolis & Kukkonen 1997)  
 5.54, 5.59, 5.37 (pH 5, 6.5, 8, HA + FA extracted from sediments of River Arno, De Paolis & Kukkonen 1997)  
 5.51, 5.74, 5.68 (pH 5, 6.5, 8, HA extracted from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)  
 4.93, 4.84, 4.85 (pH 5, 6.5, 8, FA extracted from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)  
 5.66, 5.46, 5.60 (pH 5, 6.5, 8, HA + FA from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)  
 5.22, 5.46, 5.60 (pH 5, 6.5, 8, HA extracted from water of River Arno, De Paolis & Kukkonen 1997)  
 4.67, 4.80, 4.45 (pH 5, 6.5, 8, FA extracted from water of River Arno, De Paolis & Kukkonen 1997)  
 5.21, 5.29, 5.18 (pH 5, 6.5, 8, HA + FA extracted from water of River Arno, De Paolis & Kukkonen 1997)  
 4.62, 4.52, 4.61 (pH 5, 6.5, 8, FA extracted from water of Tyrrhenian Sea, De Paolis & Kukkonen 1997)

- 5.99 (5.92–6.04), 5.53 (5.43–5.61) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 5.25–6.18 (Lake Michigan sediment, Kukkonen & Landrum 1998)
- 5.48–5.69, 5.56, 5.55, 5.49, 5.30 (log  $K_{\text{DOC}}$ : humic acid from Lake Hohlohsee in Black Forest, soil leachate, fulvic acid from brown coal-derived production effluent, fulvic acid from groundwater, fulvic acid from effluent of a waste water plant near Karlsruhe, Haitzer et al. 1999)
- 5.53 (Clay Creek sediment with organic matter content 0.45%, Bott & Standley. 2000)
- 6.23 (sediment: organic carbon OC -0.5%, average, Delle Site 2001)
- 6.39–8.17; 6.30–8.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 3.12; 6.67, 6.58, 6.79 (20°C, batch equilibrium method, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 6.15; 6.34 (Plym river sediment; plym sea sediment, batch equilibrium-LSC, Turner & Rawling 2002)
- 6.49; 6.31 (Carnon river sediment; Carnon sea sediment, batch equilibrium-LSC, Turner & Rawling 2002)

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

- Volatilization: aquatic fate rate of 300  $\text{h}^{-1}$  with  $t_{1/2} = 22$  h (Callahan et al. 1979);  
 half-lives predicted by one compartment model:  $t_{1/2} = 140$  h in river water,  $t_{1/2} = 350$  h in eutrophic pond,  $t_{1/2} = 700$  h in eutrophic lake and oligotrophic lake (Smith et al. 1978);  
 calculated  $t_{1/2} = 1500$  h for a river of 1-m deep with water velocity of 0.5  $\text{m s}^{-1}$  and wind velocity of 1  $\text{m/s}$  (Southworth 1979; Herbes et al. 1980);  
 sublimation rate constant from glass surface of  $< 1 \times 10^{-5} \text{ s}^{-1}$  was measured at 24°C at an airflow rate of 3 L/min (Cope & Kalkwarf 1987).
- Photolysis: photolysis  $t_{1/2} = 2$  h in methanol solution when irradiated at 254 nm (Lu et al. 1977);  
 $k = 0.58 \text{ h}^{-1}$  for winter at midday at 40°N latitude (Smith et al. 1978);  
 direct photochemical transformation  $t_{1/2}(\text{calc}) = 0.54$  h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis  $t_{1/2} = 3.2$  d and 13 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)
- $k(\text{aq.}) = 2.8 \times 10^{-4} \text{ s}^{-1}$  with  $t_{1/2} = 1\text{--}2$  h (Callahan et al. 1979)  
 photolytic  $t_{1/2}(\text{aq}) = 0.53$  h (quoted of EPA Report 600/7-78-074, Haque et al. 1980)  
 $k = 1.30 \text{ h}^{-1}$  (Zepp 1980)
- half-lives predicted by one compartment model:  $t_{1/2} = 3.0$  h in river water based on the photolysis rates estimated for summer sunlight,  $t_{1/2} = 7.5$  h in eutrophic pond or eutrophic lake, and  $t_{1/2} = 1.5$  h in oligotrophic lake (Smith et al. 1978; quoted, Harris 1982)
- $k = 2.8 \times 10^{-4} \text{ s}^{-1}$  with  $t_{1/2} = 1\text{--}2$  h (Callahan et al., 1979)  
 calculated direct photolysis  $k = 3.86 \times 10^{-4} \text{ s}^{-1}$  in late January with  $t_{1/2} = 0.69$  h in pure water at 366 nm and in sunlight at 23–28°C and  $k = 1.05 \times 10^{-5} \text{ s}^{-1}$  in mid-December with  $t_{1/2} = 1.1$  h at 313 nm with 1–20% acetonitrile as cosolvent in filter-sterilized natural water (Mill et al. 1981)  
 $t_{1/2} = 0.37\text{--}1.1$  h, based on estimated photolysis half-life in air (Howard et al. 1991)  
 sunlight photolysis  $t_{1/2} = 0.045$  d for mid-December (Mill & Mabey 1985)  
 half-lives on different atmospheric particulate substrates (approx. 25  $\mu\text{g/g}$  on substrate):  $t_{1/2} = 4.7$  h on silica gel,  $t_{1/2} = 1.4$  h on alumina and  $t_{1/2} = 31$  h on fly ash (Behymer & Hites 1985)  
 ozonation rate constant  $k < 6.1 \times 10^{-4} \text{ m/s}$  was measured at 24°C with  $[\text{O}_3] = 0.16$  ppm and light intensity of 1.3  $\text{kW/m}^2$  (Cope & Kalkwarf 1987)  
 first order daytime decay  $k = 0.0090 \text{ min}^{-1}$  for soot particles loading of 1000–2000  $\text{ng/mg}$  and  $k = 0.0211 \text{ min}^{-1}$  with 30–350  $\text{ng/mg}$  loading (Kamens et al. 1988)  
 photodegradation half-life was found ranging from 1 h in summer to days in winter (Valerio et al. 1991)  
 photodegradation  $k = 0.0322 \text{ min}^{-1}$  and  $t_{1/2} = 0.35$  h in ethanol-water (3:7, v/v) solution for initial concentration of 2.5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)  
 pseudo-first-order direct photolysis  $k(\text{exptl}) = 0.0322 \text{ min}^{-1}$  with the calculated  $t_{1/2} = 0.35$  h and the predicted  $t_{1/2} = 0.0416 \text{ min}^{-1}$  calculated by QSPR method, in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)  
 direct photolysis  $t_{1/2}(\text{obs}) = 0.50$  h,  $t_{1/2}(\text{calc}) = 0.57$  h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)

photochemical degradation under atmospheric conditions:  $k = (1.18 \pm 0.50) \times 10^{-4} \text{ s}^{-1}$  and  $t_{1/2} = (1.63 \pm 0.48) \text{ h}$  in diesel particulate matter, rate constant  $k = (3.09 \pm 0.23) \times 10^{-5} \text{ s}^{-1}$  and  $t_{1/2} = (6.22 \pm 0.51) \text{ h}$  in diesel particulate matter/soil mixture, and  $t_{1/2} = 0.35$  to  $1.62 \text{ h}$  in various soil components using a 900-W photo-irradiator as light source; rate constant  $k = (2.92 \pm 0.20) \times 10^{-5} \text{ s}^{-1}$  and  $t_{1/2} = (6.59 \pm 0.49) \text{ h}$  in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation  $k = 2.1 \times 10^{-3} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

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

$t_{1/2} > 340 \text{ h}$  in river water, eutrophic pond or lake and oligotrophic lake, half-lives predicted by one compartment model (Smith et al. 1978)

$k(\text{aquatic fate rate}) = 1680 \text{ M}^{-1} \text{ s}^{-1}$ , with half-life of 96 h (Callahan et al. 1979)

$t_{1/2} = 1500 \text{ h}$  for photosensitized oxygenation with singlet oxygen at near-surface natural water,  $40^\circ\text{N}$ , midday, midsummer (Zepp & Schlotzhauer 1979)

$k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $2 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982)

$k = 0.62 \times 10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  for the reaction with  $\text{O}_3$  in water at pH 7 and  $25^\circ\text{C}$  with  $t_{1/2} = 1.0 \text{ s}$  in presence of  $10^{-4} \text{ M}$  of ozone at pH 7 (Butković et al. 1983)

$k(\text{aq.}) = 3.6 \times 10^{-4} \text{ h}^{-1}$  with  $t_{1/2} = 0.5 \text{ h}$  under natural sunlight conditions;  $k(\text{aq.}) = 1.9 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$  with  $t_{1/2} = 4.3 \text{ d}$  free-radicals oxidation in air-saturated water (NRCC 1983)

photooxidation  $t_{1/2} = 0.428\text{--}4.28 \text{ h}$ , based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

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

Hydrolysis: not hydrolyzable (Mabey et al. 1982; Howard et al. 1991).

Biodegradation:

$t_{1/2} > 10000 \text{ h}$  (quoted, Smith et al. 1978)

$k = 0.2\text{--}0.9 \mu\text{mol}^{-1} \text{ mg}^{-1}$  for bacterial protein (Callahan et al. 1979)

$k = 3.4 \times 10^{-4} \text{ h}^{-1}$  with  $t_{1/2} = 83 \text{ h}$  for mixed bacterial populations in stream sediment (NRCC 1983)

$k < 3 \times 10^{-5} \text{ h}^{-1}$  with  $t_{1/2} > 2.5 \text{ yr}$ ;  $k < 3.0 \times 10^{-5} \text{ h}^{-1}$  with  $t_{1/2} > 2.5 \text{ yr}$  for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)

$k = 3.5 \times 10^{-5} \text{ h}^{-1}$  estimated in water and soil (Ryan & Cohen 1986)

$t_{1/2}(\text{aq. aerobic}) = 57 \text{ d}$  to  $1.45 \text{ yr}$  at  $10\text{--}30^\circ\text{C}$ , soil die-away test (Coover & Sims 1987; quoted, Howard et al. 1991);  $k = 0.0022 \text{ d}^{-1}$  with  $t_{1/2} = 309 \text{ d}$  for Kidman sandy loam and  $k = 0.0030 \text{ d}^{-1}$  with  $t_{1/2} = 229 \text{ d}$  for McLaren sandy loam all at  $-0.33 \text{ bar}$  soil moisture (Park et al. 1990)

$t_{1/2}(\text{aq. anaerobic}) = 228 \text{ d}$  to  $5.8 \text{ yr}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Coover & Sims 1987; quoted, Howard et al. 1991).

Biotransformation: estimated to be  $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

$k_1 = 49 \text{ h}^{-1}$ ;  $k_2 = 0.010 \text{ h}^{-1}$  (bluegill sunfish, Spacie et al. 1983)

$k_1 = 131.1 \text{ mL g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0033 \text{ h}^{-1}$  ( $4^\circ\text{C}$ , *P. hoyi*, Landrum 1988)

$k_1 = 81.3 \text{ h}^{-1}$ ;  $k_2 = 0.014 \text{ h}^{-1}$  ( $10\text{--}20^\circ\text{C}$ , *H. limbata*, Landrum & Poore 1988)

$k_1 = 16.8 \text{ h}^{-1}$ ;  $k_2 = 0.0016 \text{ h}^{-1}$  ( $4^\circ\text{C}$ , *P. hoyi*, Landrum & Poore 1988)

$k_1 = 87.8 \text{ h}^{-1}$ ;  $k_2 = 0.012 \text{ h}^{-1}$  ( $4^\circ\text{C}$ , *S. heringianus*, quoted, Landrum & Poore 1988)

$k_1 = 112.0 \text{ h}^{-1}$ ;  $k_2 = 0.013 \text{ h}^{-1}$  ( $4^\circ\text{C}$ , *Mysis relicta*, quoted, Landrum & Poore 1988)

$k_1 = 75.9 \text{ mL g}^{-1} \text{ h}^{-1}$  (*Pontoporeia hoyi*, Evans & Landrum 1989)

$k_1 = 39.9 \text{ mL g}^{-1} \text{ h}^{-1}$  (*Mysis relicta*, Evans & Landrum 1989)

$k_2 = 0.0017 \text{ h}^{-1}$  (*Amphipods*, Evans & Landrum 1989)

$k_2 = 0.0047 \text{ h}^{-1}$  (*Mysids*, Evans & Landrum 1989)

$k_1 = 0.11\text{--}0.36 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0032 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.37\text{--}1.1 \text{ h}$ , based on estimated photolysis half-life (Lyman et al. 1982; quoted, Howard et al. 1991);

half-lives under simulated atmospheric conditions:  $t_{1/2} = 5.30 \text{ h}$  in simulated sunlight,  $t_{1/2} = 0.58 \text{ h}$  in simulated sunlight + ozone (0.2 ppm),  $t_{1/2} = 0.62 \text{ h}$  in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 14 \text{ h}$  with a steady-state concn of tropospheric ozone of  $2 \times 10^{-9} \text{ M}$  in clean air (Butković et al. 1983);



- photooxidation  $t_{1/2} = 0.428\text{--}4.28$  h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- $t_{1/2} = 0.5$  h for adsorption on soot particles in an outdoor Teflon chamber with an estimated  $k = 0.0234 \text{ min}^{-1}$  at  $1 \text{ cal cm}^{-2} \text{ min}^{-1}$ ,  $10 \text{ g m}^{-3} \text{ H}_2\text{O}$  and  $20^\circ\text{C}$  (Kamens et al. 1988).
- Surface Water:  $t_{1/2} = 2$  h in methanol solution irradiated at  $254 \text{ nm}$  (Lu et al. 1977);
- half-lives predicted by one compartment model:  $t_{1/2} > 340$  h in river water, eutrophic pond or lake and oligotrophic lake (Smith et al. 1978);
- very slow, not an important process (Callahan et al. 1979);
- computed near-surface half-life for direct photochemical transformation of a natural water body  $t_{1/2} = 0.54$  h at latitude  $40^\circ\text{N}$ , midday, midsummer, and direct photolysis,  $t_{1/2} = 3.2$  d (no sediment-water partitioning) and  $t_{1/2} = 13$  d (with sediment-water partitioning) in a 5-m deep inland water body (Zepp & Schlottzauer 1979);
- $t_{1/2} = 0.37\text{--}1.1$  h, based on photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991);
- $t_{1/2} = 1.0$  s in presence of  $10^{-4} \text{ M}$  of ozone at pH 7 (Butković et al. 1983);
- $t_{1/2} = 4.3$  d free-radical oxidation in air-saturated water (NRCC 1983);
- $t_{1/2} = 0.045$  d under mid-December sunlight (Mill & Mabey 1985);
- photolysis  $t_{1/2} = 0.35$  h in aqueous solution when irradiated with a  $500 \text{ W}$  medium pressure mercury lamp (Chen et al. 1996).
- Groundwater:  $t_{1/2} = 2736\text{--}25440$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Sediment: uptake clearance from sediment  $k = (0.0023 \pm 0.001) \text{ g of dry sediment} \cdot \text{g}^{-1} \text{ of organism} \cdot \text{h}^{-1}$  for amphipod, *P. hoyi* in Lake Michigan sediments at  $4^\circ\text{C}$  (Landrum 1989);
- desorption  $t_{1/2} = 19.5$  d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
- Soil:  $t_{1/2} > 2$  d (Sims & Overcash 1983; quoted, Bulman et al. 1987);
- $t_{1/2} = 347$  d for  $5 \text{ mg/kg}$  treatment and  $t_{1/2} = 218$  d for  $50 \text{ mg/kg}$  treatment (Bulman et al. 1987);
- biodegradation  $k = 0.002 \text{ d}^{-1}$  with  $t_{1/2} = 309$  d for Kidman sandy loam soils and  $k = 0.0030 \text{ d}^{-1}$  with  $t_{1/2} = 229$  d for McLaurin sandy loam soils (Park et al. 1990);
- $t_{1/2} = 1368\text{--}12720$  h, based on aerobic soil dieaway test data at  $10\text{--}30^\circ\text{C}$  (Groenewegen & Stolp 1976; Coover & Sims 1987; quoted, Howard et al. 1991);
- $t_{1/2} > 50$  d (Ryan et al. 1988);
- $t_{1/2} = 0.3$  to  $> 300$  wk,  $8.2$  yr (literature, Luddington soil, Wild et al. 1991).
- Biota: depuration  $t_{1/2} = 18$  d by oysters (Lee et al. 1978; quoted, Verschueren 1983);
- $t_{1/2} = 67$  h in bluegill sunfish (Spacie et al. 1983);
- depuration  $t_{1/2} = 52$  h in *s. heringianus* (Frank et al. 1986);
- calculated half-lives in different tissues of sea bass:  $t_{1/2} = 12.4$  d for fat,  $t_{1/2} = 6.5$  d for kidney,  $t_{1/2} = 5.1$  d for kidney,  $t_{1/2} = 5.1$  d for intestine,  $t_{1/2} = 4.8$  d for gallbladder,  $t_{1/2} = 4.5$  d for spleen,  $t_{1/2} = 2.9$  d for muscle,  $t_{1/2} = 2.4$  d for whole body,  $t_{1/2} = 2.3$  d for gonads,  $t_{1/2} = 2.3$  d for gills, and  $t_{1/2} = 2.2$  d for liver (Lemaire et al. 1990);
- elimination  $t_{1/2} = 4.8\text{--}16$  d from mussel *Mytilus edulis*;  $t_{1/2} = 7$  d from polychaete *Abarenicola pacifica*,  $t_{1/2} = 21.7$  d from Oyster,  $t_{1/2} = 8.0$  d from clam *Mercenaria mercenaria*,  $t_{1/2} = 8$  d from clam *Rangia cuneata* (quoted, Meador et al. 1995);
- $t_{1/2} = 15\text{--}17$  d for blue mussel *Mytilus edulis* in 32-d exposure laboratory studies (Magnusson et al. 2000).

TABLE 4.1.1.43.1

Reported aqueous solubilities and Henry's law constants of benzo[a]pyrene at various temperatures

$$\ln x = A + B/(T/K) + C \cdot \ln (T/K)$$

(1)

Aqueous solubility						Henry's law constant	
May et al. 1983		Velapoldi et al. 1983		Whitehouse 1984		ten Hulscher et al. 1992	
generator column-HPLC		generator column-fluorescence		generator column-HPLC		gas stripping-HPLC/fluorescence	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	Pa m <sup>3</sup> /mol
10	0.00056	10	0.00061	8.0	0.00066	10.0	0.022
15	0.00080	15	0.00082	12.4	0.00077	20.0	0.034
20	0.00114	20	0.00113	16.7	0.00094	35.0	0.074
25	0.00162	25	0.00158	20.9	0.00116	40.1	0.092
30	0.00229	30	0.00224	25.0	0.00154	45.0	0.110
						55.0	0.239
		eq. 1	x				
		A	-677.4109				
		B	23963.0				
		C	100.767				
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.6$					
		at 25°C					
						$\ln K_{\text{AW}} = -\Delta H/RT + \Delta S/R$	
						$R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$	
						$\Delta S/R = 11.90$	
						$\Delta H/R = 4690.88$	
						enthalpy of volatilization:	
						$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 39 \pm 3$	
						entropy of volatilization, $\Delta S$ :	
						$T\Delta S/(\text{kJ} \cdot \text{mol}^{-1}) = 29 \pm 3$	
						at 20°C	

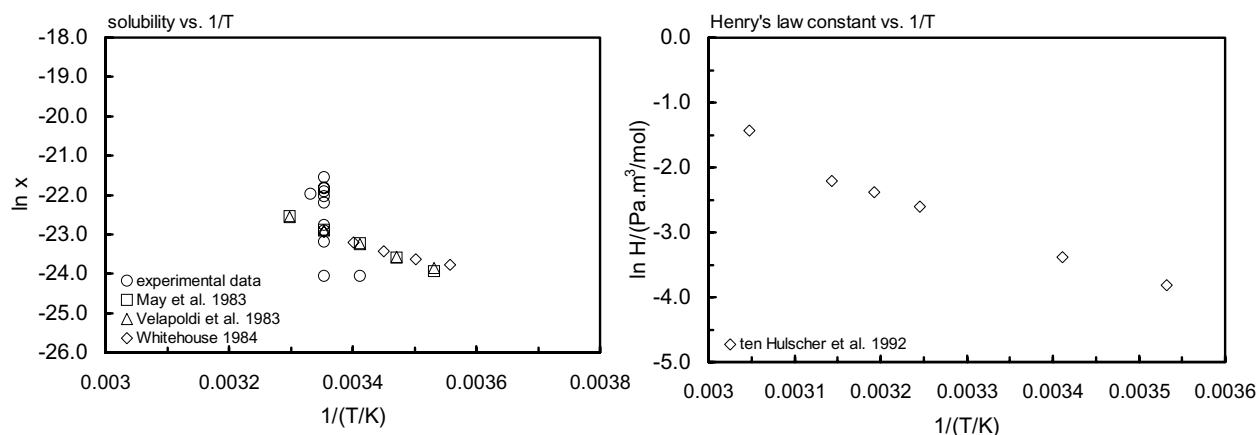
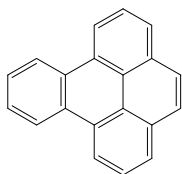


FIGURE 4.1.1.43.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for benzo[a]pyrene.

## 4.1.1.44 Benzo[e]pyrene



Common Name: Benzo[e]pyrene

Synonym: B[e]P, 4,5-benzopyrene

Chemical Name: 4,5-benzopyrene

CAS Registry No: 192-97-2

Molecular Formula:  $C_{20}H_{12}$

Molecular Weight: 252.309

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

181.4 (Lide 2003)

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

311 (Lide 2003)

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

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

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

16.57 (exptl., Chickos et al. 1999)

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

42.30 (differential scanning calorimetry, Hinckley et al. 1990)

36.5 (Passivirta et al. 1999)

Fugacity Ratio at  $25^{\circ}\text{C}$  (assuming  $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$ ), F: 0.0292 (mp at  $181.4^{\circ}\text{C}$ )

0.010 (calculated, Passivirta et al. 1999)

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

0.0035 ( $27^{\circ}\text{C}$ , shake flask-nephelometry, Davis et al. 1942)

0.00732 (shake flask-UV/fluorescence, Barone et al. 1967)

0.00014, 0.000172, 0.0000252 (HPLC-relative retention correlation, different stationary and phases, Locke 1974)

0.0050\* ( $23^{\circ}\text{C}$ , shake flask-fluorescence, measured range  $8.6\text{--}31.7^{\circ}\text{C}$ , Schwarz 1977)

0.00732, 0.004; 0.0063 (quoted values; lit. mean, Pearlman et al. 1984)

$\log S_L$  ( $\text{mol}/\text{L}$ ) =  $-1.398 - 866.8/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$\ln x = -11.8754 - 2916.84/(T/K)$ ; temp range  $5\text{--}50^{\circ}\text{C}$  (regression eq. of literature data, Shiu & Ma 2000)

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

$7.40 \times 10^{-7}$  (Knudsen effusion method, extrapolated, Murray et al. 1974)

$\log (P/\text{mmHg}) = 9.736 - 6220/(T/K)$ ; temp range  $359\text{--}423 \text{ K}$  (Knudsen effusion method, Murray et al. 1974)

$7.58 \times 10^{-7}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 11.7417 - 6220/(T/K)$ ; temp range  $358\text{--}423 \text{ K}$  (Antoine eq., Stephenson & Malanowski 1987)

$3.20 \times 10^{-7}$ ,  $1.28 \times 10^{-5}$  ( $20^{\circ}\text{C}$ , literature solid  $P_s$ , converted to supercooled liquid  $P_L$  with  $\Delta S_{\text{fus}}$  Bidleman & Foreman 1987)

$8.59 \times 10^{-5}$  ( $P_{\text{GC}}$ , GC-RT correlation with  $p,p'$ -DDT as reference standard, Hinckley et al. 1990)

$2.53 \times 10^{-5}$ ,  $1.02 \times 10^{-5}$  (supercooled liquid values  $P_L$ , converted from literature  $P_s$  with different  $\Delta S_{\text{fus}}$  values, Hinckley et al. 1990)

$\log (P_L/\text{Pa}) = 11.11 - 4803/(T/K)$  (GC-RT correlation, Hinckley et al. 1990)

$1.29 \times 10^{-5}$  (supercooled liquid values  $P_L$ , calculated from Yamasaki et al. 1984, Finizio et al. 1997)

$1.78 \times 10^{-5}$ ;  $1.78 \times 10^{-6}$  (quoted supercooled liquid  $P_L$  from Hinckley et al. 1990; converted to solid  $P_s$  with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.15 - 5333/(T/K)$  (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 10.14 - 4467/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ( $Pa\ m^3/mol$  at  $25^\circ C$  and reported temperature dependence equations):

0.02 (calculated-P/C, Mackay et al. 1992)

$\log [H/(Pa\ m^3/mol)] = 11.64 - 3660/(T/K)$  (Passivirta et al. 1999)

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

6.44 (calculated-MCI  $\chi$  as per Rekker & De Kort 1979, Ruepert et al. 1985)

7.40 (calculated- $K_{OC}$ , Broman et al. 1991)

6.44 (TLC retention time correlation, De Voogt et al. 1990)

6.44 (recommended, Sangster 1993)

6.10 (quoted, Meador et al. 1995)

5.68 (calculated, Passivirta et al. 1999)

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

11.13 (calculated, Finizio et al. 1997)

Bioconcentration Factor,  $\log BCF$ :

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

7.20 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)

4.00 (predicted dissolved  $\log K_{OC}$ , Broman et al. 1991)

6.11–7.90; 7.20–8.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

5.84; 6.12, 6.11, 6.62  $20^\circ C$ , batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants or Half-Lives:

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

$k_1 = 0.13\text{--}0.36\ mg\ g^{-1}\ h^{-1}$ ;  $k_2 = 0.0031\ h^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: half-lives under simulated atmospheric conditions:  $t_{1/2} = 21.10\ h$  in simulated sunlight,  $t_{1/2} = 5.38\ h$  in simulated sunlight + ozone (0.2 ppm),  $t_{1/2} = 7.6\ h$  in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: elimination  $t_{1/2} = 6.9\text{--}14.4\ d$  from mussel *Mytilus edulis*;  $t_{1/2} = 30.1\ d$  from Oyster,  $t_{1/2} = 4.7\ d$  from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

**TABLE 4.1.1.44.1**

**Reported aqueous solubilities of benzo[e]pyrene at various temperatures**

Schwarz 1977

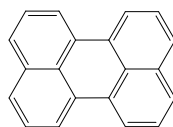
shake flask-fluorescence

$t/^\circ C$	$S/g\cdot m^{-3}$
8.6	$3.25 \times 10^{-3}$
14.0	$3.58 \times 10^{-3}$
17.0	$4.44 \times 10^{-3}$
17.5	$3.94 \times 10^{-3}$

**TABLE 4.1.1.44.1** (*Continued*)

Schwarz 1977	
shake flask-fluorescence	
<i>t</i> /°C	<i>S</i> /g·m <sup>-3</sup>
20.2	$4.79 \times 10^{-3}$
23.2	$5.35 \times 10^{-3}$
23.0	$5.07 \times 10^{-3}$
29.2	$6.38 \times 10^{-3}$
29.2	$6.48 \times 10^{-3}$
31.7	$6.81 \times 10^{-3}$
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 25.56$	
at 25°C	

## 4.1.1.45 Perylene



Common Name: Perylene

Synonym: peri-dinaphthalene

Chemical Name: perylene

CAS Registry No: 198-55-0

Molecular Formula:  $C_{20}H_{12}$

Molecular Weight: 252.309

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

277.76 (Lide 2003)

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

503 (Pearlman et al. 1984)

Density ( $g/cm^3$  at  $25^{\circ}C$ ):

1.35 (Lide 2003)

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

186.9 ( $25^{\circ}C$ , calculated-density)

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

23.51 (quoted, Tsonopoulos & Prausnitz 1971)

31.753 (Ruelle & Kesselring 1997)

31.88 (exptl., Chickos et al. 1999)

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

42.68 (quoted, Tsonopoulos & Prausnitz 1971)

57.4 (Passivirta et al. 1999)

67.87, 43.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.00331 (mp at  $277.76^{\circ}C$ )

0.00268 (calculated, Passivirta et al. 1999)

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

0.0005 ( $27^{\circ}C$ , shake flask-nephelometry Davis et al. 1942)

< 0.0005 (Weimer & Prausnitz 1965)

0.00011 ( $20^{\circ}C$ , shake flask-UV, Eisenbrand & Baumann 1970)

0.0004 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0003 (average lit. value, Pearlman et al. 1984)

0.0007 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)

$\log [S_L/(mol/L)] = -0.306 - 1662/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

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

$\log (P/mmHg) = 13.95 - 7260/(T/K)$ ; temp range  $110-180^{\circ}C$  (Knudsen effusion method, Hoyer & Peperle 1958)

$5.31 \times 10^{-9}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 13.075 - 7260/(T/K)$ ; temp range  $383-453 K$  (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 12.9379 - 7210/(T/K)$ ; temp range  $383-516 K$  (Antoine eq.-II, Stephenson & Malanowski 1987)

$7.00 \times 10^{-7}$  (quoted, Riederer 1990)

$1.84 \times 10^{-8*}$  (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range  $118-210^{\circ}C$ , Oja & Suuberg 1998)

$\ln (P/Pa) = 35.702 - 15955/(T/K)$ ; temp range  $391-424 K$  (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)

$1.40 \times 10^{-8}$ ;  $5.22 \times 10^{-6}$  (quoted solid  $P_s$  from Mackay et al. 1992; converted to supercooled liquid  $P_L$  with fugacity ratio  $F$ , Passivirta et al. 1999)

$\log (P_s/Pa) = 12.53 - 6074/(T/K)$  (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.53 - 4414/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$4.88 \times 10^{-6}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -4694/(T/K) + 10.43$ ;  $\Delta H_{vap} = -89.9 \text{ kJ}\cdot\text{mol}^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at  $25^\circ\text{C}$  and the report temperature dependence equations):

0.440 (calculated-P/C, Riederer 1990)

$\log [H/(\text{Pa m}^3/\text{mol})] = 9.84 - 2752/(T/K)$ , (Passivirta et al. 1999)

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

6.30, 5.10 (HPLC-RV predicted, Brooke et al. 1986)

5.30 (HPLC-RV measured, Brooke et al. 1986)

5.82 (HPLC-RT correlation, Wang et al. 1986)

6.25 (recommended, Sangster 1989, 1994)

6.40 (Bayona et al. 1991)

5.82 (recommended, Hansch et al. 1995)

6.50 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

6.25; 6.53 (quoted lit.; calculated, Passivirta et al. 1999)

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

Bioconcentration Factor,  $\log BCF$ :

3.86, 3.73 (*Daphnia pulex*, kinetic estimation, Southworth et al. 1978)

4.36 (activated sludge, Freitag et al. 1984)

3.30, 4.36, < 1.0 (algae, activated sludge, fish, Klein et al. 1984)

3.85 (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

3.30, 4.36, < 1.0 (algae, activated sludge, fish, Freitag et al. 1985)

3.86 (*Daphnia magna*, Newsted & Giesy 1987)

1.196, -0.398 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient,  $\log K_{oc}$  at  $25^\circ\text{C}$  or as indicated:

6.39–7.93 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)  
5.88; 6.73, 6.63, 6.76 ( $20^\circ\text{C}$ , batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

6.30; 5.89; 4.15–6.38 (calculated- $K_{ow}$ ; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)

6.05 at pH 4, 5.98 at pH 7, 5.71 at pH 10 in 0.001 M NaCl; 6.01 at pH 4, 5.95 at pH 7, 5.29 at pH 10 in 0.01 M NaCl; 5.98 at pH 4, 5.67 at pH 7, 4.86 at pH 10 in 0.1 M NaCl; 5.97 at pH 4, 5.61 at pH 7, 4.78 at pH 10 in 1 mM  $\text{Ca}^{2+}$  in 0.1 M total ionic strength solutions (shake flask/fluorescence, dissolved humic substances-humic acid; Schlautman & Morgan 1993)

5.17 at pH 4 in 0.001 M NaCl; 5.14 at pH 4 in 0.01 M NaCl; 5.08 at pH 4 in 0.1 M NaCl; 5.11 at pH 4 in 1 mM  $\text{Ca}^{2+}$  in 0.1 M total ionic strength solutions (shake flask/fluorescence, dissolved humic substances-fulvic acid; Schlautman & Morgan 1993a, b)

5.82 at pH 4, < 4.49 at pH 7, < 4.18 at pH 10 in 0.001 M NaCl; 5.65 at pH 4, < 4.46 at pH 7, < 3.85 at pH 10 in 0.01 M NaCl; 5.67 at pH 4, < 4.17 at pH 7, < 3.78 at pH 10 in 0.1 M NaCl; 5.74 at pH 4, 5.02 at pH 7, 4.43 at pH 10 in 1 mM  $\text{Ca}^{2+}$  in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substances-humic acid; Schlautman & Morgan 1993b)

< 3.48 at pH 4 in 0.001 M NaCl; < 3.30 at pH 4 in 0.01 M NaCl; < 3.48 at pH 4 in 0.1 M NaCl; < 3.48 at pH 4 in 1 mM  $\text{Ca}^{2+}$  in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substances-fulvic acid; Schlautman & Morgan 1993b)

6.00 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

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

Volatilization: sublimation  $k < 1 \times 10^{-5} \text{ s}^{-1}$  from glass surface was measured at  $24^\circ\text{C}$  at an airflow rate of 3 L/min (Cope & Kalkwarf 1987).

## Photolysis:

half-lives on different atmospheric particulate substrates (appr.  $25 \mu\text{g/g}$  on substrate):  $t_{1/2} = 3.9 \text{ h}$  on silica gel,  $t_{1/2} = 1.2 \text{ h}$  on alumina and  $t_{1/2} = 35 \text{ h}$  on fly ash (Behymer & Hites 1985)

ozonation  $k < 4.7 \times 10^{-5} \text{ m/s}$  was measured from glass surface at  $24^\circ\text{C}$  with  $[\text{O}_3] = 0.16 \text{ ppm}$  and light intensity of  $1.3 \text{ kW/m}^2$  (Cope & Kalkwarf 1987)

photodegradation  $k = 0.0152 \text{ min}^{-1}$  and  $t_{1/2} = 0.78 \text{ h}$  in ethanol-water (2:3, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

$k(\text{expt}) = 0.0152 \text{ min}^{-1}$  the pseudo-first-order rate constant with the calculated  $t_{1/2} = 0.78 \text{ h}$  and the predicted  $k = 0.0406 \text{ min}^{-1}$ , calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

$t_{1/2} = 0.53 \text{ h}$  (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001)

Photodegradation  $k = 4.4 \times 10^{-4} \text{ s}^{-1}$  in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

## Hydrolysis:

## Oxidation:

## Biodegradation:

## Biotransformation:

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

$k_1 = 752 \text{ h}^{-1}$ ;  $k_2 = 0.139 \text{ h}^{-1}$  (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.88 \text{ h}^{-1}$ ;  $\log k_2 = -0.86 \text{ h}^{-1}$  (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 0.12\text{--}0.38 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0034 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

## Half-Lives in the Environment:

Air: direct photolysis  $t_{1/2} = 0.53 \text{ h}$  (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis  $t_{1/2} = 0.78 \text{ h}$  (reported in units of minutes) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

## Groundwater:

## Sediment:

## Soil:

Biota: elimination half-lives:  $t_{1/2} = 2.0 \text{ d}$  from rainbow trout,  $t_{1/2} = 26.2 \text{ d}$  from clam *Mya arenaria*,  $t_{1/2} = 6.3\text{--}13.3 \text{ d}$  from mussel *Mytilus edulis*;  $t_{1/2} = 9.2 \text{ d}$  from Oyster,  $t_{1/2} = 1.2 \text{ d}$  from shrimp,  $t_{1/2} = 5.7 \text{ d}$  from polychaete *Nereis virens*,  $t_{1/2} = 8.0 \text{ d}$  from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.45.1

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

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

Hoyer & Peperle 1958		Oja & Suuberg 1998	
effusion		Knudsen effusion	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
data presented by equation		124.10	0.0114
eq. 1	P/mmHg	127.37	0.0164
A	13.95	131.82	0.0249
B	7260	135.96	0.0373



TABLE 4.1.1.45.1 (Continued)

Hoyer & Peperle 1958		Oja & Suuberg 1998	
effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
for temp range 110–180°C		141.87	0.0638
mp/°C	270.5–273.5	mp/K	551
$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 140.1$		eq. 1a	P/Pa
		A	35.702
		B	15955
		for temp range 391–424 K	
		$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 132.6$	

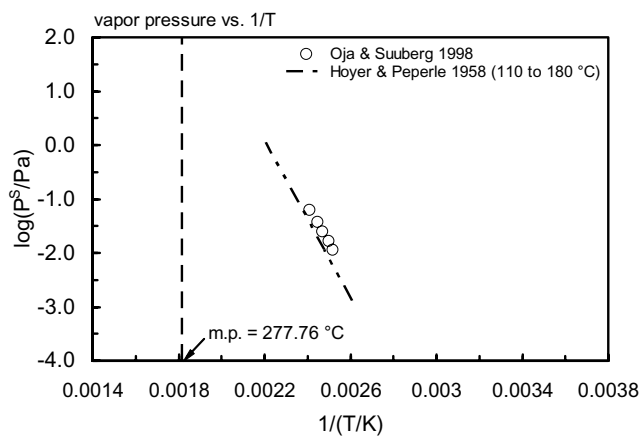
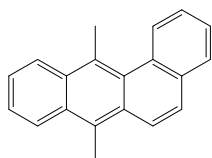


FIGURE 4.1.1.45.1 Logarithm of vapor pressure versus reciprocal temperature for perylene.

## 4.1.1.46 7,12-Dimethylbenz[a]anthracene



Common Name: 7,12-Dimethylbenz[a]anthracene

Synonym: 7,12-dimethylbenz[a]anthracene, 9,10-dimethyl-1,2-benzanthracene, 7,12-dimethylbenzanthracene

Chemical Name: 7,12-dimethylbenz[a]anthracene

CAS Registry No: 57-97-6

Molecular Formula:  $C_{20}H_{16}$

Molecular Weight: 256.341

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

122.5 (Lide 2003)

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

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

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

245.8 (Ruelle & Kesselring 1997)

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

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

104.56 (Kelley & Rice 1964)

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

22.09 (Kelley & Rice 1964)

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.111 (mp at  $122.5^{\circ}C$ )

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

0.043 ( $27^{\circ}C$ , shake flask-nephelometry, Davis et al. 1942)

0.061 (shake flask-fluorescence, Mackay & Shiu 1977)

0.053 ( $24^{\circ}C$ , shake flask-nephelometry, Hollifield 1979)

0.025 ( $24^{\circ}C$ , shake flask-LSC, Means et al. 1979)

0.0244 (shake flask-LSC, Means et al. 1980b)

0.043, 0.061, 0.053; 0.054 (quoted lit. values; lit. mean, Pearlman et al. 1984)

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

$3.73 \times 10^{-7}$  (solid vapor pressure, extrapolated, effusion method, Kelley & Rice 1974)

$3.70 \times 10^{-6}$  (extrapolated, supercooled liquid value  $P_L$ , Kelley & Rice 1974)

$\log(P_s/mmHg) = 15.108 - 7051/(T/K)$ ; temp range:  $106-122^{\circ}C$  (effusion method, Kelley & Rice 1964)

$\log(P_L/mmHg) = 12.232 - 5987/(T/K)$ ; temp range:  $122-135^{\circ}C$  (effusion method, Kelley & Rice 1964)

$3.84 \times 10^{-7}$  (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 14.233 - 7051/(T/K)$ ; temp range 379–396 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$6.78 \times 10^{-6}$  (extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.70417 - 5629.911/(T/K)$ ; temp range 379–390 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.357 - 5897/(T/K)$ , temp range 396–408 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$6.38 \times 10^{-6}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -4643/(T/K) + 10.38$ ;  $\Delta H_{vap} = -88.9$  kJ $\cdot$ mol $^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa  $m^3/mol$ ):

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

5.98 (shake flask-LSC, concn. ratio, Means et al. 1979)

5.80 (shake flask-LSC, Means et al. 1980b)

6.16	(UNIFAC activity coeff., Banerjee & Howard 1988)
5.80	(recommended, Sangster 1989)
5.89	(recommended, Sangster 1993)
5.80	(recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

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

5.68	(average of 3 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1979)
5.37	(average of 12 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1980b)

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

Volatilization:

Photolysis:

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: photooxidation  $t_{1/2} = 0.32\text{--}3.2$  h estimated, based on estimated rate constant for the reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991); photooxidation  $t_{1/2}(\text{aq.}) = 1.57\text{--}157$  yr estimated, based on measured rate constant for the reaction with singlet oxygen in benzene (Stevens et al. 1974; quoted, Howard et al. 1991).

Biodegradation: biodegradation  $k = 0.0339\text{ d}^{-1}$  with  $t_{1/2} = 20$  d for Kidman sandy loam soil and  $k = 0.0252\text{ d}^{-1}$  with  $t_{1/2} = 28$  d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2}(\text{aq. aerobic}) \sim 480\text{--}672$  h, based on aerobic soil die-away test data (Sims 1990; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) \sim 1920\text{--}2688$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.32\text{--}3.2$  h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

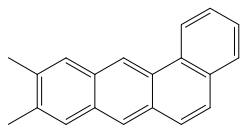
Surface water:  $t_{1/2} = 480\text{--}672$  h, based on aerobic soil die-away test data (Howard et al. 1991).

Groundwater:  $t_{1/2} = 960\text{--}1344$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation rate constant  $k = 0.0339\text{ d}^{-1}$  with  $t_{1/2} = 20$  d for Kidman sandy loam soil and  $k = 0.0252\text{ d}^{-1}$  with  $t_{1/2} = 28$  d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} \sim 480\text{--}672$  h, based on aerobic soil die-away test data (Howard et al. 1991).

**4.1.1.47 9,10-Dimethylbenz[a]anthracene**

Common Name: 9,10-Dimethylbenz[a]anthracene

Synonym:

Chemical Name: 9,10-dimethylbenz[a]anthracene

CAS Registry No: 56-56-4

Molecular Formula: C<sub>20</sub>H<sub>16</sub>

Molecular Weight: 256.341

Melting Point (°C):

122 (Yalkowsky et al. 1983; Ruelle & Kesselring 1997)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

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

245.8 (Ruelle & Kesselring 1997)

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

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

54.81 (Kelley & Rice 1974)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.112 (mp at 122°C)

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C or as indicated):

0.0435 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.0435 (recommended, Shaw 1989)

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

log (P/mmHg) = 15.108 – 7051/(T/K); temp range: 106–135°C (effusion method, Kelley & Rice 1964)

log (P/mmHg) = 12.232 – 5897/(T/K) (liquid, effusion method, Kelley & Rice 1964)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

6.93 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

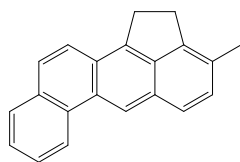
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K<sub>OC</sub>:

Environmental Fate Rate Constants, k or Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

## 4.1.1.48 3-Methylcholanthrene



Common Name: 3-Methylcholanthrene

Synonym: 20-methylcholanthrene, 1,2-dihydro-3-methyl-benz[j]aceanthrylene

Chemical Name: 3-methylcholanthrene

CAS Registry No: 56-49-5

Molecular Formula:  $C_{21}H_{16}$

Molecular Weight: 268.352

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

180 (Bjørseth 1983)

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

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

1.28 (Lide 2003)

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

247.8 (Ruelle & Kesselring 1997)

209.6 ( $20^{\circ}C$ , calculated-density)

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0301 (mp at  $180^{\circ}C$ )

0.003 (Mackay et al. 1980)

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

0.0015 (Weimer & Prausnitz 1965)

0.0029 (shake flask-fluorescence, Mackay & Shiu 1977)

0.00323 (shake flask-liquid scintillation counting, Means et al. 1980)

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

$\log(P/mmHg) = 13.168 - 6643/(T/K)$ ; temp range  $128-152^{\circ}C$  (effusion method, Kelley & Rice 1964)

$1.03 \times 10^{-7}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 12.293 - 6643/(T/K)$ ; temp range  $401-425 K$  (Antoine eq., Stephenson & Malanowski 1987)

$1.48 \times 10^{-6}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -4901/(T/K) + 10.61$ ;  $\Delta H_{vap} = -93.8 kJ \cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ( $Pa m^3/mol$ ):

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

6.42 (shake flask-LSC, Means et al. 1980)

7.11 (calculated-f const., Valvani & Yalkowsky 1980)

6.69 (calculated-S and mp, Mackay et al. 1980)

7.11 (Hansch & Leo 1985)

6.45, 7.07 (calculated-UNIFAC, calculated-fragment const., Banerjee & Howard 1988)

$6.75 \pm 0.50$  (recommended, Sangster 1989)

6.45 (recommended, Sangster 1993)

6.42 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

4.12 (*Daphnia magna*, McCarthy et al. 1985)

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

6.09 (soil/sediment, sorption isotherm by batch equilibrium-LSC, Means et al. 1980b)  
 6.25 (average of 14 soil/sediment samples, sorption isotherm by shake flask-LSC, Means et al. 1980)  
 6.09, 6.10 (calculated-regression of  $K_p$  versus substrate properties, calculated- $K_{OW}$ , Means et al. 1980)  
 4.02 (soil, calculated- $K_{OW}$ , Briggs 1981)  
 6.18 (soil, calculated- $K_{OW}$ , Means et al. 1982)  
 5.07 (soil, calculated- $K_{OW}$ , Chiou et al. 1983)

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

Volatilization:

Photolysis:

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: photooxidation  $t_{1/2} = 0.317\text{--}3.17$  h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aerobic  $t_{1/2} = 14616\text{--}33600$  h, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991);  
 anaerobic  $t_{1/2} = 58464\text{--}134400$  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:  $t_{1/2} = 0.317\text{--}3.17$  h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 14616\text{--}33600$  h, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991).

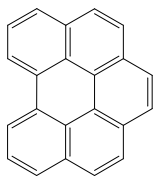
Groundwater:  $t_{1/2} = 29232\text{--}672000$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 14616\text{--}33600$  h, based on estimated mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991).

Biota:

## 4.1.1.49 Benzo[ghi]perylene



Common Name: Benzo[ghi]perylene

Synonym: 1,12-benzoperylene, benzoperylene

Chemical Name: 1,12-benzoperylene

CAS Registry No: 191-24-2

Molecular Formula:  $C_{22}H_{12}$

Molecular Weight: 276.330

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

272.5 (Lide 2003)

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

525 (Pearlman et al. 1984)

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

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

233.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

17.365 (Ruelle & Kesselring 1997)

17.37 (exptl., Chickos et al. 1999)

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

31.34, 43.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

31.4 (Passivirta et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ,  $F = 0.00373$  (mp at  $272.5^{\circ}C$ ))

0.039 (calculated,  $\Delta S_{fus} = 31.4 J/mol K$ , Passivirta et al. 1999)

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

0.00026 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0007 (generator column-HPLC/fluor., Wise et al. 1981)

0.00083 (quoted, Pearlman et al. 1984)

0.000137 (generator column-HPLC/fluor., De Maagd et al. 1998)

$\log [S_L/(mol/L)] = -2.073 - 908.7/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

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

$1.39 \times 10^{-8}$  (Knudsen effusion method, Murray et al. 1974)

$\log (P/atm) = 9.519 - 6674/(T/K)$ ; temp range: 389–468 K (Knudsen effusion method, Murray et al. 1974)

$1.33 \times 10^{-8}$  ( $20^{\circ}C$ , estimated, Callahan et al. 1979)

$6.69 \times 10^{-7}$  (Yamasaki et al. 1984)

$1.38 \times 10^{-8}$ ;  $7.51 \times 10^{-9}$  (extrapolated-Antoine eq. I, II, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 11.5247 - 6674/(T/K)$ ; temp range 389–468 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 10.945 - 6580/(T/K)$ ; temp range 391–513 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$7.20 \times 10^{-6}$ ;  $1.84 \times 10^{-6}$  (quoted solid  $P_S$  from Mackay et al. 1992; converted to supercooled liquid  $P_L$  with fugacity ratio  $F$ , Passivirta et al. 1999)

$\log (P_S/Pa) = 12.40 - 5824/(T/K)$  (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 10.76 - 4915/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$4.28 \times 10^{-7}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -5018/(T/K) + 10.46$ ;  $\Delta H_{vap} = -96.1 kJ \cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

0.027\* ( $20^\circ\text{C}$ , gas stripping-HPLC/fluorescence, measured range  $10\text{--}55^\circ\text{C}$ , ten Hulscher et al. 1992)

$\log (H/(\text{Pa m}^3/\text{mol})) = 12.83 - 4006/(T/K)$  (Passivirta et al. 1999)

0.0278 ( $20^\circ\text{C}$ , selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = -0.651 - 1258/(T/K)$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

7.10 (RP-TLC- $k'$  correlation, Bruggeman et al. 1982)

7.05 (HPLC-RT correlation, Rapaport et al. 1984)

6.63 (HPLC-RT correlation, Wang et al. 1986)

6.90 (recommended, Sangster 1989, 1993)

7.04 (TLC retention time correlation, De Voogt et al. 1990)

6.63 (recommended, Hansch et al. 1995)

6.22 (range  $5.95\text{--}6.38$ ) (shake flask/slow stirring-HPLC/fluor., De Maagd et al. 1998)

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

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

5.54 (microorganisms-water, calculated from  $K_{\text{OW}}$ , Mabey et al. 1982)

4.45 (*Daphnia magna*, Newsted & Giesy 1987)

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

6.70 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)

7.215 ( $10^\circ\text{C}$ ), 7.08, 6.93 ( $20^\circ\text{C}$ ), 6.68 ( $35^\circ\text{C}$ ), 6.46, 6.51 ( $45^\circ\text{C}$ ) ( $\log K_{\text{DOC}}$  - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)

6.80 ( $20^\circ\text{C}$ ,  $\log K_{\text{POC}}$  - particulate organic material from lake, Lüers & ten Hulscher 1996)

6.82–8.25; 6.20–9.20 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

5.87; 6.84, 6.82, 7.26 ( $20^\circ\text{C}$ , batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

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

Volatilization:

Photolysis: half-lives on different atmospheric particulate substrates (approx.  $25\text{ }\mu\text{g/g}$  on substrate):  $t_{1/2} = 7.0\text{ h}$  on silica gel,  $t_{1/2} = 22\text{ h}$  on alumina and  $t_{1/2} = 29\text{ h}$  on fly ash (Behymer & Hites 1985);

first order daytime photodegradation rate constants for adsorption on wood soot particles in an outdoor Teflon chamber:  $k = 0.0077\text{ min}^{-1}$  with  $1000\text{--}2000\text{ ng/mg}$  loading and  $k = 0.0116\text{ min}^{-1}$  with  $30\text{--}350\text{ ng/mg}$  loading (Kamens et al. 1988);

direct photolysis  $t_{1/2}(\text{obs}) = 0.89\text{ h}$ ,  $t_{1/2}(\text{calc}) = 0.86\text{ h}$  predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: rate constants  $k < 60\text{ M}^{-1}\text{ h}^{-1}$  for singlet oxygen and  $k < 6\text{ M}^{-1}\text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982); photooxidation  $t_{1/2} = 0.321\text{--}3.21\text{ h}$ , based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aerobic  $t_{1/2} = 14160\text{--}15600\text{ h}$ , based on aerobic soil die-away test data at  $10\text{--}30^\circ\text{C}$  (Coover & Sims 1987; quoted, Howard et al. 1991); anaerobic  $t_{1/2} = 56640\text{--}62400\text{ h}$ , based on aerobic soil die-away test data at  $10\text{--}30^\circ\text{C}$  (Coover & Sims 1987; quoted, Howard et al. 1991).

Biotransformation: estimated to be  $3 \times 10^{-12}\text{ mL cell}^{-1}\text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

$k_1 = 0.076\text{--}0.21\text{ mg g}^{-1}\text{ h}^{-1}$ ;  $k_2 = 0.0012\text{--}0.0014\text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)



## Half-Lives in the Environment:

Air:  $t_{1/2} = 0.321\text{--}3.21$  h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);  $t_{1/2} = 0.6$  h for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated first order rate constant  $k = 0.0179 \text{ min}^{-1}$  at  $1 \text{ cal cm}^{-2} \text{ min}^{-1}$ ,  $10 \text{ g/m}^3 \text{ H}_2\text{O}$  and  $20^\circ\text{C}$  (Kamens et al. 1988).

Surface water:  $t_{1/2} = 14160\text{--}15600$  h, based on aerobic soil die-away test data at  $10\text{--}30^\circ\text{C}$  (Coover & Sims 1987; quoted, Howard et al. 1991).

Groundwater:  $t_{1/2} = 28320\text{--}31200$  h, based on aerobic soil die-away test data at  $10\text{--}30^\circ\text{C}$  (Coover & Sims 1987; quoted, Howard et al. 1991).

Sediment:

Soil:  $t_{1/2} = 14160\text{--}15600$  h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$t_{1/2} > 50$  d (Ryan et al. 1988);

mean  $t_{1/2} = 9.1$  yr for Luddington soil (Wild et al. 1991).

Biota: elimination  $t_{1/2} = 12.4$  d from Oyster,  $t_{1/2} = 4.8$  d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

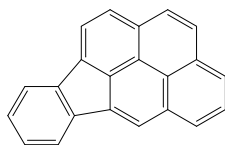
**TABLE 4.1.1.49.1**

**Reported Henry's law constants of benzo[ghi]perylene at various temperatures**

**ten Hulscher et al. 1992**

**gas stripping-HPLC/fluor.**

$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10.0	0.019
20.0	0.027
35.0	0.052
40.1	0.054
45.0	0.066
55.0	0.087
enthalpy of volatilization:	
$\Delta H_{\text{vol}}/(\text{kJ}\cdot\text{mol}^{-1}) = 26.1 \pm 1.0$	
entropy of volatilization, $\Delta S$	
$T\Delta S_{\text{vol}}/(\text{kJ}\cdot\text{mol}^{-1}) = 15.9 \pm 1.3$	
at $20^\circ\text{C}$	
$\ln K_{\text{AW}} = -\Delta H_{\text{vol}}/RT + \Delta S_{\text{vol}}/R$	
$R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$	

4.1.1.50 Indeno[1,2,3-*cd*]pyrene

Common Name: Indeno[1,2,3-*cd*]pyrene

Synonym: 2,3-*o*-phenylenepyrene,

Chemical Name: indeno[1,2,3-*cd*]pyrene

CAS Registry No: 193-39-5

Molecular Formula: C<sub>22</sub>H<sub>12</sub>

Molecular Weight: 276.330

Melting Point (°C):

162 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup>):

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

233.8 (Ruelle & Kesselring 1997, Passivirta et al. 1999)

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

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

21.51 (Chickos et al. 1999)

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

49.41, 36.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

56.5 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0453 (mp at 162°C)

0.043 (Passivirta et al. 1999)

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C and the reported temperature dependence equations):

0.00019 (generator column-HPLC/UV, Wise et al. 1981)

0.000438; 0.0023, 0.000191 (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

log [S<sub>L</sub>/(mol/L)] = -0.758 - 1631/(T/K) (supercooled liquid, Passivirta et al. 1999)

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

1.33 × 10<sup>-7</sup> (estimated, Callahan et al. 1979)

1.00 × 10<sup>-8</sup>; 2.32 × 10<sup>-7</sup> (quoted solid P<sub>s</sub> from Mackay et al. 1992; converted to supercooled liquid P<sub>L</sub> with fugacity ratio F, Passivirta et al. 1999)

log (P<sub>s</sub>/Pa) = 12.56 - 6126/(T/K) (solid, Passivirta et al. 1999)

log (P<sub>L</sub>/Pa) = 9.60 - 4839/(T/K) (supercooled liquid, Passivirta et al. 1999)

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

0.029\* (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)

log [H/(Pa m<sup>3</sup>/mol)] = 10.36 - 3208/(T/K) (Passivirta et al. 1999)

0.0285 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

log K<sub>AW</sub> = 0.033 - 1455/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

7.66 (calculated-π substituent const., Callahan et al. 1979)

8.20 (calculated, Broman et al. 1991)

6.72 (calculated, Passivirta et al. 1999)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

- 8.00 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 6.93 (10°C), 6.88, 6.84 (20°C), 6.42 (35°C), 6.32, 6.31 (45°C) ( $\log K_{DOC}$  - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
- 6.80 (20°C,  $\log K_{POC}$  - particulate organic material from lake, Lüers & ten Hulscher 1996)

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

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

$k_1 = 0.067\text{--}0.20 \text{ mg g}^{-1} \text{ h}^{-1}$ ;  $k_2 = 0.0010\text{--}0.0013 \text{ h}^{-1}$  (freshwater oligochaete from sediment, Van Hoof et al. 2001)

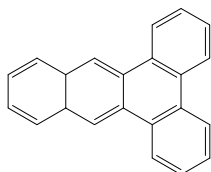
Half-Lives in the Environment:

**TABLE 4.1.1.50.1**  
**Reported Henry's law constants of indeno[123-cd]pyrene at various temperatures**

ten Hulscher et al. 1992

gas stripping-HPLC/fluor.

$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10.0	0.018
20.0	0.029
35.0	0.057
40.1	0.061
45.0	0.077
55.0	0.105
enthalpy of volatilization: $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 30.0 \pm 1.1$	
entropy of volatilization, $\Delta S$ : $T\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 19.9 \pm 1.3$	
at 20°C	
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$	
$R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$	

4.1.1.51 Dibenz[*a,c*]anthracene

Common Name: Dibenz[*a,c*]anthracene

Synonym: 1,2:3,4-Dibenzanthracene, naphtho-2',3':9,10-phenanthrene

Chemical Name: dibenz[*a,c*]anthracene

CAS Registry No: 215-58-7

Molecular Formula: C<sub>22</sub>H<sub>14</sub>

Molecular Weight: 278.346

Melting Point (°C):

205 (Bjørseth 1983; Lide 2003)

Boiling Point (°C):

518 (Weast 1982–83)

Density (g/cm<sup>3</sup> at 20°C):

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

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

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

25.82 (exptl., Chickos et al. 1999)

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

46.65, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0171 (mp at 205°C)

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

0.0016 (generator column-HPLC/UV, Billington et al. 1988)

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

1.30 × 10<sup>-9</sup>\* (effusion method, extrapolated, De Kruif 1980)

log (P/Pa) = 16.25 – 7322.2/(T/K); temp range: 152–179°C (torsion-effusion, de Kruif 1980)

log (P/Pa) = 16.011 – 7207.2/(T/K); temp range: 152–179°C (weighing-effusion, de Kruif 1980)

log (P/Pa) = 16.131 – 7265/(T/K); temp range: 152–179°C (mean, de Kruif 1980)

3.44 × 10<sup>-7</sup> (supercooled liquid P<sub>L</sub>, calibrated GC-RT correlation, Lei et al. 2002)

log (P<sub>L</sub>/Pa) = -5094/(T/K) + 10.62; ΔH<sub>vap</sub> = -97.5 kJ·mol<sup>-1</sup> (GC-RT correlation, Lei et al. 2002)

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

7.19 (calculated, Miller et al. 1985)

7.11 (calculated-MCI χ as per Rekker & De Kort 1979, Ruepert et al. 1985)

7.19 (recommended, Sangster 1989, 1993)

7.11 (TLC retention time correlation, De Voogt et al. 1990)

8.0068 (calculated-UNIFAC group contribution, Chen et al. 1993)

6.17 (recommended, Hansch et al. 1995)

6.40 ± 0.19, 6.48 ± 0.78 (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

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

6.54 (humic acid, HPLC- $k'$  correlation, Nielsen et al. 1997)

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

Half-Lives in the Environment:

Air: half-lives under simulated atmospheric conditions:  $t_{1/2} = 9.20$  h in simulated sunlight,  $t_{1/2} = 4.60$  h in simulated sunlight + ozone (0.2 ppm),  $t_{1/2} = 3.82$  h in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983).

**TABLE 4.1.1.51.1**

**Reported vapor pressures of dibenz[a,c]anthracene at various temperatures and the coefficients for the vapor pressure equations**

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

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

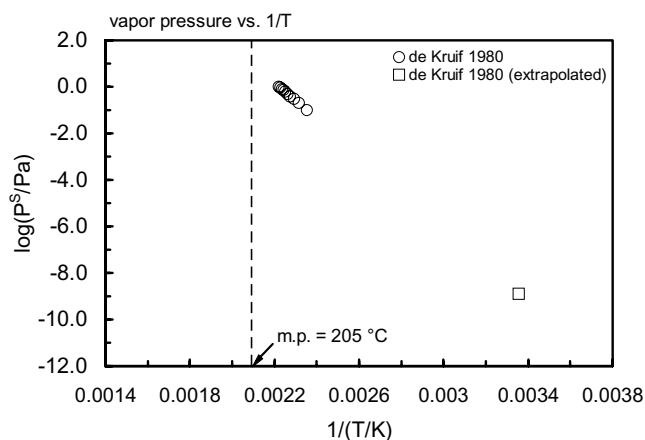
$$\log P = A - B/(C + T/K) \quad (3)$$

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

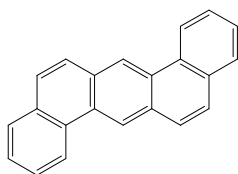
de Kruif 1980

torsion-, weighing effusion

$t/^{\circ}\text{C}$	$P/\text{Pa}$
151.65	0.1
158.52	0.2
163.08	0.3
166.38	0.4
168.97	0.5
171.11	0.6
172.94	0.7
174.53	0.8
175.95	0.9
177.22	1.0
298.15	$1.3 \times 10^{-9}$
extrapolated	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 138.0$	



**FIGURE 4.1.1.51.1** Logarithm of vapor pressure versus reciprocal temperature for dibenz[a,c]anthracene.

4.1.1.52 Dibenz[*a,h*]anthracene

Common Name: Dibenz[*a,h*]anthracene

Synonym: DB[*a,h*]A, 1,2,5,6-dibenzanthracene, 1,2:5,6-dibenzanthracene

Chemical Name: 1,2:5,6-dibenzanthracene

CAS Registry No: 53-70-3

Molecular Formula:  $C_{22}H_{14}$

Molecular Weight: 278.346

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

269.5 (Lide 2003)

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

524 (Weast 1977)

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

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

252.6 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

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

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

31.165 (Ruelle & Kesselring 1997)

31.16 (exptl., Chickos et al. 1999)

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

58.26, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

57.3 (Passivirta et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.00399 (mp at  $269.5^{\circ}C$ )

0.00389 (calculated, Passivirta et al. 1999)

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

0.0005 ( $27^{\circ}C$ , shake flask-nephelometry, Davis et al. 1942)

0.0006 (shake flask-UV, Klevens 1950)

0.0025 (shake flask-LSC, Means et al. 1980b)

0.00056 (lit. mean, Pearlman et al. 1984)

$\log [S_L/(mol/L)] = -1.409 - 1631/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

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

$1.33 \times 10^{-8}$  ( $20^{\circ}C$ , estimated, Callahan et al. 1979)

$3.70 \times 10^{-10}$ \* (effusion method, De Kruif 1980)

$\log (P/Pa) = 16.049 - 7395.4/(T/K)$ ; temp range:  $163-189^{\circ}C$  (torsion-effusion, de Kruif 1980)

$\log (P/Pa) = 15.876 - 7312/(T/K)$ ; temp range:  $163-189^{\circ}C$  (weighing-effusion, de Kruif 1980)

$\log (P/Pa) = 15.962 - 7730/(T/K)$ ; temp range:  $163-189^{\circ}C$  (mean, de Kruif 1980)

$4.25 \times 10^{-10}$  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.515 - 7420/(T/K)$ ; temp range  $403-513\ K$  (Antoine eq., Stephenson & Malanowski 1987)

$3.70 \times 10^{-10}$ ;  $9.31 \times 10^{-8}$  (quoted solid  $P_s$  from Mackay et al. 1992; converted to supercooled liquid  $P_L$  with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.82 - 5824/(T/K)$  (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.82 - 5002/(T/K)$  (supercooled liquid, Passivirta et al. 1999)

$2.51 \times 10^{-7}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -5193/(T/K) + 10.82$ ;  $\Delta H_{vap} = -99.4\ kJ\cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m<sup>3</sup>/mol at 25°C and reported temperature dependence equations):

- 0.0074 (calculated-P/C, Mabey et al. 1982)
- 0.0076 (calculated-P/C, Eastcott et al. 1988)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 11.23 - 3371/(T/K)$ , (Passivirta et al. 1999)

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

- 6.50 (shake flask-LSC, Means et al. 1980b)
- 6.88 (HPLC-RT/MS, Burkhard et al. 1985)
- 5.80 (Hansch & Leo 1985)
- 6.75 ± 0.40 (recommended, Sangster 1989, 1993)
- 7.11 (TLC retention time correlation, De Voogt et al. 1990)
- 6.60 (shake flask-UV, pH 7.4, Alcorn et al. 1993)
- 6.50 (recommended, Hansch et al. 1995)
- 6.54 ± 0.19, 6.60 ± 0.78 (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)

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

Bioconcentration Factor,  $\log BCF$ :

- 5.84 (microorganisms-water, calculated from  $K_{OW}$ , Mabey et al. 1982)
- 4.63 (activated sludge, Freitag et al. 1984)
- 3.38, 4.63, 1.0 (algae, activated sludge, fish, Freitag et al. 1985)
- 4.00 (*Daphnia magna*, Newsted & Giesy 1987)

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

- 6.31 (average of 14 soil/sediment samples, equilibrium sorption isotherms by shake flask-LSC, Means et al. 1980b)
- 6.22, 6.18 (calculated-regression of  $k_p$  versus substrate properties, calculated- $K_{OW}$ , Means et al. 1980b)
- 6.22; 6.11, 5.30, 5.62 (quoted; calculated- $K_{OW}$ , calculated-S and mp, calculated-S, Karickhoff 1981)
- 6.52 (calculated- $K_{OW}$ , Mabey et al. 1982)
- 5.20 (calculated, Pavlou 1987)
- 6.31; 6.44; 3.75–5.77 (soil, quoted exptl.; calculated-MCI  $^1\chi$ , calculated- $K_{OW}$  range, Sabljic 1987a,b)
- 5.77 (soil, calculated- $K_{OW}$  based on model of Karickhoff et al. 1979, Sabljic 1987b)
- 5.66 (soil, calculated- $K_{OW}$  based on model of Means et al. 1982, Sabljic 1987b)
- 4.60 (soil, calculated- $K_{OW}$  based on model of Chiou et al. 1983, Sabljic 1987b)
- 4.61 (soil, calculated- $K_{OW}$  based on model of Kenaga 1980, Sabljic 1987b)
- 3.75 (soil, calculated- $K_{OW}$  based on model of Briggs 1981, Sabljic 1987b)
- 6.22 (calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 6.44 (humic acid, HPLC-k' correlation, Nielsen et al. 1997)
- 6.00; 6.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
- 6.76–8.42; 5.80–8.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 6.03; 7.0, 6.76, 7.32 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

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

Volatilization:

- Photolysis: atmospheric and aqueous photolysis  $t_{1/2} = 782$  h, based on measured rate of photolysis in heptane under November sunlight (Muel & Saguim 1985; quoted, Howard et al. 1991) and  $t_{1/2} = 6$  h after adjusting the ratio of sunlight photolysis in water versus heptane (Smith et al. 1978; Muel & Saguim 1985; quoted, Howard et al. 1991);
- pseudo-first-order direct photolysis rate constant  $k(\text{exptl}) = 0.014 \text{ min}^{-1}$  with the calculated  $t_{1/2} = 0.83$  h and the predicted  $k = 0.0216 \text{ min}^{-1}$  calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);
- direct photolysis  $t_{1/2}(\text{obs.}) = 0.31$  h,  $t_{1/2} = 0.38$  h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Oxidation: rate constant  $k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $k = 1.5 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$  for peroxy radical (Mabey et al. 1982);

photooxidation  $t_{1/2} = 0.428\text{--}4.28 \text{ h}$ , based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aerobic  $t_{1/2} = 8664\text{--}22560 \text{ h}$ , based on aerobic soil die-away test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);

$k = 0.0019 \text{ d}^{-1}$  with  $t_{1/2} = 361 \text{ d}$  for Kidman sandy loam and  $k = 0.0017 \text{ d}^{-1}$  with  $t_{1/2} = 420 \text{ d}$  for McLarin sandy loam all at  $-0.33 \text{ bar}$  soil moisture (Park et al. 1990).

Biotransformation: estimated to be  $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$  for bacteria (Mabey et al. 1982).

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

#### Half-Lives in the Environment:

Air: half-lives under simulated atmospheric conditions:  $t_{1/2} = 9.6 \text{ h}$  in simulated sunlight,  $t_{1/2} = 4.8 \text{ h}$  in simulated sunlight + ozone (0.2 ppm),  $t_{1/2} = 2.71 \text{ h}$  in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 0.428\text{--}4.28 \text{ h}$ , based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 6\text{--}782 \text{ h}$ , based on sunlight photolysis half-life in water (Smith et al. 1978; Muel & Saguem 1985; quoted, Howard et al. 1991);

photolysis  $t_{1/2} = 0.83 \text{ h}$  in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996).

Groundwater:  $t_{1/2} = 17328\text{--}45120 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation rate constant  $k = 0.0019 \text{ d}^{-1}$  with  $t_{1/2} = 361 \text{ d}$  for Kidman sandy loam soil and  $k = 0.117 \text{ d}^{-1}$  with  $t_{1/2} = 420 \text{ d}$  for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} \sim 8664\text{--}22560 \text{ h}$ , based on aerobic soil dieaway test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);

mean  $t_{1/2} = 20.607 \text{ wk}$  (quoted, Wild et al. 1991).

Biota:

**TABLE 4.1.1.52.1**

**Reported vapor pressures of dibenz[a,h]anthracene 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)		

**de Kruif 1980**

**torsion-, weighing effusion**

$t/^{\circ}\text{C}$	$P/\text{Pa}$
160.38	0.1
168.21	0.2
172.93	0.3
176.33	0.4
179.01	0.5
181.22	0.6
183.11	0.7
184.76	0.8



TABLE 4.1.1.52.1 (Continued)

de Kruif 1980	
torsion-, weighing effusion	
t/°C	P/Pa
186.22	0.9
187.54	1.0
25.0	$3.7 \times 10^{-10}$
	extrapolated
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 140.0$	

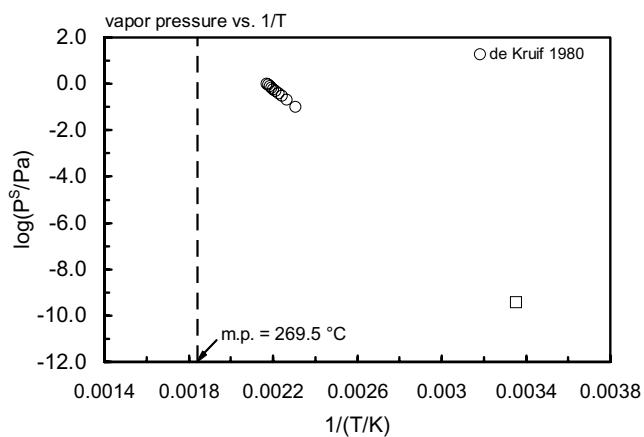
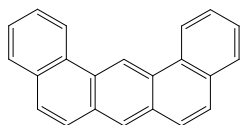


FIGURE 4.1.1.52.1 Logarithm of vapor pressure versus reciprocal temperature for dibenz[a,h]anthracene.

**4.1.1.53 Dibenz[*a,j*]anthracene**

Common Name: Dibenz[*a,j*]anthracene

Synonym: 1,2:7,8-dibenzanthracene, 1,2:7,8-dibenzanthracene, *a,a'*-dibenzanthracene, dinaphthanthracene

Chemical Name: dibenz[*a,j*]anthracene

CAS Registry No: 58-70-3

Molecular Formula: C<sub>22</sub>H<sub>14</sub>

Molecular Weight: 278.346

Melting Point (°C):

197.5 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

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

222.8 (Ruelle & Kesselring 1997)

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

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

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

Fugacity Ratio at 25°C (assuming  $\Delta S = 56$  J/mol K), F: 0.0203 (mp at 197.5°C)

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C or as indicated):

0.012 (27°C, shake flask-nephelometry, Davis et al. 1942; quoted, Shaw 1989)

0.012 (quoted, Yalkowsky et al. 1983; Pearlman et al. 1984)

0.000041, 0.00022 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C):

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

7.19 (calculated-fragment const., Yalkowsky et al. 1983)

7.11 (calculated-MCI  $\chi$  as per Rekker & De Kort 1979, Ruepert et al. 1985)

7.11 (TLC retention time correlation, De Voogt et al. 1990)

7.11 (quoted and recommended, Sangster 1993)

6.54 ± 0.19, 6.44 ± 0.75 (HPLC-*k'* correlation: ODS column; Diol column, Helweg et al. 1997; quoted, Nielsen et al. 1997)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

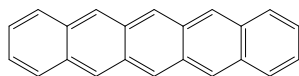
Sorption Partition Coefficient, log K<sub>oc</sub>:

6.58 (humic acid, HPLC-*k'* correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, *k* or Half-Lives, *t*<sub>1/2</sub>:

Half-Lives in the Environment:

## 4.1.1.54 Pentacene



Common Name: Pentacene

Synonym: 2,3,6,7-dibenzanthracene, 2,3:6,7-dibenzanthracene

Chemical Name: pentacene

CAS Registry No: 135-48-8

Molecular Formula:  $C_{22}H_{14}$

Molecular Weight: 278.346

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

270–271 (Weast 1982–83)

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

290–300 (sublimation, Weast 1982–83)

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

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

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

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

35.19 (Chickos et al. 1999)

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

55.22, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F: 0.00395 (mp at  $270^{\circ}C$ )

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

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

$1.0 \times 10^{-13}$ \* (effusion method, De Kruif 1980)

$\log(P_s/kPa) = 12.725 - 8260/(T/K)$ ; temp range 444–566 K (Antoine eq., Stephenson & Malanowski 1987)

$1.19 \times 10^{-12}$ \* (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range  $170$ – $210^{\circ}C$ , Oja & Suuberg 1998)

$\log(P/Pa) = 35.823 - 18867/(T/K)$ ; temp range 443–483 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

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

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

7.19 (calculated-f const., Miller et al. 1985)

7.19 (recommended, Sangster 1989, 1993)

7.11 (TLC retention time correlation, De Voogt et al. 1990)

8.0068 (calculated-UNIFAC group contribution, Chen et al. 1993)

7.19 (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,  $t_{1/2}$ :

Half-Lives in the Environment:

TABLE 4.1.1.54.1

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

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<b>de Kruif 1980</b>		<b>Oja &amp; Suuberg 1998</b>	
<b>torsion-, weighing effusion</b>		<b>Knudsen effusion</b>	
<b>t/°C</b>	<b>P/Pa</b>	<b>t/°C</b>	<b>P/Pa</b>
220.51	0.1	171.33	0.00161
229.8	0.2	184.8	0.00413
235.4	0.3	185.99	0.00421
239.45	0.4	190.98	0.00760
242.63	0.5	200.29	0.0171
245.27	0.6	203.1	0.0157
247.51	0.7	212.6	0.0515
249.47	0.8		
251.22	0.9	mp/K	> 573
252.79	1.0		
25.0	$1.0 \times 10^{-13}$	eq. 1a	P/Pa
	extrapolated	A	35.823
		B	18823
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 155.0$		for temp range 443–483 K	
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 155.9$	

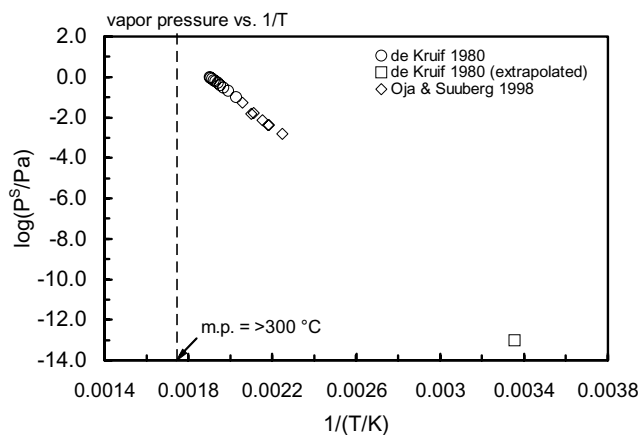
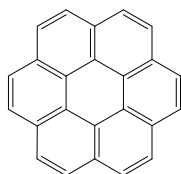


FIGURE 4.1.1.54.1 Logarithm of vapor pressure versus reciprocal temperature for pentacene.

## 4.1.1.55 Coronene



Common Name: Coronene

Synonym: hexabenzobenzene

Chemical Name: coronene

CAS Registry No: 191-07-1

Molecular Formula:  $C_{24}H_{12}$

Molecular Weight: 300.352

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

437.4 (Lide 2003)

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

525 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$  at  $25^{\circ}C$ ):

1.371 (Lide 2003)

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

244.8 (Ruelle & Kesselring 1997)

219.1 ( $25^{\circ}C$ , calculated-density)

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

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

19.202 (Ruelle & Kesselring 1997)

19.2 (exptl., Chickos et al. 1999)

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

27.02, 42.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ),  $F: 8.99 \times 10^{-5}$  (mp at  $437.4^{\circ}C$ )

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

0.00014 (shake flask-fluorescence, Mackay & Shiu 1977)

0.00014 (average lit. value, Pearlman et al. 1984)

0.00010 (generator column-HPLC/UV, Billington et al. 1988)

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):

$\log(P/mmHg) = 12.62 - 7675/(T/K)$ ; temp range  $160\text{--}240^{\circ}C$  (Knudsen effusion method, Hoyer & Peperle 1958)

$1.95 \times 10^{-10}$  (Knudsen effusion method, extrapolated, Murray et al. 1974)

$\log(P/atm) = 9.110 - 7100/(T/K)$ ; temp range  $427\text{--}510\ K$  (Knudsen effusion method, Murray et al. 1974)

$2.00 \times 10^{-10}$  (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.1157 - 7100/(T/K)$ ; temp range  $427\text{--}510\ K$  (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.886 - 5764/(T/K)$ ; temp range not specified (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.318 - 5362/(T/K)$ ; temp range not specified (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$2.89 \times 10^{-10}$ \* (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range  $148\text{--}231^{\circ}C$ , Oja & Suuberg 1998)

$\log(P/Pa) = 31.72 - 16006/(T/K)$ ; temp range  $421\text{--}504\ K$  (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

$2.55 \times 10^{-8}$  (supercooled liquid  $P_L$ , calibrated GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -5446/(T/K) + 10.67$ ;  $\Delta H_{vap} = -104.2\ kJ\cdot mol^{-1}$  (GC-RT correlation, Lei et al. 2002)

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

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

7.64	(average lit. value, Yalkowsky et al. 1983)
7.64	(calculated-MCI $\chi$ as per Rekker & De Kort 1979, Ruepert et al. 1985)
8.20, 6.70	(HPLC-RV correlation, different mobile phases, Brooke et al. 1986)
5.40	(shake flask/slow stirring-GC, Brooke et al. 1986)
6.50	(recommended, Sangster 1989, 1993)
7.64	(TLC retention time correlation, De Voogt et al. 1990)
8.0	(calculated- $K_{\text{OC}}$ , Broman et al. 1991)
5.40, 6.70	(Hansch et al. 1995)

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

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

7.80	(Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
5.0	(predicted dissolved $\log K_{\text{OC}}$ , Broman et al. 1991)

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

Half-Lives in the Environment:

Soil: mean  $t_{1/2} = 16.5$  yr for Luddington soil (Wild et al. 1991).

**TABLE 4.1.1.55.1**

**Reported vapor pressures of coronene 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)		

Hoyer & Peperle 1958		Murray et al. 1974		Oja & Suuberg 1998	
effusion		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
data presented by equation		data presented by graph and		147.9	0.00191
eq. 1	P/mmHg	eq. 1	P/atm	163.6	0.00686
A	12.62	A	9.110	178.1	0.0236
B	7676	B	7100	196.9	0.0895
for temp range 160–240°C		for temp range 427–510 K		109.9	0.222
				210.0	0.309
$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 147.0$		25.0	$2.0 \times 10^{-10}$	231.11	0.927
			extrapolated		
				mp/K	711
		mp/°C	~440		
				eq. 1a	P/Pa
		$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 135.9$		A	31.72
		at av. temp measurements		B	16006
				temp range 421–504 K	
				$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 133.1$	

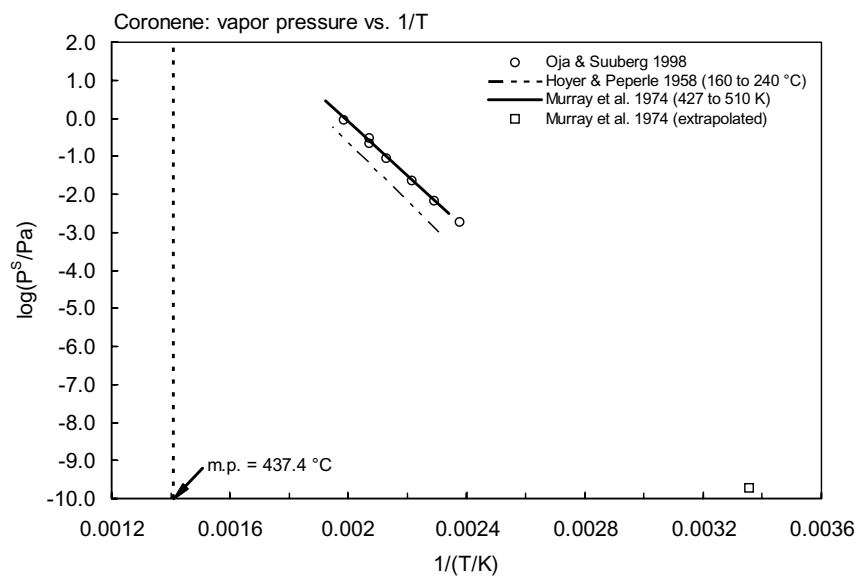
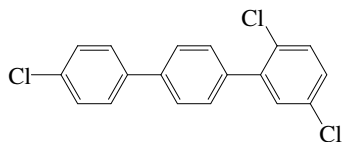


FIGURE 4.1.1.55.1 Logarithm of vapor pressure versus reciprocal temperature for coronene.

### 4.1.2 CHLORINATED POLYNUCLEAR AROMATIC HYDROCARBONS

#### 4.1.2.1 2,4'',5-Trichloro-*p*-terphenyl



Common Name: 2,4'',5-Trichloro-*p*-terphenyl

Synonym:

Chemical Name:

CAS Registry No: 61576-93-0

Molecular Formula: C<sub>18</sub>H<sub>11</sub>Cl<sub>3</sub>

Molecular Weight: 333.639

Melting Point (°C):

92 (Dickhut et al. 1994)

Boiling Point (°C):

Density (g/cm<sup>3</sup>):

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

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

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

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

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.22 (mp at 92°C)

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C or as indicated):

3.8 × 10<sup>-4</sup>; 3.37 × 10<sup>-4</sup> (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)  
1.01 × 10<sup>-4</sup>, 6.56 × 10<sup>-4</sup>, 8.56 × 10<sup>-4</sup> (5, 25, 30°C, generator column-GC, Dickhut et al. 1994)

Vapor Pressure (Pa at 25°C):

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

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

Octanol/Air Partition Coefficient, log K<sub>oa</sub>:

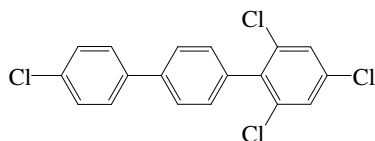
Bioconcentration Factor, log BCF or log K<sub>B</sub>:

Sorption Partition Coefficient, log K<sub>oc</sub>:

Environmental Fate Rate Constants, k and Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:



4.1.2.2 2,4,4'',6-Tetrachloro-*p*-terphenyl

Common Name: 2,4,4'',6-Tetrachloro-*p*-terphenyl

Synonym:

Chemical Name:

CAS Registry No:

Molecular Formula:  $C_{18}H_{11}Cl_4$

Molecular Weight: 368.084

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

114 (Dickhut et al. 1994)

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

Density ( $g/cm^3$ ):

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

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.134 (m.p at  $114^{\circ}C$ )

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

$1.79 \times 10^{-4}$ ;  $7.91 \times 10^{-5}$  (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)

$5.91 \times 10^{-5}$ ,  $1.74 \times 10^{-4}$ ,  $4.07 \times 10^{-4}$  (5, 25,  $40^{\circ}C$ , generator column-GC, Dickhut et al. 1994)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

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,  $\log BCF$  or  $\log K_B$ :

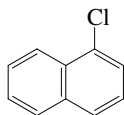
Sorption Partition Coefficient,  $\log K_{OC}$ :

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

Half-Lives in the Environment:

### 4.1.3 POLYCHLORINATED NAPHTHALENES

#### 4.1.3.1 1-Chloronaphthalene



Common Name: 1-Chloronaphthalene

Synonym: PCN-1,  $\alpha$ -chloronaphthalene

Chemical Name: 1-chloronaphthalene

CAS Registry No: 90-13-1

Molecular Formula:  $C_{10}H_7Cl$

Molecular Weight: 162.616

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

−2.5 (Lide 2003)

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

259 (Lide 200)

Density ( $g/cm^3$ ):

1.1938 ( $20^{\circ}C$ , Weast 1982–83; Windholz 1983; Budavari 1989)

1.1976, 1.1938 ( $15^{\circ}C$ ,  $20^{\circ}C$ , Riddick et al. 1986)

1.188 ( $25^{\circ}C$ , Lide 2003)

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

136.2 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

22.4 (shake flask-fluorescence, Mackay & Shiu 1981)

19.0; 8.93 (quoted; calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

2.87 (quoted, Crookes & Howe 1993, Alcock et al. 1999)

6.75; 36.3 (quoted exptl value; calculated-molar volume, Wang et al. 1992)

19.1; 25.8 (quoted; calculated-group contribution method, Kühne et al. 1995)

19.1; 25.2 (quoted; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

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

133.3\* ( $80.6^{\circ}C$ , static-Hg manometer, measured range  $80.6$ – $269.3^{\circ}C$ , Kahlbaum 1898)

133.3\* ( $80.6^{\circ}C$ , summary of literature data, temp range  $80.6$ – $269.3^{\circ}C$ , Stull 1947)

3.055 (extrapolated from Antoine eq., temp range  $353$ – $533 K$ , Stephenson & Malanowski 1987)

$\log (P/kPa) = 6.15143 - [1861.65/(T/K - 83.337)]$ ; temp range:  $353$ – $533 K$  (Antoine eq., Stephenson & Malanowski 1987)

2.133 (estimated, Crookes & Howe 1993)

$1.2 \times 10^{-4}$  (estimated, Alcock et al. 1999)

3.597, 3.84 (calibrated GC-RT correlation, GC-RT correlation,  $P_L$  supercooled liquid values, Lei et al. 1999)

$\log (P_L/Pa) = -3058/(T/K) + 10.81$  (HPLC-RT correlation, Lei et al. 1999)

5.588 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log (P_L/Pa) = -3054/(T/K) + 9.97$ ; (regression with GC-RT from literature, supercooled liquid, Lei et al. 1999)

6.89\* ( $23.15^{\circ}C$ , transpiration method, measured range  $289.1$ – $332.3 K$ , Verevkin 2003)

$\ln (P/P^\circ) = 299.001/R - 83941.481/R \cdot (T/K) - (73.5/R) \cdot \ln[(T/K)/298.15]$ , where  $P^\circ = 101.325$  kPa, gas constant  $R = 8.31451$  J·K<sup>-1</sup>·mol<sup>-1</sup> (vapor pressure eq. from transpiration measurement, temp range 289.1–332.3 K, Verevkin 2003)

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25°C):

- 35.5 (gas stripping-GC, Mackay & Shiu 1981)  
36.3 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, log  $K_{OW}$  at 25°C and the reported temperature dependence equations:

- 3.80 (HPLC-k'correlation, Hanai et al. 1981)  
4.08 (calculated-fragment constant, Yalkowsky et al. 1983)  
3.90 (shake flask, Opperhuizen 1987)  
4.08 (estimated, Abernethy & Mackay 1987)  
3.80 (calculated-molar volume, Wang et al. 1992)  
4.24 (recommended, Hansch et al. 1995)  
4.0; 3.97 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)  
 $\log K_{OW} = 0.841 + 940.09/(T/K)$ , temp range 5–55°C (temperature dependence HPLC-k'correlation, Lei et al. 2000)  
4.06 (GC-RT correlation, Hackenberg et al. 2003)

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

- 6.39, 6.10, 5.52, 5.30, 5.13 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)  
 $\log K_{OA} = 58300/(2.303 \cdot RT) - 4.40$ ; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, log BCF or log  $K_B$ :

- 2.28 (*Cyprinus carpio*, for monochloronaphthalenes, Matsuo 1984; quoted, Crookes & Howe 1993)

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

- 2.97 (estimated for mono-chloronaphthalenes, Crookes & Howe 1993)

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

Half-Lives in the Environment:

**TABLE 4.1.3.1.1**

**Reported vapor pressures of 1-chloronaphthalene at various temperatures and the coefficients for the vapor pressure equations**

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^\circ\text{C}) & (2) & \ln P = A - B/(C + t/^\circ\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & \ln P/P^\circ = A - B/(T/K) - C \cdot \ln [(T/K)/298.15] & (4a) \end{array}$$

Kahlbaum 1898		Stull 1947		Verevkin 2003	
static-Hg manometer		summary of lit. data		transpiration-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
80.6	133.3	80.6	133.3	15.95	3.57
104.8	666.6	104.8	666.6	5.55	1.47
118.6	1333	118.6	1333	7.15	1.75
134.7	2666	134.4	2666	13.85	3.12
140.3	2333	153.2	5333	20.05	5.29
145.1	3999	165.6	7999	23.15	6.89
149.4	4666	180.4	13332	26.05	8.43
153.0	5333	204.2	26664	30.25	11.51

(Continued)

TABLE 4.1.3.1.1 (Continued)

Kahlbaum 1898		Stull 1947		Verevkin 2003	
static-Hg manometer		summary of lit. data		transpiration-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
159.3	6666	230.8	53329	32.15	14.07
171.4	9999	269.3	101325	35.35	18.30
180.4	13332	mp/°C	-20	38.35	24.71
204.2	26664			40.35	28.10
218.3	39997			41.15	29.56
230.8	53329			44.05	35.53
240.5	66661			47.05	46.62
248.6	79993			50.15	55.93
255.5	93326			53.15	69.72
269.3	101325			56.15	84.66
				59.15	105.54
				eq. 4a	P/kPa
				P <sup>o</sup>	101.325 kPa
				A	299.011/R
				B	83941.481/R
				C	73.5/R
				R = 8.314 J K <sup>-1</sup> mol <sup>-1</sup>	
				$\Delta H_v / (\text{kJ mol}^{-1}) = 62.03$	
				at 298.15 K	

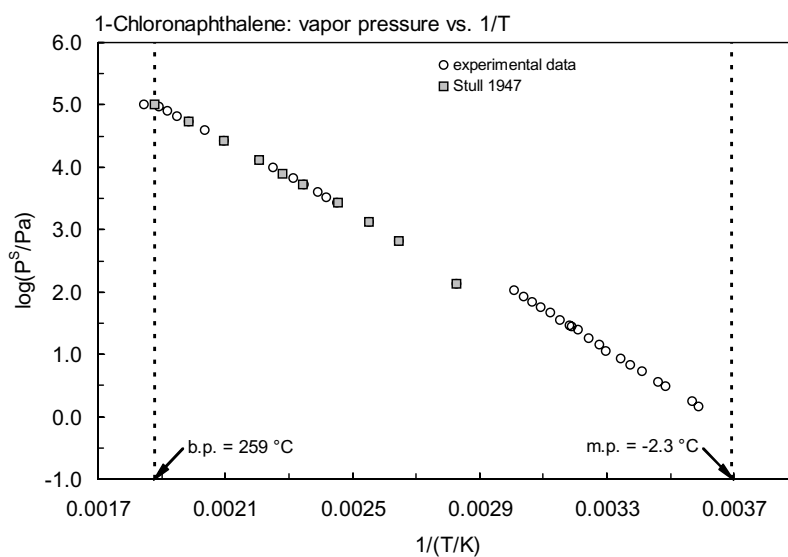
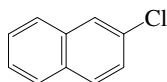


FIGURE 4.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chloronaphthalene.

## 4.1.3.2 2-Chloronaphthalene



Common Name: 2-Chloronaphthalene

Synonym: PCN-2,  $\beta$ -chloronaphthalene

Chemical Name: 2-chloronaphthalene

CAS Registry No: 91-58-7

Molecular Formula:  $C_{10}H_7Cl$

Molecular Weight: 162.616

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

58 (Lide 2003)

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

256 (Weast 1982–83; Windholz 1983; Budavari 1989; Järnberg et al. 1994; Lide 2003)

Density ( $g/cm^3$ ):

1.1377 (71 $^{\circ}C$ , Weast 1982–83; Lide 2003)

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

142.9 (71 $^{\circ}C$ , calculated from density, Stephenson & Malanowski 1987)

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

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

3.346 (Ruelle & Kesselring 1997)

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

Fugacity Ratio at 25 $^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ , F: 0.474 (mp at 58 $^{\circ}C$ ))

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

11.7 (shake flask-fluorescence, Mackay & Shiu 1981)

0.924 (shake flask, Opperhuizen et al. 1985, 1986)

8.93 (calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

16.3 (calculated-group contribution method, Kühne et al. 1995)

7.80 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

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

5.34 (supercooled liquid value, extrapolated from Antoine eq., temperature range 400–435 K, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.8608 - [3021.2/(T/K)]$ ; temp range 400–435 K (Antoine eq., Stephenson & Malanowski 1987)

3.679, 3.84 (supercooled liquid values  $P_L$ : calibrated GC-RT correlation, GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3054/(T/K) + 10.81$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

2.526 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3054/(T/K) + 9.97$  (regression with GC-RT data from literature, Lei et al. 1999)

2.301\* (24.15 $^{\circ}C$ , transpiration method, measured range 280.2–330.7 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 301.255/R - 87496.950/R \cdot (T/K) - (39.5/R) \cdot \ln[(T/K)/298.15]$ , where  $P^{\circ} = 101.325\ kPa$ , gas constant  $R = 8.31451\ J \cdot K^{-1} \cdot mol^{-1}$  (vapor pressure eq. from transpiration measurement, solid, temp range 280.2–330.7 K, Verevkin 2003)

53.71\* (59.05 $^{\circ}C$ , transpiration method, measured range 332.2–362.2 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 294.501/R - 84197.803/R \cdot (T/K) - (73.5/R) \cdot \ln[(T/K)/298.15]$ , where  $P^{\circ} = 101.325\ kPa$ , gas constant  $R = 8.31451\ J \cdot K^{-1} \cdot mol^{-1}$  (vapor pressure eq. from transpiration measurements, liquid, temp range 332.2–362.2 K, Verevkin 2003)

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

31.9 (gas stripping-GC, Mackay & Shiu 1981)

33.5 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C and the reported temperature dependence equations:

- 4.80 (calculated-fragment constant, Yalkowsky et al. 1983)
- 4.19 (HPLC-RT correlation, Opperhuizen et al. 1985, 1986)
- 4.08 (estimated, Abernethy & Mackay 1987)
- 3.98 (shake flask, Opperhuizen 1987)
- 4.07 (selected, Isnard & Lambert 1988; 1989)
- 4.6024 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 4.14 (selected, Hansch et al. 1995)
- 3.90; 3.91 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
- $\log K_{OW} = 0.821 + 924.42/(T/K)$ , temp range 5–55°C (temperature dependence HPLC- $k'$  correlation, Lei et al. 2000)

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

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

- 6.36, 6.08, 5.50, 5.28, 5.11 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
- $\log K_{OA} = 58000/(2.303 \cdot RT) - 4.40$ ; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

- 2.28 (*Cyprinus carpio*, for monochloronaphthalenes, Matsuo 1981)
- 3.63 (guppies, Opperhuizen et al. 1985)
- 3.63, 4.81 (whole fish, fish lipid, Gobas et al. 1987)
- 4.52 (guppy, lipid-weight based, Gobas et al. 1989)
- 3.63; 3.06 (quoted means; calculated- $K_{OW}$  and  $S_0$ , Banerjee & Baughman 1991)
- 3.63 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)
- 2.496, 2.721 (calculated-MCI  $\chi$ , calculated- $K_{OW}$ , Lu et al. 1999)

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

- 2.97 (estimated for monochloronaphthalenes, Crookes & Howe 1993)

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

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis: laboratory determined hydrolysis rate constant  $k = (9.5 \pm 2.8) \times 10^{-6} \text{ h}^{-1}$  at neutral conditions, calculated  $t_{1/2} = 8.3 \text{ yr}$  at pH 7 (Ellington et al. 1988).

Biodegradation:

Biotransformation:

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

- $k_1 = 7.3 \times 10^2 \text{ d}^{-1}$ ;  $k_2 = 3.1 \times 10^{-1} \text{ d}^{-1}$  (guppy, Opperhuizen et al. 1985; quoted, Connell & Hawker 1988)
- $\log k_1 = 2.83 \text{ d}^{-1}$ ;  $\log k_2 = -0.51 \text{ d}^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: experimentally measured abiotic disappearance  $t_{1/2} = 11.3 \text{ d}$  in two different soil types, a Captina silt loam (Typic Fragiudult) and McLaurin sandy loam (Typic Paleudults) (Anderson et al. 1991).

Biota:  $t_{1/2} = 2.3 \text{ d}$  (female guppies, Opperhuizen et al. 1985, quoted, Crookes & Howe 1993)

TABLE 4.1.3.2.1

Reported vapor pressures of 2-chloronaphthalene at various temperatures and the coefficients for the vapor pressure equations

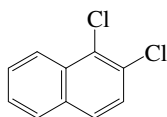
$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \ln P/P^{\circ} = A - B/(T/K) - C \cdot \ln[(T/K)/298.15] & (4a) \end{array}$$

Verevkin 2003

transpiration-GC

t/°C	P/Pa	t/°C	P/Pa
	solid		liquid
7.05	0.342	59.05	53.71
10.15	0.494	62.05	64.43
15.05	0.881	65.05	77.53
17.05	1.103	68.05	95.98
19.05	1.394	71.05	111.91
21.05	1.716	74.05	134.91
24.15	2.301	77.05	161.0
27.15	3.162	80.05	190.2
29.05	3.854	83.05	223.41
30.15	4.361	85.05	252.43
32.05	5.167	89.05	310.78
34.05	6.297		
36.05	7.569	$\Delta H_v/(\text{kJ mol}^{-1}) = 62.3 \pm 1.1$	
38.05	9.386	at 298.15 K	
40.05	10.941		
42.05	13.466	eq. 4a	P/kPa
44.04	15.786	P <sup>o</sup>	101.325 kPa
46.05	18.715	A	294.501/R
48.05	22.307	B	84197.803/R
50.05	26.990	C	73.5/R
52.05	31.158	R = 8.314 J K <sup>-1</sup> mol <sup>-1</sup>	
54.05	36.801		
56.05	43.420		
57.55	49.194		
eq. 4a	P/kPa		
P <sup>o</sup>	101.325 kPa		
A	301.255/R		
B	87496.95/R		
C	39.5/R		
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 75.72$			
at 298.15 K			

## 4.1.3.3 1,2-Dichloronaphthalene



Common Name: 1,2-Dichloronaphthalene

Synonym: PCN-3

Chemical Name: 1,2-dichloronaphthalene

CAS Registry No: 2050-69-3

Molecular Formula:  $C_{10}H_6Cl_2$

Molecular Weight: 197.061

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

36 (Lide 2003)

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

295.6 (Lide 2003)

Density ( $g/cm^3$ ): 1.3147 (49 $^{\circ}C$ , Weast 1982–83; Lide 2003)

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

156 (Ruelle & Kesselring 1997)

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

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

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

Fugacity Ratio at 25 $^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.78 (mp at 36 $^{\circ}C$ )

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

0.137 (generator column-GC/ECD, Opperhuizen 1987)

4.31 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

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

0.344; 0.333 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3172/(T/K) + 10.18$ ; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.301 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3172/(T/K) + 10.11$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25 $^{\circ}C$  and the reported temperature dependence equations:

4.40 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.42 (shake flask, Opperhuizen 1987; quoted, Sangster 1993, Crookes & Howe 1993, Hansch et al. 1995)

4.66 (selected, Alcock et al. 1999)

4.60; 4.45 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 1.064 + 1060.21/(T/K)$ , temp range 5–55 $^{\circ}C$  (temperature dependence HPLC- $k'$  correlation, Lei et al. 2000)

4.69 (GC-RT correlation, Hackenberg et al. 2003)

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

6.93 (generator column-GC, Harner & Bidleman 1998)

7.35, 7.01, 6.44, 6.13, 5.91 (10, 20, 30, 40, 50 $^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 66000/(2.303 \cdot RT) - 4.800$ ; temp range 10–50 $^{\circ}C$  (GC-RT correlation, Su et al. 2002)

6.89; 7.01 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

3.40 (fish, Opperhuizen et al. 1985)

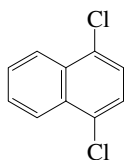
Sorption Partition Coefficient,  $\log K_{OC}$ :

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

Half-Lives in the Environment:



## 4.1.3.4 1,4-Dichloronaphthalene



Common Name: 1,4-Dichloronaphthalene

Synonym: PCN-5

Chemical Name: 1,4-dichloronaphthalene

CAS Registry No: 1825-31-6

Molecular Formula:  $C_{10}H_6Cl_2$

Molecular Weight: 197.061

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

67.5 (Lide 2003)

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

288 (Lide 2003)

Density ( $g/cm^3$ ):

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

156.0 (Ruelle & Kesselring 1997)

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

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

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

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.383 (mp at  $288^{\circ}C$ )

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

0.314 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.314 (generator column-GC/ECD, Opperhuizen et al. 1987)

4.02 (calculated-TSA, Dickhut et al. 1994)

1.98 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

0.173 (estimated, Crookes & Howe 1993)

$9.98 \times 10^{-6}$  (estimated, Alcock et al. 1999)

0.428; 0.416 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3067/(T/K) + 9.92$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.353 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3067/(T/K) + 10.17$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$  at  $25^{\circ}C$  and the reported temperature dependence equations:

4.88 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.66 (shake flask, Opperhuizen 1987; quoted, Gobas et al. 1987; 1989; Clark et al. 1990; Sangster 1993; Crookes & Howe 1993; Hansch et al. 1995; Devillers et al. 1996; Alcock et al. 1999)

4.79 (calculated, Oliver & Niimi 1984; Oliver 1987)

4.80; 4.57 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 1.269 + 1049.8/(T/K)$ , temp range  $5-55^{\circ}C$  (temperature dependence HPLC- $k'$  correlation, Lei et al. 2000)

4.56 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{oa}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations:

6.93 (generator column-GC/MS, Harner & Bidleman 1998)

7.52, 7.13, 6.72, 6.38, 6.13 (10, 20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -3.97 + 3248/(T/K)$ , temp range: 10–50°C (generator column-GC/MS, Harner & Bidleman 1998)  
6.78; 6.91 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log  $K_B$ :

3.75 (*Oncorhynchus mykiss*, Oliver & Niimi 1984)  
3.36 (female guppies, Opperhuizen et al. 1985)  
3.80 (Opperhuizen et al. 1985)  
4.04 (Opperhuizen et al. 1985)  
3.36, 4.54 (guppies: whole fish, fish lipid, Gobas et al. 1987)  
3.75 (rainbow trout, Oliver & Niimi 1984; Oliver 1987)  
5.18 (guppy, lipid-weight based, Gobas et al. 1989)  
3.36; 4.63 (quoted means; calculated- $K_{OW}$  and  $S_0$ , Banerjee & Baughman 1991)  
3.75 (*Oncorhynchus mykiss*, under flow-through condition, quoted Devillers et al. 1996)  
3.36 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log  $K_{OC}$ :

Environmental Fate Rate Constants, k and Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Photooxidation: rate constant  $k = 5.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the gas-phase reactions with OH radical at  $298 \pm 2 \text{ K}$  (Atkinson 1989).

Hydrolysis:

Biodegradation:

Biotransformation:

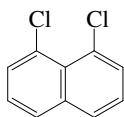
Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$k_1 = 1.2 \times 10^3 \text{ d}^{-1}$ ;  $k_2 = 1.1 \times 10^{-1} \text{ d}^{-1}$  (guppies, Opperhuizen et al. 1985)  
 $\log k_1 = 3.04 \text{ d}^{-1}$ ;  $\log k_2 = -0.96 \text{ d}^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota:  $t_{1/2} = 6.2 \text{ d}$  (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

## 4.1.3.5 1,8-Dichloronaphthalene



Common Name: 1,8-Dichloronaphthalene

Synonym: PCN-9

Chemical Name: 1,8-dichloronaphthalene

CAS Registry No: 2050-74-0

Molecular Formula:  $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ( $^{\circ}C$ ):

89 (Weast 1982-83; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

sublimation (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

156.0 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.236 (mp at  $89^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.315 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.059 (generator column-GC/ECD, Opperhuizen et al. 1987)

0.309 (Isnard & Lambert 1988, 1989; quoted, Crookes & Howe 1993)

1.27 (calculated-molar volume mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and the reported temperature dependence equation):

0.198 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3169/(T/K) + 9.93$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

4.41 (HPLC-RT, Opperhuizen et al. 1985)

4.19 (shake flask-GC, Opperhuizen 1987; quoted, Sangster 1993; Hansch et al. 1995)

5.4348 (calculated-UNIFAC, Chen et al. 1993)

4.85 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

3.79 (guppies, Opperhuizen et al. 1985)

3.79. 4.96 (guppies: whole fish, fish lipid, Gobas et al. 1987)

4.95 (guppy, lipid-weight based, Gobas et al. 1989)

3.79 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

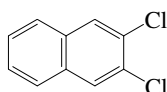
$k_1 = 9.8 \times 10^2 d^{-1}$ ;  $k_2 = 1.6 \times 10^{-1} d^{-1}$  (guppies, Opperhuizen et al. 1985)

$\log k_1 = 2.97 d^{-1}$ ;  $\log k_2 = -0.80 d^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: elimination  $t_{1/2} = 4.3 d$  (guppies, Opperhuizen et al. 1985; Crookes & Howe 1993)

## 4.1.3.6 2,3-Dichloronaphthalene



Common Name: 2,3-Dichloronaphthalene

Synonym: PCN-10

Chemical Name: 2,3-dichloronaphthalene

CAS Registry No: 2050-75-1

Molecular Formula:  $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ( $^{\circ}C$ ):

120 (Weast 1982-83; Ruelle & Kesselring 1997; Lide 2003)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

156.0 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (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  $25^{\circ}C$ ):

0.0862 (generator column-GC/ECD, Opperhuizen et al. 1985; 1987)

0.623 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and the reported temperature dependence equation):

0.333 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3169/(T/K) + 10.15$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

4.71 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.51 (shake flask, Opperhuizen 1987)

4.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

4.04 (guppies, Opperhuizen et al. 1985)

4.04, 5.22 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.08 (guppy, lipid-weight based, Gobas et al. 1989)

4.04 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

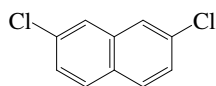
$k_1 = 1.6 \times 10^3 d^{-1}$ ;  $k_2 = 1.4 \times 10^{-1} d^{-1}$  (guppies, Opperhuizen et al. 1985)

$\log k_1 = 3.05 d^{-1}$ ;  $\log k_2 = -0.85 d^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: elimination  $t_{1/2} = 5.1 d$  (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

## 4.1.3.7 2,7-Dichloronaphthalene



Common Name: 2,7-Dichloronaphthalene

Synonym: PCN-12

Chemical Name: 2,7-dichloronaphthalene

CAS Registry No: 2198-77-8

Molecular Formula:  $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ( $^{\circ}C$ ):

115 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

156.0 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ , F: 0.131 (mp at  $115^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.236 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.235 (reported as 2,8-dichloronaphthalene, generator column-GC/ECD, Opperhuizen 1987)

0.699 (calculated-molar volume mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

0.344 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3169/(T/K) + 10.16$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

4.81 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.56 (shake flask-GC, Opperhuizen 1987)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  and reported temperature dependence equation:

7.28, 6.95, 6.38, 6.08, 5.85 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 65400/(2.303 \cdot RT) - 4.80$ ; temp range  $10-50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

4.04 (guppies, Opperhuizen et al. 1985; Crookes & Howe 1993, Lu et al. 1999)

4.04 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.11 (guppy, lipid-weight based, Gobas et al. 1989)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

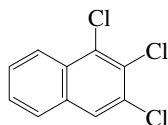
$k_1 = 1.6 \times 10^3 d^{-1}$ ;  $k_2 = 1.4 \times 10^{-1} d^{-1}$  (guppies, Opperhuizen et al. 1985)

$\log k_1 = 3.08 d^{-1}$ ;  $\log k_2 = -0.85 d^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: depuration  $t_{1/2} = 5.1 d$  (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

## 4.1.3.8 1,2,3-Trichloronaphthalene



Common Name: 1,2,3-Trichloronaphthalene

Synonym: PCN-13

Chemical Name: 1,2,3-trichloronaphthalene

CAS Registry No: 50402-52-3

Molecular Formula:  $C_{10}H_5Cl_3$

Molecular Weight: 231.506

Melting Point ( $^{\circ}C$ ):

81–84 (Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

210.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

0.071; 0.0652 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3551/(T/K) + 10.76$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0791 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3485/(T/K) + 10.59$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  and reported temperature dependence equation:

8.24, 7.85, 7.30, 6.91, 6.63 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 73200/(2.303 \cdot RT) - 5.20$ ; temp range  $10$ – $50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

7.66; 7.72 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

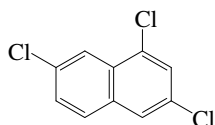
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.9 1,3,7-Trichloronaphthalene



Common Name: 1,3,7-Trichloronaphthalene

Synonym: PCN-21

Chemical Name: 1,3,7-trichloronaphthalene

CAS Registry No: 55720-37-1

Molecular Formula:  $C_{10}H_5Cl_3$

Molecular Weight: 231.506

Melting Point ( $^{\circ}C$ ):

113 (Crookes & Howe 1993)

Boiling Point ( $^{\circ}C$ ): 274

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

168.9 (Ruelle & Kesselring 1997)

210.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (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  $25^{\circ}C$ ):

0.0644 (generator column-GC/ECD, Opperhuizen et al. 1985, 1987)

0.049 (Opperhuizen et al. 1986)

2.85 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

0.127 (estimated, Crookes & Howe 1993)

$7.10 \times 10^{-6}$  (estimated, Alcock et al. 1999)

0.114 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3485/(T/K) + 10.74$  (regression with GC-RT from literature, Lei et al. 1999)

$0.0778 - P_S, 0.359 - P_L$  (estimated for trichloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

5.59 (HPLC-RT correlation, Opperhuizen et al. 1985)

5.60 (selected, Opperhuizen et al. 1986)

5.35 (shake flask, Opperhuizen 1987)

5.08 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

3.94 (*Cyprinus carpio*, for trichloronaphthalenes, Matsuo 1981)

4.43 (guppies, Opperhuizen et al. 1985)

4.43, 5.61 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.96 (guppy, lipid-weight based, Gobas et al. 1989)

4.08 (calculated- $K_{OW}$  and solubility, Banerjee & Baughman 1991)

4.43 (*Poecilia reticulata*, under static and semi-static conditions, Devillers et al. 1996)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$$k_1 = 2.3 \times 10^3 \text{ d}^{-1}; k_2 = 8.4 \times 10^{-2} \text{ d}^{-1} \text{ (guppy, Opperhuizen et al. 1985)}$$

$$k_1 = 1.7 \times 10^3 \text{ d}^{-1} \text{ (estimated, Opperhuizen et al. 1985)}$$

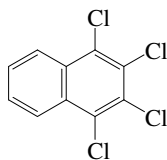
$$\log k_1 = 3.14 \text{ d}^{-1}; \log k_2 = -1.64 \text{ d}^{-1} \text{ (guppy, Gobas et al. 1989)}$$

Half-Lives in the Environment:

$$\text{Biota: } t_{1/2} = 8.3 \text{ d (guppies, Opperhuizen et al. 1985; quoted, Crookes \& Howe 1993)}$$



## 4.1.3.10 1,2,3,4-Tetrachloronaphthalene



Common Name: 1,2,3,4-Tetrachloronaphthalene

Synonym: PCN-27

Chemical Name: 1,2,3,4-tetrachloronaphthalene

CAS Registry No: 20020-02-4

Molecular Formula:  $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ( $^{\circ}C$ ):

199 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

181.8 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0196 (mp at  $199^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.00426 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.0042 (generator column-GC/ECD, Opperhuizen 1987)

0.0172 (calculated-AQUAFAC, Myrdal et al. 1995)

0.016 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

0.0197; 0.0173 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3825/(T/K) + 11.12$ ; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0162(supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3825/(T/K) + 10.96$  (regression with GC-RT from literature, Lei et al. 1999)

0.00536 –  $P_S$ ; 0.0975 –  $P_L$  (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$  at  $25^{\circ}C$  and the reported temperature dependence equations:

5.94 (HPLC-RT correlation, Opperhuizen et al. 1985)

5.90 (HPLC-RT correlation, Opperhuizen et al. 1985)

5.75 (shake flask-GC, Opperhuizen 1987)

6.30; 5.76 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 1.832 + 1347.46/(T/K)$ , temp range  $5-55^{\circ}C$  (temperature dependence HPLC- $k'$  correlation, Lei et al. 2000)

5.91 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equation:

9.03, 8.59, 8.05, 7.59, 7.26 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 79500/(2.303 \cdot RT) - 5.60$ ; temp range  $10-50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

8.30; 8.29 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log  $K_B$ :

3.94	( <i>Cyprinus carpio</i> , Matsuo 1981)
3.71	( <i>Oncorhynchus mykiss</i> , Oliver & Niimi 1984)
4.52	(guppies, Opperhuizen et al. 1985)
4.50	(fish, Opperhuizen et al. 1985)
4.66, 5.71	(whole fish, fish lipid, Gobas et al. 1987)
3.71	(rainbow trout, mean value, Oliver & Niimi 1985)
5.96	(guppy, lipid-weight based, Gobas et al. 1989)

Sorption Partition Coefficient, log  $K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$k_1 = 3.3 \times 10^3 \text{ d}^{-1}$ ;  $k_2 = 9.9 \times 10^{-2} \text{ d}^{-1}$  (guppy, Opperhuizen et al. 1985)

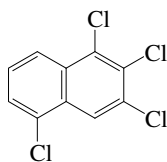
$k_1 = 1.3 \times 10^3 \text{ d}^{-1}$  (estimated, Opperhuizen et al. 1985)

$\log k_1 = 3.70 \text{ d}^{-1}$ ;  $\log k_2 = -1.08 \text{ d}^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota:  $t_{1/2} = 7 \text{ d}$  (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

## 4.1.3.11 1,2,3,5-Tetrachloronaphthalene



Common Name: 1,2,3,5-Tetrachloronaphthalene

Synonym: PCN-28

Chemical Name: 1,2,3,5-tetrachloronaphthalene

CAS Registry No: 53555-63-8

Molecular Formula:  $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ( $^{\circ}C$ ):

141 (Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0728 (mp at  $141^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

0.0203; 0.0179 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3836/(T/K) + 11.17$ ; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0205 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3800/(T/K) + 11.06$  (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

5.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equation:

8.98, 8.55, 8.00, 7.55, 7.22 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 79100/(2.303 \cdot RT) - 5.60$ ; temp range  $10$ – $50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

8.29; 8.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

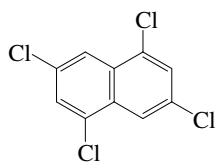
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{oc}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.12 1,3,5,7-Tetrachloronaphthalene



Common Name: 1,3,5,7-Tetrachloronaphthalene

Synonym: PCN-42

Chemical Name: 1,3,5,7-tetrachloronaphthalene

CAS Registry No: 53555-64-9

Molecular Formula:  $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ( $^{\circ}C$ ):

179 (Crookes & Howe 1993)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

181.8 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0308 (mp at  $179^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.00426 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.0040 (generator column-GC/ECD, Opperhuizen 1987)

0.0237 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

0.0480 (estimated, Crookes & Howe 1993)

$2.70 \times 10^{-6}$  (estimated, Alcock et al. 1999)

0.0415 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3800/(T/K) + 11.36$  (regression with GC-RT from literature, Lei et al. 1999)

$0.00536 - P_S$ ;  $0.0975 - P_L$  (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

6.38 (HPLC-RT correlation, Opperhuizen et al. 1985)

6.40 (Opperhuizen 1986)

6.19 (shake flask, Opperhuizen 1987; selected, Hansch et al. 1995)

5.54 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equation:

8.39 (estimated value for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

8.58, 8.18, 7.62, 7.21, 6.90 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 75000/(2.303 \cdot RT) - 5.40$ ; temp range  $10-50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

4.53 (guppies, Opperhuizen et al. 1985)

4.50 (guppies, Opperhuizen et al. 1985)

5.06, 5.71 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.81 (guppy, lipid-weight based, Gobas et al. 1989)  
4.53; 4.37 (quoted means; calculated- $K_{OW}$  and S, Banerjee & Baughman 1991)  
4.701, 4.961 (calculated-MCI  $\chi$ , calculated- $K_{OW}$ , Lu et al. 1999)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

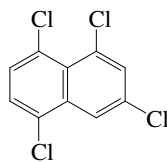
$k_1 = 7.5 \times 10^2 \text{ d}^{-1}$ ;  $k_2 = 2.2 \times 10^{-2} \text{ d}^{-1}$  (guppies, Opperhuizen et al. 1985)

$\log k_1 = 2.97 \text{ d}^{-1}$ ;  $\log k_2 = -1.66 \text{ d}^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota:  $t_{1/2} = 30 \text{ d}$  (guppies, Opperhuizen et al. 1985)

## 4.1.3.13 1,3,5,8-Tetrachloronaphthalene



Common Name: 1,3,5,8-Tetrachloronaphthalene

Synonym: PCN-43

Chemical Name: 1,3,5,8-tetrachloronaphthalene

CAS Registry No: 31604-28-1

Molecular Formula:  $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ( $^{\circ}C$ ):

131 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

181.8 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (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  $25^{\circ}C$ ):

0.00825 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.0030 (Opperhuizen 1986)

0.0082 (generator column-GC/ECD, Opperhuizen 1987)

0.0716 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

0.0208 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3800/(T/K) + 11.07$  (regression with GC-RT from literature, Lei et al. 1999)

$0.00536 - P_S$ ;  $0.0975 - P_L$  (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

5.96 (HPLC-RT correlation, Opperhuizen et al. 1985; selected, Sangster 1993)

6.00 (Opperhuizen et al. 1985; Opperhuizen 1986)

5.76 (shake flask, Opperhuizen 1987; selected, Hansch et al. 1995)

5.81 (selected, Gobas et al. 1987, 1989)

5.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations:

8.39 (value for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

8.98, 8.55, 8.00, 7.55, 7.22 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 79100/(2.303 \cdot RT) - 5.60$ ; temp range  $10-50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

4.40 (guppies, Opperhuizen et al. 1985)

4.69, 5.57 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.62 (guppy, lipid-weight based, Gobas et al. 1989)

4.701, 4.582 (calculated-MCI  $\chi$ , calculated- $K_{OW}$ , Lu et al. 1999)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$$k_1 = 1.2 \times 10^3 \text{ d}^{-1}; k_2 = 4.5 \times 10^{-2} \text{ d}^{-1} \quad (\text{guppies, Opperhuizen et al. 1985})$$

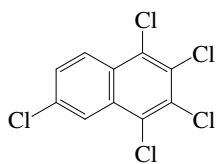
$$k_1 = 1.4 \times 10^3 \text{ d}^{-1} \quad (\text{fish, Opperhuizen 1986})$$

$$\log k_1 = 3.10 \text{ d}^{-1}; \log k_2 = -1.35 \text{ d}^{-1} \quad (\text{guppy, Gobas et al. 1989})$$

Half-Lives in the Environment:

$$\text{Biota: } t_{1/2} = 15.5 \text{ d (guppies, Opperhuizen et al. 1985)}$$

## 4.1.3.14 1,2,3,4,6-Pentachloronaphthalene



Common Name: 1,2,3,4,6-Pentachloronaphthalene

Synonym: PCN-50

Chemical Name: 1,2,3,4,6-pentachloronaphthalene

CAS Registry No: 67922-25-2

Molecular Formula:  $C_{10}H_3Cl_5$

Molecular Weight: 300.396

Melting Point ( $^{\circ}C$ ):

147 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0635 (mp at  $147^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$ ):

0.00562; 0.00475 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4123/(T/K) + 11.58$ ; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0055 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4116/(T/K) + 11.55$  (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at  $25^{\circ}C$  and the reported temperature dependence equations:

7.0; 6.27 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 2.166 + 1446.69/(T/K)$ , temp range  $5-55^{\circ}C$  (temperature dependence HPLC-k' correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and the reported temperature dependence equations:

8.91 (generator column-GC/MS, Harner & Bidleman 1998)

9.73, 9.20, 8.63, 8.11, 7.75 (10, 20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.63 + 4629/(T/K)$ , temp range:  $10-50^{\circ}C$  (generator column-GC/MS, Harner & Bidleman 1998)

8.92; 8.85 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

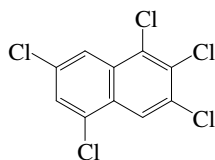
Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:



## 4.1.3.15 1,2,3,5,7-Pentachloronaphthalene



Common Name: 1,2,3,5,7-Pentachloronaphthalene

Synonym: PCN-52

Chemical Name: 1,2,3,5,7-pentachloronaphthalene

CAS Registry No: 53555-65-0

Molecular Formula:  $C_{10}H_3Cl_5$

Molecular Weight: 300.396

Melting Point ( $^{\circ}C$ ):

171 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

313 (estimated, Crookes & Howe 1993)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0369 (mp at  $171^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.0073 (estimated, Crookes & Howe 1993)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

$4.266 \times 10^{-3}$  (estimated, Crookes & Howe 1993)

$2.40 \times 10^{-6}$  (estimated, Alcock et al. 1999)

0.00696; 0.00593 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4082/(T/K) + 11.53$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00798 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4082/(T/K) + 11.71$  (regression with GC-RT data from literature, Lei et al. 1999)

0.0–133 –  $P_S$ ; 0.0277 –  $P_L$  (estimated for pentachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

5.46 (selected, Hawker 1990)

6.87 (estimated, Crookes & Howe 1993, quoted, Alcock et al. 1999)

6.87 (quoted, Falandysz et al. 1997)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations:

8.73 (generator-column-GC, Harner & Bidleman 1998)

9.50, 9.04, 8.47, 7.97, 7.63 (10, 20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.02 + 4394/(T/K)$ ; temp range: 10– $50^{\circ}C$  (generator column-GC/MS, Harner & Bidleman 1998)

9.00 (estimated, Kaupp & McLachlan 1999)

8.82; 8.76 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

4.23 (selected, Hawker 1990)

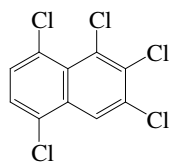
Sorption Partition Coefficient,  $\log K_{oc}$ :

4.36 (estimated, Crookes & Howe 1993)

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.16 1,2,3,5,8-Pentachloronaphthalene



Common Name: 1,2,3,5,8-Pentachloronaphthalene

Synonym: PCN-53

Chemical Name: 1,2,3,5,8-pentachloronaphthalene

CAS Registry No: 150224-24-1

Molecular Formula:  $C_{10}H_3Cl_5$

Molecular Weight: 300.396

Melting Point ( $^{\circ}C$ ):

174–176 (Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

0.00394; 0.00329 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4204/(T/K) + 11.70$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00428 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4116/(T/K) + 11.44$  (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at  $25^{\circ}C$  and the temperature dependence equations:

6.80; 6.13 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 2.305 + 1431.02/(T/K)$ , temp range  $5-55^{\circ}C$  (temperature dependence HPLC-k' correlation, Lei et al. 2000)

6.46 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations:

9.13 (generator column-GC/MS, Harner & Bidleman 1998)

9.97, 9.44, 8.86, 8.34, 7.96 (10, 20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.59 + 4684/(T/K)$ ; temp range:  $10-50^{\circ}C$  (generator column-GC/MS, Harner & Bidleman 1998)

9.10; 9.01 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

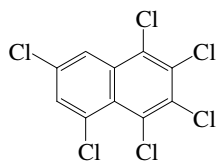
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.17 1,2,3,4,5,7-Hexachloronaphthalene



Common Name: 1,2,3,4,5,7-Hexachloronaphthalene

Synonym: PCN-64

Chemical Name: 1,2,3,4,5,7-hexachloronaphthalene

CAS Registry No: 67927-67-4

Molecular Formula:  $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ( $^{\circ}C$ ):

194 (Crookes & Howe 1993)

164–166 (Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

331 (estimated, Crookes & Howe 1993)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.022 (mp at  $194^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.00011 (estimated, Crookes & Howe 1993)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

$9.47 \times 10^{-4}$  (estimated, Crookes & Howe 1993)

$5.30 \times 10^{-8}$  (estimated, Alcock et al. 1999)

0.00134 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 11.99$  (regression with GC-RT data from literature, Lei et al. 1999)

$0.000257 - P_S$ ;  $0.00809 - P_L$  (estimated for hexachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

7.58 (estimated, Crookes & Howe 1993, quoted, Alcock et al. 1999)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and the reported temperature dependence equations:

9.80 (generator-column-GC, Harner & Bidleman 1998)

10.07, 9.57, 8.95, 8.54 (20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.77 + 4393/(T/K)$ ; temp range:  $20$ – $50^{\circ}C$  (generator column-GC/MS, Harner & Bidleman 1998)

10.02 (value for hexachloronaphthalenes, Kaupp & McLachlan 1999)

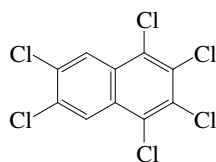
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.18 1,2,3,4,6,7-Hexachloronaphthalene



Common Name: 1,2,3,4,6,7-Hexachloronaphthalene

Synonym: PCN-66

Chemical Name: 1,2,3,4,6,7-hexachloronaphthalene

CAS Registry No: 103426-96-6

Molecular Formula:  $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ( $^{\circ}C$ ):

205-206 (Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

Enthalpy of Sublimation,  $\Delta H_{subl}$  (kJ/mol):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and the reported temperature dependence equations):

0.0015; 0.00121 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4411/(T/K) + 11.97$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00157 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 12.06$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$  at  $25^{\circ}C$  and the temperature dependence equations:

7.70; 6.79 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 2.489 + 1556.37/(T/K)$ ; temp range  $5-55^{\circ}C$  (temperature dependence HPLC-k' correlation, Lei et al. 2000)

6.77 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations:

9.70 (generator column-GC/MS, Harner & Bidleman 1998)

10.58, 10.01, 9.46, 8.84, 8.42 (10, 20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -7.09 + 5003/(T/K)$ ; temp range:  $10-50^{\circ}C$  (generator column-GC/MS, Harner & Bidleman 1998)

9.58; 9.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

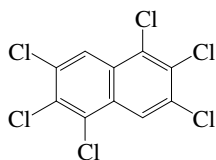
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.19 1,2,3,5,6,7-Hexachloronaphthalene



Common Name: 1,2,3,5,6,7-Hexachloronaphthalene

Synonym: PCN-67

Chemical Name: 1,2,3,5,6,7-hexachloronaphthalene

CAS Registry No: 103426-97-7

Molecular Formula:  $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ( $^{\circ}C$ ):

234–235 (Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$ ):

0.00150; 0.00121 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4411/(T/K) + 11.97$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00157 (supercooled liquid  $P_L$ , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 12.06$  (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  and reported temperature dependence equation:

9.70 (generator column-GC/MS, Harner & Bidleman 1998)

10.58, 10.01, 9.46, 8.84, 8.42 (10, 20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -7.09 + 5003/(T/K)$ ; temp range: 10– $50^{\circ}C$  (generator column-GC/MS, Harner & Bidleman 1998)

9.58; 9.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

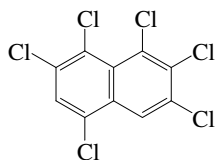
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.20 1,2,3,5,7,8-Hexachloronaphthalene



Common Name: 1,2,3,5,7,8-Hexachloronaphthalene

Synonym: PCN-69

Chemical Name: 1,2,3,5,7,8-hexachloronaphthalene

CAS Registry No: 103426-94-4

Molecular Formula:  $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ( $^{\circ}C$ ):

148–149 (Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$  and the reported temperature dependence equations):

0.00124; 0.0010 (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4441/(T/K) + 11.99$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00134(supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 11.99$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$  at  $25^{\circ}C$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$  at  $25^{\circ}C$  and the reported temperature dependence equations:

7.50; 6.69 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 2.413 + 1535.48/(T/K)$ ; temp range  $5-55^{\circ}C$  (temperature dependence HPLC-k' correlation, Lei et al. 2000)

6.87 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equation:

9.83 (generator column-GC/MS, Harner & Bidleman 1998)

10.09, 9.62, 8.99, 8.57 (20, 30, 40,  $50^{\circ}C$ , generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.64 + 4909/(T/K)$ ; temp range:  $20-50^{\circ}C$  (generator column-GC, Harner & Bidleman 1998)

9.67; 9.53 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

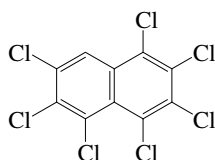
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.21 1,2,3,4,5,6,7-Heptachloronaphthalene



Common Name: 1,2,3,4,5,6,7-Heptachloronaphthalene

Synonym: PCN-73

Chemical Name: 1,2,3,4,5,6,7-heptachloronaphthalene

CAS Registry No: 58863-14-2

Molecular Formula:  $C_{10}HCl_7$

Molecular Weight: 369.287

Melting Point ( $^{\circ}C$ ):

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

293.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.00062 (generator column-GC/ECD, Opperhuizen 1985; quoted, Opperhuizen 1986)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

$5.44 \times 10^{-4} - P_S$ ;  $0.00258 - P_L$  (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)

$2.93 \times 10^{-4}$ ,  $2.78 \times 10^{-4}$  (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4745/(T/K) + 12.38$  (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.000278 (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4745/(T/K) + 12.37$  (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at  $25^{\circ}C$  and the reported temperature dependence equations:

8.20 (HPLC-RT, Opperhuizen et al. 1985; quoted, Opperhuizen 1986)

7.69 (calculated-fragment const., Burreau et al. 1997)

8.20; 7.18 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 2.638 + 1660.82/(T/K)$ ; temp range  $5-55^{\circ}C$  (HPLC- $k'$  correlation, Lei et al. 2000)

7.33 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equation:

11.52, 10.96, 10.44, 9.75, 9.28 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 99500/(2.303 \cdot RT) - 6.80$ ; temp range  $10-50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

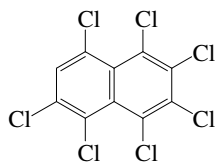
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.3.22 1,2,3,4,5,6,8-Heptachloronaphthalene



Common Name: 1,2,3,4,5,6,8-Heptachloronaphthalene

Synonym: PCN-74

Chemical Name: 1,2,3,4,5,6,8-heptachloronaphthalene

CAS Registry No: 58863-15-3

Molecular Formula:  $C_{10}HCl_7$

Molecular Weight: 369.287

Melting Point ( $^{\circ}C$ ):

194 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ( $^{\circ}C$ ):

348 (estimated, Crookes & Howe 1993)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

293.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.022 (mp at  $194^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.00004 estimated, Crookes & Howe 1993; quoted, Alcock et al. 1999)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equation):

$3.73 \times 10^{-4}$  (estimated, Crookes & Howe 1993)

$2.10 \times 10^{-8}$  (estimated, Alcock et al. 1999)

$2.46 \times 10^{-4}$  (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4748/(T/K) + 12.31$  (regression with GC-RT from literature, Lei et al. 1999)

$5.44 \times 10^{-4} - P_S$ ;  $0.00258 - P_L$  (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

8.30 (estimated, Crookes & Howe 1993, quoted, Alcock et al. 1999)

8.50; 7.46 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equation:

11.56, 10.99, 10.47, 9.79, 9.31 (10, 20, 30, 40,  $50^{\circ}C$ , GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 99800/(2.303 \cdot RT) - 6.80$ ; temp range  $10-50^{\circ}C$  (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

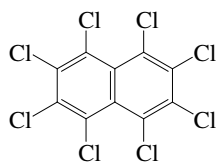
Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:



## 4.1.3.23 Octachloronaphthalene



Common Name: Octachloronaphthalene

Synonym: PCN-75

Chemical Name: octachloronaphthalene

CAS Registry No: 2234-13-1

Molecular Formula:  $C_{10}Cl_8$

Molecular Weight: 403.731

Melting Point ( $^{\circ}C$ ):

197.5 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

365 (estimated, Crookes & Howe 1993)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

314.8 (calculated-Le Bas method at normal boiling point)

233.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0203 (mp at  $197.5^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.000078, 0.00008 (generator column-GC/ECD, Opperhuizen 1986)

0.00008 (generator column-GC/ECD, Opperhuizen 1987)

0.00008; 0.00027 (quoted; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

$1.33 \times 10^{-4}$  (estimated, Crookes & Howe 1993)

$7.50 \times 10^{-9}$  (estimated, Alcock et al. 1999)

$7.61 \times 10^{-5}$ ,  $5.60 \times 10^{-5}$  (supercooled liquid  $P_L$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -5021/(T/K) + 12.72$  (Antoine eq., GC-RT correlation, supercooled liquid, Lei et al. 1999)

$6.84 \times 10^{-5}$  (supercooled liquid  $P_L$ , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -5021/(T/K) + 12.82$  (regression with GC-RT from literature, Lei et al. 1999)

$1.60 \times 10^{-5} - P_S$ ;  $8.71 \times 10^{-4} - P_L$  (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$  at  $25^{\circ}C$  and the reported temperature dependence equations.

6.50 (calculated, Kaiser 1983)

8.40 (HPLC-RT correlation, Opperhuizen et al. 1985)

8.50 (Opperhuizen 1986)

6.42 (shake flask, Opperhuizen)

7.90 (calculated, Banerjee & Baughman 1991)

8.50, 7.47 (calibrated HPLC- $k'$  correlation, HPLC- $k'$  correlation, Lei et al. 2000)

$\log K_{ow} = 2.998 + 1660.82/(T/K)$ , temp range  $5-55^{\circ}C$  (temperature dependence HPLC- $k'$  correlation, Lei et al. 2000)

7.70 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient,  $\log K_{OA}$  at 25°C or as indicated and the reported temperature dependence equations:

12.39, 11.78, 11.27, 10.51, 9.98 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 10600/(2.303 \cdot RT) - 7.20$ ; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

2.50 (*Oncorhynchus mykiss*, Oliver & Niimi 1985; quoted, Crookes & Howe 1993)

2.52 (rainbow trout, mean value, Oliver & Niimi 1985)

5.0 (calculated- $K_{OW}$  and  $S_0$ , Banerjee & Baughman 1991)

2.52 (*Oncorhynchus mykiss*, under flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient,  $\log K_{OC}$ :

5.38 (estimated, Crookes & Howe 1993)

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis:

Photooxidation:  $t_{1/2} = 1608$ – $16082$  h based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aerobic biodegradation  $t_{1/2} = 4320$ – $8760$  h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991);

anaerobic biodegradation  $t_{1/2} = 17280$ – $35040$  h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

Half-Lives in the Environment:

Air: photooxidation  $t_{1/2} = 1608$ – $16082$  h in air based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 4320$ – $8760$  h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 8640$ – $17520$  h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

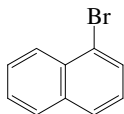
Sediment:

Soil:  $t_{1/2} = 4320$ – $8760$  h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

Biota:

#### 4.1.4 BROMINATED POLYNUCLEAR AROMATIC HYDROCARBONS

##### 4.1.4.1 1-Bromonaphthalene



Common Name: 1-Bromonaphthalene

Synonym:  $\alpha$ -bromonaphthalene

Chemical Name: 1-bromonaphthalene

CAS Registry No: 90-11-9

Molecular Formula:  $C_{10}H_7Br$

Molecular Weight: 207.067

Melting Point ( $^{\circ}C$ ):

6.1 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

281 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

1.4834 (Dean 1992)

1.4785 (Lide 2003)

Molar Volume ( $cm^3/mol$ ):

140.6 ( $30^{\circ}C$ , calculated from density, Stephenson & Malanowski 1987)

140.0 ( $20^{\circ}C$ , calculated-density)

170.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

39.33 (at normal bp, Hon et al. 1976)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$ , F: 1.0

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

9.95 (Yalkowsky et al. 1983)

7.72 (calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

9.08, 9.80, 13.35, and 18.98 (4, 10, 25, and  $40^{\circ}C$ , generator column-UV spec., Dickhut et al. 1994)

25.3 (calculated-TSA, Dickhut et al. 1994)

14.0 (calculated-group contribution method, Kühne et al. 1995)

23.3 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

266.6\* ( $97.9^{\circ}C$ , static-Hg manometer, measured range  $97.9$ – $281.1^{\circ}C$ , Kahlbaum 1898)

133\* ( $84.2^{\circ}C$ , summary of literature data, temp range  $84.2$ – $281.1^{\circ}C$ , Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 13274.9/(T/K)] + 8.131285$ ; temp range  $84.2$ – $281.1^{\circ}C$ , (Antoine eq., Weast 1972–73)

18681\* ( $196.27^{\circ}C$ , ebulliometry, measured range  $97.9$ – $285.92^{\circ}C$ , Hon et al. 1976)

$\log(P/mmHg) = 5.38175 - 929.64/(91.06 + t/^{\circ}C)$ ; temp range:  $196.27$ – $285.93^{\circ}C$  (Antoine eq., twin ebulliometry, Hon et al. 1976)

0.713\*, 1.07\* (torsion effusion, measured range  $295$ – $359 K$ , Urbani et al. 1980)

$\log(P/kPa) = (6.90 - 2950/(T/K))$ , temp range  $295$ – $359 K$  (torsion and Knudsen effusion, Urbani et al. 1980)

$\log(P/mmHg) = 7.00350 - 1927.05/(186.0 + t/^{\circ}C)$ ; temp range: liquid (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.56365 - 2303.73/[-48.841 + (T/K)]$ ; temp range  $357$ – $555 K$  (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 4.50679 - 929.871/[182.045 + (T/K)]$ , temp range 469–559 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

2.754\* (30.15°C, transpiration method, measured range 303.3–336.3 K, Verevkin 2003)

$\ln (P/P^\circ) = 299.001/R - 8.3941.481/R \cdot (T/K) - (73.5/R) \cdot \ln[(T/K)/298.15]$ , where  $P^\circ = 101.325 \text{ kPa}$ , gas constant  $R = 8.31451 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  (vapor pressure eq. from transpiration measurement, temp range 303.3–336.3 K, Verevkin 2003)

Henry's Law Constant ( $\text{Pa} \cdot \text{m}^3/\text{mol}$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

4.35 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log \text{BCF}$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 4.1.4.1.1**

**Reported vapor pressures of 1-bromonaphthalene 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)		

1.

Kahlbaum 1898		Stull 1947		Hon et al. 1976		Urbani et al. 1980	
static method-manometer		summary of literature data		ebulliometry		torsion effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						Run A.01	
97.9	266.6	84.2	133.3	196.27	18681	25	0.713
117.5	666.6	117.5	666.6	213.14	28206	28	0.950
134.0	1333	133.6	1333	228.08	39235	30	1.37
151.3	2666	150.2	2666	234.45	44740	33	1.31
157.2	3333	170.2	5333	244.51	54504	34	1.43
162.3	3999	183.5	7999	245.13	55150	40	2.85
166.7	4666	198.8	13332	250.71	61192	42	3.05
170.5	5333	224.2	26664	256.24	67574	45	3.62
177.1	6666	252.2	53329	262.78	75759	46	3.72
189.6	9999	281.1	101325	275.35	93151	47	4.16
198.8	13332			279.49	99510	48	4.51
223.8	26664	mp/°C	5.5	281.40	102474	49	4.75
239.7	39997			284.04	106737	50	4.99
252.0	53329			285.92	109863	52	5.82
261.6	66661					58	7.78
269.8	79993			bp/°C	280.56	61	8.94
277.2	93326					66	12.8

TABLE 4.1.4.1.1 (Continued)

Kahlbaum 1898		Stull 1947		Hon et al. 1976		Urbani et al. 1980	
static method-manometer		summary of literature data		ebulliometry		torsion effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
281.1	101325			eq. 2	P/mmHg	74	20.2
				A	5.38157	77	24.3
				B	929.64	86	42.0
				C	91.06		
				$\Delta H_v/(\text{kJ mol}^{-1}) = 39.33$ at bp			

2.

Urbani et al. 1980 (Continued)				Verevkin 2003			
torsion effusion		Knudsen effusion		transpiration-GC			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
Run A.02							
50	8.33	42	4.95	30.15	2.754		
53	8.54	49	9.26	33.15	3.466		
55	10.4	50	8.97	36.15	4.388		
58	12.5	54	11.6	39.14	5.529		
58	11.7	60	16.1	42.15	7.095		
67	17.3	65	18.4	45.15	8.644		
Run A.04		70	28.3	48.15	10.97		
26	1.07			51.25	13.66		
34	1.72	For Knudsen effusion:		54.15	16.64		
36	2.32	eq. 1	P/kPa	57.15	20.95		
38	2.61	A	$6.33 \pm 0.33$	60.15	25.50		
43	3.86	B	$2710 \pm 110$	63.15	30.34		
50	6.18						
51	6.21			$\Delta H_v/(\text{kJ mol}^{-1}) = 63.91$			
55	7.00			at 298.15 K			
60	8.58						
63	10.3			eq. 4a	P/kPa		
68	12.9			P <sup>0</sup>	101.325 kPa		
70	17.5			A	303.761/R		
82	38.7	Overall temp dependence eq.		B	89574.863/R		
		eq. 1	P/kPa	C	78.8/R		
for torsion effusion:		A	$6.90 \pm 1.1$	$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$			
eq. 1	P/kPa	B	$2950 \pm 300$				
A	$6.96 \pm 0.18$						
B	$2980 \pm 57$	$\Delta H_v/(\text{kJ mol}^{-1}) = 56 \pm 6$					

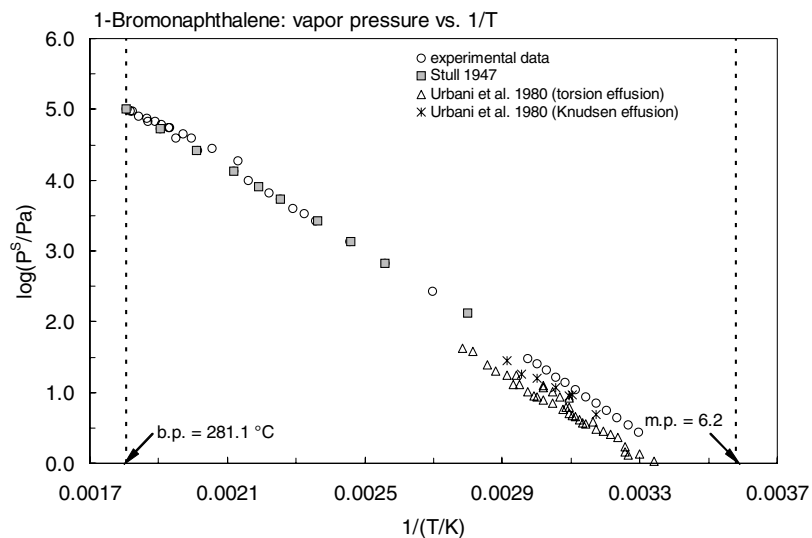
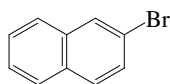


FIGURE 4.1.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1-bromonaphthalene.

## 4.1.4.2 2-Bromonaphthalene



Common Name: 2-Bromonaphthalene

Synonym:  $\beta$ -bromonaphthalene

Chemical Name: 2-bromonaphthalene

CAS Registry No: 580-13-2

Molecular Formula:  $C_{10}H_7Br$

Molecular Weight: 207.067

Melting Point ( $^{\circ}C$ ):

55.9 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

281.5 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

146.3 (Ruelle & Kesselring 1997)

170.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

11.97 (Ruelle & Kesselring 1997)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.498 (mp at  $55.9^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

8.27 (Yalkowsky et al. 1983)

7.72 (calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

3.80, 8.04, 15.76 (4, 25,  $40^{\circ}C$ , generator column-UV spec., Dickhut et al. 1994)

10.1 (calculated-TSA, Dickhut et al. 1994)

9.04 (calculated-group contribution method, Kühne et al. 1995)

8.06 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

0.501\* ( $25.15^{\circ}C$ , solid I, transpiration method-GC, measured range 280.4–318.3 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 314.110/R - 94001.596/R \cdot (T/K) - (41.6/R) \cdot \ln[(T/K)/298.15]$ , where  $P^{\circ} = 101.325$  kPa, gas constant  $R = 8.31451$  J·K $^{-1}$ ·mol $^{-1}$  (solid I, vapor pressure eq. from transpiration measurement, temp range 280.4–318.3 K, Verevkin 2003)

7.34\* ( $46.05^{\circ}C$ , solid-II, transpiration method-GC, measured range 319.2–328.2 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 302.672/R - 90417.272/R \cdot (T/K) - (41.6/R) \cdot \ln[(T/K)/298.15]$ , where  $P^{\circ} = 101.325$  kPa, gas constant  $R = 8.31451$  J·K $^{-1}$ ·mol $^{-1}$  (solid II, vapor pressure eq. from transpiration measurements, temp range 319.2–328.2 K, Verevkin 2003)

18.75\* ( $57.05^{\circ}C$ , liquid, transpiration method-GC, measured range 330.2–360.2 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 303.761/R - 89574.863/R \cdot (T/K) - (78.8/R) \cdot \ln[(T/K)/298.15]$ , where  $P^{\circ} = 101.325$  kPa, gas constant  $R = 8.31451$  J·K $^{-1}$ ·mol $^{-1}$  (liquid, vapor pressure eq. from transpiration measurements, temp range 330.2–360.2 K, Verevkin 2003)

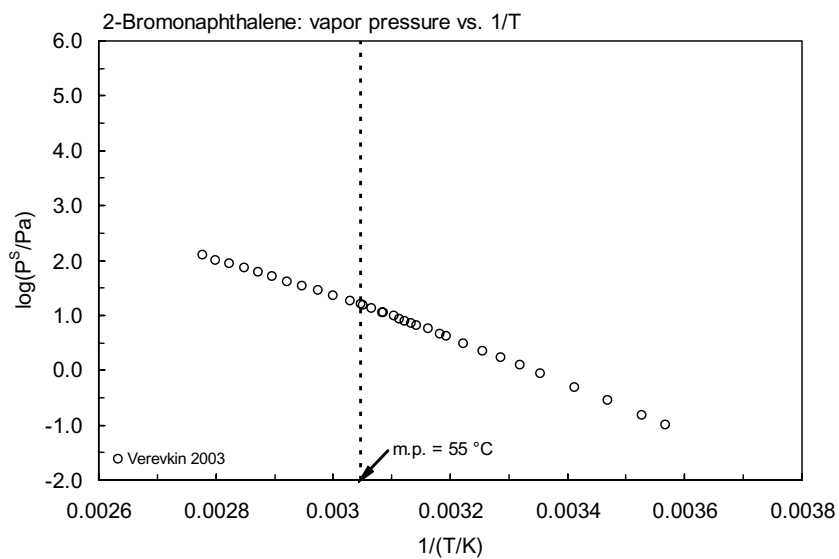
Henry's Law Constant (Pa·m $^3$ /mol):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

4.35 (calculated-fragment const., Yalkowsky et al. 1983)

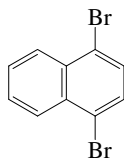






**FIGURE 4.1.4.2.1** Logarithm of vapor pressure versus reciprocal temperature for 2-bromonaphthalene.

## 4.1.4.3 1,4-Dibromonaphthalene



Common Name: 1,4-Dibromonaphthalene

Synonym:

Chemical Name: 1,4-dibromonaphthalene

CAS Registry No: 83-53-4

Molecular Formula:  $C_{10}H_6Br_2$

Molecular Weight: 285.963

Melting Point ( $^{\circ}C$ ):

83 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

310 (Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

194.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.27 (mp at  $83^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated):

0.125, 0.35, and 0.866 (4, 25, and  $40^{\circ}C$ , generator column-GC/ECD, Dickhut et al. 1994)

1.92 (calculated-TSA, Dickhut et al. 1994)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

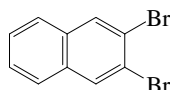
Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants, k or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**4.1.4.4 2,3-Dibromonaphthalene**

Common Name: 2,3-Dibromonaphthalene

Synonym:

Chemical Name: 2,3-dibromonaphthalene

CAS Registry No:

Molecular Formula:  $C_{10}H_6Br_2$

Molecular Weight: 285.963

Melting Point ( $^{\circ}C$ ):

140 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

194.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0744 (mp at  $140^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.0554, 0.138, and 0.352 (4, 25, and  $40^{\circ}C$ , generator column-GC/ECD, Dickhut et al. 1994)

0.432 (calculated-TSA, Dickhut et al. 1994)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

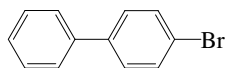
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.4.5 4-Bromobiphenyl



Common Name: 4-Bromobiphenyl

Synonym:

Chemical Name: 4-bromobiphenyl

CAS Registry No: 92-66-0

Molecular Formula:  $C_{12}H_9Br$

Molecular Weight: 233.103

Melting Point ( $^{\circ}C$ ):

91.5 (Lide 2003)

Boiling Point ( $^{\circ}C$ ):

310 (Weast 1983–84; Stephenson & Malanowski 1987, Lide 2003)

Density ( $g/cm^3$  at  $25^{\circ}C$ ):

0.9327 (Weast 1983–84, Lide 2003)

Molar Volume ( $cm^3/mol$ ):

176.1 (Ruelle & Kesselring 1997)

250.0 ( $25^{\circ}C$ , calculated-density)

207.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

26.86 (Doucette & Andren 1988)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.223 (mp at  $91.5^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations.):

0.235, 0.653, 0.874 ( $4.9, 25, 40^{\circ}C$ , generator column-GC, Doucette & Andren 1988a)

$S/(mol/L) = 9.36 \times 10^{-7} \exp(0.037 \cdot t/^{\circ}C)$  (generator column-GC/ECD, temp range  $4.9$ – $40^{\circ}C$ , Doucette & Andren 1988a); or

$\log x = -1436/(T/K) - 1.541$ , temp range  $4.9$ – $40^{\circ}C$  (generator column-GC/ECD, Doucette & Andren 1988a)

0.546 (calculated-TSA, Dickhut et al. 1994)

0.256 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$  and reported temperature dependence equations):

$\log (P_L/kPa) = 2.24643 - 2174.97/[(T/K) - 70.067]$ ; (Antoine eq., liquid state, temp range  $371$ – $583 K$ , Stephenson & Malanowski 1987)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

4.96; 4.89, 5.00 (generator column-GC; calculated-group contribution method, estimated-TSA and  $K_{OW}$ , Doucette & Andren 1987)

4.96; 4.89, 4.83, 5.10, 5.14, 5.10 (generator column-GC; calculated- $\pi$  const., HPLC-RT correlation, calculated-MW, calculated-MCI  $\chi$ , calculated-TSA and  $K_{OW}$ , Doucette & Andren 1988b)

4.96 (recommended, Sangster 1993)

4.95 (Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

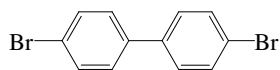
Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

## 4.1.4.6 4,4'-Dibromobiphenyl



Common Name: 4,4'-Dibromobiphenyl

Synonym: PBB-15, 4,4'-dibromo-1,1'-biphenyl

Chemical Name: 4,4'-dibromobiphenyl

CAS Registry No: 92-86-4

Molecular Formula:  $C_{12}H_8Br_2$

Molecular Weight: 312.000

Melting Point ( $^{\circ}C$ ):

164 (Ruelle & Kesselring 1997, Lide 2003)

Boiling Point ( $^{\circ}C$ ):

357.5 (Lide 2003)

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

192.2 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0433 (mp at  $164^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations):

0.00574 (generator column-GC, Gobas et al. 1988)

0.104 (quoted, Chessells et al. 1992)

0.0164 (calculated-MCI  $\chi$ , Ruelle & Kesselring et al. 1997)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{OW}$ :

5.72; 5.75, 5.57 (generator column-GC; calculated-group contribution method, estimated-TSA and  $K_{OW}$ , Doucette & Andren 1987)

5.72; 5.75, 5.85, 6.14, 5.81, 5.68 (generator column-GC; calculated- $\pi$  const., HPLC-RT correlation, calculated-MW, calculated-MCI  $\chi$ , calculated-TSA and  $K_{OW}$ , Doucette & Andren 1988b)

5.72 (HPLC-RT correlation, Gobas et al. 1988,)

5.72 (recommended, Sangster 1993)

4.67 (calculated-UNIFAC, Chen et al. 1993)

5.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

5.43 (guppy, lipid weight-based, Gobas et al. 1989)

4.19; 5.43 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)

3.825, 4.365 (calculated-MCI  $\chi$ ,  $K_{OW}$ , Lu et al. 1999)

Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

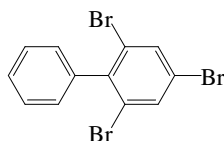
Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$\log k_1 = 3.35$   $d^{-1}$  (guppy, Gobas et al. 1989)

$\log k_2 = -0.91$   $d^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

## 4.1.4.7 2,4,6-Tribromobiphenyl



Common Name: 2,4,6-Tribromobiphenyl

Synonym: PBB-30

Chemical Name: 2,4,6-tibromobiphenyl

CAS Registry No: 59080-33-0

Molecular Formula:  $C_{12}H_7Br_3$

Molecular Weight: 390.896

Melting Point ( $^{\circ}C$ ):

64 (Ruelle & Kesselring 1997)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

208.3 (Ruelle & Kesselring 1997)

254.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.414 (mp at  $64^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.016 (generator column-GC, Gobas et al. 1988)

0.0131 (quoted, Chessells et al. 1992)

0.054 (calculated-MCI  $\chi$ , Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

6.03 (HPLC-RT correlation, Gobas et al. 1988, 1989)

6.03; 4.78 (quoted; calculated-UNIFAC, Chen et al. 1993)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

5.06 (guppy, lipid weight-based, Gobas et al. 1989)

3.97; 5.06 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)

4.408, 4.645 (calculated-MCI  $\chi$ ,  $K_{ow}$ , Lu et al. 1999)

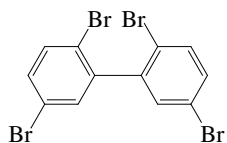
Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$\log k_1 = 3.05 d^{-1}$ ;  $\log k_2 = -0.83 d^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

**4.1.4.8 2,2',5,5'-Tetrabromobiphenyl**

Common Name: 2,2',5,5'-Tetrabromobiphenyl

Synonym: PBB-52

Chemical Name: 2,2',5,5'-tetrabromobiphenyl

CAS Registry No: 59080-37-4

Molecular Formula:  $C_{12}H_6Br_4$

Molecular Weight: 469.792

Melting Point ( $^{\circ}C$ ):

144 (Ruelle & Kesselring 1997)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

224.4 (Ruelle & Kesselring 1997)

277.8 (calculated-Le Bas at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.068 (mp at  $144^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

0.00429 (generator column-GC, Gobas et al. 1988)

0.0545 (quoted, Chessells et al. 1992)

0.00409 (calculated-AQUAFAC, Myrdal et al. 1995)

0.00246 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

6.50 (HPLC-RT correlation, Gobas et al. 1988,)

4.88 (calculated-UNIFAC group contribution, Chen et al. 1993)

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

6.16 (guppy, lipid weight-based, Gobas et al. 1989)

4.62; 6.16 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)

5.097; 6.16 (calculated-MCI  $\chi$ ,  $K_{ow}$ , Lu et al. 1999)

Sorption Partition Coefficient,  $\log K_{oc}$ :

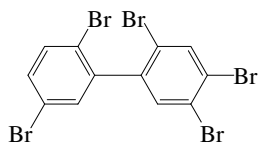
Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$\log k_1 = 2.96 d^{-1}$ ;  $\log k_2 = -2.02 d^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

## 4.1.4.9 2,2',4,5,5'-Pentabromobiphenyl



Common Name: 2,2',4,5,5'-Pentabromobiphenyl

Synonym:

Chemical Name: 2,2',4,5,5'-pentabromobiphenyl

CAS Registry No: 6788-96-4

Molecular Formula:  $C_{12}H_5Br_5$

Molecular Weight: 548.688

Melting Point ( $^{\circ}C$ ):

157 (Dickhut et al. 1994; Ruelle & Kesselring 1997)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$  at  $20^{\circ}C$ ):

Molar Volume ( $cm^3/mol$ ):

301.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

45.44 (Doucette & Andren 1988)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0507 (mp at  $157^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$  or as indicated and reported temperature dependence equations.):

$1.032 \times 10^{-4}$ ,  $4.42 \times 10^{-4}$ ,  $9.82 \times 10^{-4}$  ( $4.9$ ,  $25$ ,  $40^{\circ}C$ , generator column-GC/ECD, Doucette & Andren 1988a)

$S/(mol/L) = 1.52 \times 10^{-10} \exp(0.063 \cdot t/^{\circ}C)$  (generator column-GC, temp range  $4-40^{\circ}C$ , Doucette & Andren 1988a)

$\log x = -2374/(T/K) - 2.373$ , temp range  $4-40^{\circ}C$  (generator column-GC, Doucette & Andren 1988a)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

77.10 (generator column-GC Doucette & Andren 1987)

77.10; 8.76 (generator column-GC; HPLC-RT correlation, Doucette & Andren 1988b)

7.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

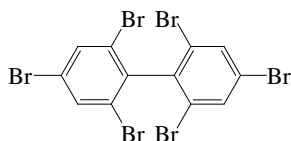
Sorption Partition Coefficient,  $\log K_{OC}$ :

Environmental Fate Rate Constants,  $k$  or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:



## 4.1.4.10 2,2',4,4',6,6'-Hexabromobiphenyl



Common Name: 2,2',4,4',6,6'-Hexabromobiphenyl

Synonym: 2,2',4,4',6,6'-HBB

Chemical Name: 2,2',4,4',6,6'-hexabromobiphenyl

CAS Registry No: 59261-08-4

Molecular Formula:  $C_{12}H_4Br_6$

Molecular Weight: 627.584

Melting Point ( $^{\circ}C$ ):

176 (Gobas et al. 1988; Ruelle & Kesselring 1997)

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

256.6 (Ruelle & Kesselring 1997)

324.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.033 (mp at  $176^{\circ}C$ )

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

$6.23 \times 10^{-4}$  (generator column-GC, Gobas et al. 1988)

0.0210 (lit. mean, Chessells et al. 1992)

$1.04 \times 10^{-4}$  (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at  $25^{\circ}C$ ):

$8.033 \times 10^{-6}$  (for hexabrominated biphenyl, GC-RT correlation, Watanabe & Tatsukawa 1989)

$4.52 \times 10^{-10}$  (quoted, Pijnenburg et al. 1995)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

7.50 (for hexabrominated biphenyl, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

7.20 (HPLC-RT correlation, Gobas et al. 1987, 1989)

7.20; 5.09 (quoted; calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient,  $\log K_{OA}$ :

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

5.85 (guppy, lipid weight-based, Gobas et al. 1989)

4.26 (calculated- $K_{ow}$ , Chessells et al. 1992)

Sorption Partition Coefficient,  $\log K_{OC}$ :

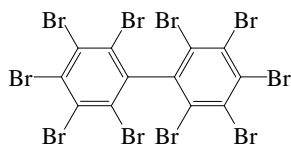
Environmental Fate Rate Constants,  $k$  and Half-Lives,  $t_{1/2}$ :

Bioconcentration and Uptake and Elimination Rate Constants ( $k_1$  and  $k_2$ ):

$\log k_1 = 2.51 d^{-1}$ ;  $\log k_2 = -2.15 d^{-1}$  (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

## 4.1.4.11 Decabromobiphenyl



Common Name: Decabromobiphenyl

Synonym: PBB-209

Chemical Name:

CAS Registry No: 13654-09-6

Molecular Formula:  $C_{12}Br_{10}$

Molecular Weight: 943.168

Melting Point ( $^{\circ}C$ ):

Boiling Point ( $^{\circ}C$ ):

Density ( $g/cm^3$ ):

Molar Volume ( $cm^3/mol$ ):

417.6 (calculated-Le Bas method at normal boiling point)

Heat of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F:

Water Solubility ( $g/m^3$  or  $mg/L$  at  $25^{\circ}C$ ):

Vapor Pressure (Pa at  $25^{\circ}C$ ):

$> 1.33 \times 10^{-9}$  (GC-RT correlation, Watanabe & Tatsukawa 1989)

$< 7.4 \times 10^{-4}$  (quoted, Pijnenburg et al. 1995)

Henry's Law Constant ( $Pa \cdot m^3/mol$ ):

Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

8.58; 12.63, 9.36 (generator column-GC; calculated-group contribution method, estimated-TSA and  $K_{ow}$ , Doucette & Andren 1987)

8.58; 10.42, 13.87, 8.46, 8.69, 7.10 (generator column-GC; calculated- $\pi$  const., HPLC-RT correlation, calculated-MW, calculated-MCI  $\chi$ , calculated-TSA and  $K_{ow}$ , Doucette & Andren 1988b)

8.60 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

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:

## 4.2 SUMMARY TABLES AND QSPR PLOTS

**TABLE 4.2.1**  
Summary of physical properties of polynuclear aromatic hydrocarbons (PAHs)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p.°C	b.p.°C	Fugacity ratio, F at 25°C*	Molar volume, V <sub>M</sub> cm <sup>3</sup> /mol	
							MW/ρ at 20°C	Le Bas
Indan	496-11-7	C <sub>9</sub> H <sub>10</sub>	118.175	-51.38	177.97	1	123.0	143.7
Naphthalene	91-20-3	C <sub>10</sub> H <sub>8</sub>	128.171	80.26	217.9	0.287	125.0	147.6
1-Methyl-	90-12-0	C <sub>11</sub> H <sub>10</sub>	142.197	-30.43	244.7	1	139.4	169.8
2-Methyl-	91-57-6	C <sub>11</sub> H <sub>10</sub>	142.197	34.6	241.1	0.805	141.4	169.8
1,2-Dimethyl-	573-98-8	C <sub>12</sub> H <sub>12</sub>	156.223	0.8	266.5	1		192.0
1,3-Dimethyl-	575-41-7	C <sub>12</sub> H <sub>12</sub>	156.223	-6	263	1	154.0	192.0
1,4-Dimethyl-	571-58-4	C <sub>12</sub> H <sub>12</sub>	156.223	7.6	268	1	153.7	192.0
1,5-Dimethyl-	571-61-9	C <sub>12</sub> H <sub>12</sub>	156.223	82	265	0.276		192.0
2,3-Dimethyl-	581-40-8	C <sub>12</sub> H <sub>12</sub>	156.223	105	268	0.164	155.8	192.0
2,6-Dimethyl-	581-42-0	C <sub>12</sub> H <sub>12</sub>	156.223	112	262	0.140	155.8	192.0
1-Ethyl-	1127-76-0	C <sub>12</sub> H <sub>12</sub>	156.223	-10.9	258.6	1	155.0	192.0
2-Ethyl-	939-27-5	C <sub>12</sub> H <sub>12</sub>	156.223	-7.4	258	1	157.4	192.0
1,4,5-Trimethyl-	2131-41-1	C <sub>13</sub> H <sub>14</sub>	170.250	63	285	0.424		214.2
Biphenyl	92-52-4	C <sub>12</sub> H <sub>10</sub>	154.207	68.93	256.1	0.371	148.3	184.6
4-Methyl-	644-08-6	C <sub>13</sub> H <sub>12</sub>	168.234	49.5	267.5	0.575		206.8
4,4'-Dimethyl-	613-33-2	C <sub>14</sub> H <sub>14</sub>	182.261	125	295	0.104		229.0
Diphenylmethane	101-81-5	C <sub>13</sub> H <sub>12</sub>	168.234	25.4	265	0.991	167.2	206.8
Bibenzyl	103-29-7	C <sub>14</sub> H <sub>14</sub>	182.261	52.5	284	0.537		229.0
<i>trans</i> -Stilbene	103-30-0	C <sub>14</sub> H <sub>12</sub>	180.245	124.2	307	0.106	185.7	221.6
Acenaphthylene	208-96-8	C <sub>12</sub> H <sub>8</sub>	150.192	91.8	280	0.221		165.7
Acenaphthene	83-32-9	C <sub>12</sub> H <sub>10</sub>	154.207	93.4	279	0.213	126.2	173.1
Fluorene	86-73-7	C <sub>13</sub> H <sub>10</sub>	166.218	114.77	295	0.132		187.9
1-Methylfluorene	1730-37-6	C <sub>14</sub> H <sub>12</sub>	180.245	87	318	0.246		210.1
Phenanthrene	85-01-8	C <sub>14</sub> H <sub>10</sub>	178.229	99.24	340	0.187		199.2
1-Methyl-	832-69-9	C <sub>15</sub> H <sub>12</sub>	192.256	123	354	0.109		221.4
Anthracene	120-12-7	C <sub>14</sub> H <sub>10</sub>	178.229	215.76	339.9	0.0134		196.7
2-Methyl-	613-12-7	C <sub>15</sub> H <sub>12</sub>	192.256	209	359	0.0157		218.9
9-Methyl-	779-02-2	C <sub>15</sub> H <sub>12</sub>	192.256	81.5		0.279		218.9
9,10-Dimethyl-	781-43-1	C <sub>16</sub> H <sub>14</sub>	206.282	183.6	360	0.0278		241.1

(Continued)

TABLE 4.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V <sub>M</sub> cm <sup>3</sup> /mol	
							MW/ρ at 20°C	Le Bas
Pyrene	129-00-0	C <sub>16</sub> H <sub>10</sub>	202.250	150.62	404	0.0585		213.8
Fluoranthene	206-44-0	C <sub>16</sub> H <sub>10</sub>	202.250	110.19	384	0.146		217.3
Benzo[ <i>a</i> ]fluorene	238-84-6	C <sub>17</sub> H <sub>12</sub>	216.227	189.5	405	0.0243		239.5
Benzo[ <i>b</i> ]fluorene	243-17-4	C <sub>17</sub> H <sub>12</sub>	216.227	212	401	0.0146		239.5
Chrysene	218-01-9	C <sub>18</sub> H <sub>12</sub>	228.288	255.5	448	0.00548	179.2	250.8
Triphenylene	217-59-4	C <sub>18</sub> H <sub>12</sub>	228.288	197.8	425	0.0202		250.8
<i>o</i> -Terphenyl	84-15-1	C <sub>18</sub> H <sub>14</sub>	230.304	56.2	332	0.494		273.2
<i>m</i> -Terphenyl	92-06-8	C <sub>18</sub> H <sub>14</sub>	230.304	87	363	0.246	192.1	273.2
<i>p</i> -Terphenyl	92-94-4	C <sub>18</sub> H <sub>14</sub>	230.304	213.9	376	0.0140		273.2
Naphthacene	92-24-0	C <sub>18</sub> H <sub>12</sub>	228.288	357	sublim	0.00055		250.8
Benz[ <i>a</i> ]anthracene	56-55-3	C <sub>18</sub> H <sub>12</sub>	228.288	160.5	438	0.0468		248.3
Benzo[ <i>b</i> ]fluoranthene	205-99-2	C <sub>20</sub> H <sub>12</sub>	252.309	168	481	0.0395		268.9
Benzo[ <i>j</i> ]fluoranthene	205-82-3	C <sub>20</sub> H <sub>12</sub>	252.309	166	480	0.0414		268.9
Benzo[ <i>k</i> ]fluoranthene	207-08-9	C <sub>20</sub> H <sub>12</sub>	252.309	217	480	0.0131		268.9
Benzo[ <i>a</i> ]pyrene	50-32-8	C <sub>20</sub> H <sub>12</sub>	252.309	181.1	495	0.0294		262.9
Benzo[ <i>e</i> ]pyrene	192-97-2	C <sub>20</sub> H <sub>12</sub>	252.309	181.4	311	0.0292		262.9
Perylene	198-55-0	C <sub>20</sub> H <sub>12</sub>	252.309	277.76	503	0.00331		262.9
7,12-DMBA	57-97-6	C <sub>20</sub> H <sub>16</sub>	256.341	122.5		0.111		292.7
9,10-DMBA	56-56-35	C <sub>20</sub> H <sub>16</sub>	256.341	122		0.112		292.7
3-MCA	56-49-5	C <sub>21</sub> H <sub>16</sub>	268.352	180		0.0301	209.6	296.0
Benzo[ghi]perylene	191-24-2	C <sub>22</sub> H <sub>12</sub>	276.330	272.5		0.00373		277.5
Indeno[1,2,3- <i>c,d</i> ]pyrene	193-39-5	C <sub>22</sub> H <sub>12</sub>	276.330	162		0.0453		283.5
Dibenz[ <i>a,c</i> ]anthracene	215-58-7	C <sub>22</sub> H <sub>14</sub>	278.346	205		0.0171		299.9
Dibenz[ <i>a,h</i> ]anthracene	53-70-3	C <sub>22</sub> H <sub>14</sub>	278.346	269.5	524	0.00399		299.9
Dibenz[ <i>a,j</i> ]anthracene	224-41-9	C <sub>22</sub> H <sub>14</sub>	278.346	197.5		0.0203		299.9
Pentacene	135-48-8	C <sub>22</sub> H <sub>14</sub>	278.346	> 300 dec				299.9
Coronene	191-07-1	C <sub>24</sub> H <sub>12</sub>	300.352	437.4	525	0.00009		292.1
2,4'',5-Trichloro- <i>p</i> -terphenyl	61576-93-0	C <sub>18</sub> H <sub>11</sub> Cl <sub>3</sub>	333.639	92		0.220		335.9
2,4,4'',6-Tetrachloro- <i>p</i> -terphenyl		C <sub>18</sub> H <sub>10</sub> Cl <sub>4</sub>	368.084	114		0.134		356.8
1-Chloronaphthalene	90-13-1	C <sub>10</sub> H <sub>7</sub> Cl	162.616	-2.5	259	1	136.2	168.5
2-Chloronaphthalene	91-58-7	C <sub>10</sub> H <sub>7</sub> Cl	162.616	58	256	0.474		168.5
1,2-Dichloronaphthalene	2050-69-3	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>	197.061	36	296.5	0.780		189.4
1,4-Dichloronaphthalene	1825-31-6	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>	197.061	67.5	288	0.383		189.4
1,8-Dichloronaphthalene	2050-74-0	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>	197.061	89	sublim	0.236		189.4

2,3-Dichloronaphthalene	2050–75–1	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>	197.061	120		0.117		189.4
2,7-Dichloronaphthalene	2198–77–8	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>	197.061	115		0.131		189.4
1,2,3-Trichloronaphthalene	50402–52–3	C <sub>10</sub> H <sub>5</sub> Cl <sub>3</sub>	231.506	81–84		0.273		210.3
1,3,7-Trichloronaphthalene	55720–37–1	C <sub>10</sub> H <sub>5</sub> Cl <sub>3</sub>	231.506	113	274	0.137		210.3
1,2,3,4-Tetrachloronaphthalene	20020–02–4	C <sub>10</sub> H <sub>4</sub> Cl <sub>4</sub>	265.951	199		0.0196		231.2
1,2,3,5-Tetrachloronaphthalene	53555–63–8	C <sub>10</sub> H <sub>4</sub> Cl <sub>4</sub>	265.951	141		0.0728		231.2
1,3,5,7-Tetrachloronaphthalene	53555–64–9	C <sub>10</sub> H <sub>4</sub> Cl <sub>4</sub>	265.951	179		0.0308		231.2
1,3,5,8-Tetrachloronaphthalene	31604–28–1	C <sub>10</sub> H <sub>4</sub> Cl <sub>4</sub>	265.951	131		0.0912		231.2
1,2,3,4,6-Pentachloronaphthalene	67922–25–2	C <sub>10</sub> H <sub>3</sub> Cl <sub>5</sub>	300.396	147		0.0635		252.1
1,2,3,5,7-Pentachloronaphthalene	53555–65–0	C <sub>10</sub> H <sub>3</sub> Cl <sub>5</sub>	300.396	171	313	0.0369		252.1
1,2,3,5,8-Pentachloronaphthalene	150224–24–1	C <sub>10</sub> H <sub>3</sub> Cl <sub>5</sub>	300.396	174–176		0.0340		252.1
1,2,3,4,5,7-Hexachloronaphthalene	67927–67–4	C <sub>10</sub> H <sub>2</sub> Cl <sub>6</sub>	334.842	194	331	0.0220		273.0
1,2,3,4,6,7-Hexachloronaphthalene	103426–96–6	C <sub>10</sub> H <sub>2</sub> Cl <sub>6</sub>	334.842	205–206		0.0340		273.0
1,2,3,5,6,7-Hexachloronaphthalene	103426–97–7	C <sub>10</sub> H <sub>2</sub> Cl <sub>6</sub>	334.842	234–235		0.00880		273.0
1,2,3,5,7,8-Hexachloronaphthalene	103426–94–4	C <sub>10</sub> H <sub>2</sub> Cl <sub>6</sub>	334.842	148–149		0.0614		273.0
1,2,3,4,5,6,7-Heptachloro-	58863–14–2	C <sub>10</sub> HCl <sub>7</sub>	369.287					293.9
1,2,3,4,5,6,8-Heptachloro-	58863–15–3	C <sub>10</sub> HCl <sub>7</sub>	369.287	194	348	0.0220		293.9
Octachloronaphthalene	2234–13–1	C <sub>10</sub> Cl <sub>8</sub>	403.731	197.5	365	0.0203		314.8
1-Bromonaphthalene	90–11–9	C <sub>10</sub> H <sub>7</sub> Br	207.067	6.1	281	1	140.0	170.9
2-Bromonaphthalene	580–13–1	C <sub>10</sub> H <sub>7</sub> Br	207.067	55.9	281.5	0.498		170.9
1,4-Dibromonaphthalene	83–53–4	C <sub>10</sub> H <sub>6</sub> Br <sub>2</sub>	285.963	83	310	0.270		194.2
2,3-Dibromonaphthalene	13214–70–5	C <sub>10</sub> H <sub>6</sub> Br <sub>2</sub>	285.963	140		0.0744		194.2
4-Bromobiphenyl	92–66–0	C <sub>12</sub> H <sub>9</sub> Br	233.103	91.5	310	0.223		207.9
4,4'-Dibromobiphenyl	92–86–4	C <sub>12</sub> H <sub>8</sub> Br <sub>2</sub>	312.000	164	357.5	0.0433		231.2
2,4,6-Tribromobiphenyl	59080–33–0	C <sub>12</sub> H <sub>7</sub> Br <sub>3</sub>	390.896	64		0.414		254.5
2,2',5,5'-Tetrabromobiphenyl	59080–37–4	C <sub>12</sub> H <sub>6</sub> Br <sub>4</sub>	469.792	144		0.0680		277.8
2,2',4,5,5'-Pentabromobiphenyl	6788–96–4	C <sub>12</sub> H <sub>5</sub> Br <sub>5</sub>	548.688	157		0.0507		301.1
2,2',4,4',6,6'-Hexabromobiphenyl	59261–08–4	C <sub>12</sub> H <sub>4</sub> Br <sub>6</sub>	627.584	176		0.0330		324.4
Decabromobiphenyl	13654–09–6	C <sub>12</sub> Br <sub>10</sub>	943.168					417.6

Note:

3-MCA	3-Methylcholanthrene
7,12-DMBA	7,12-Dimethylbenz[ <i>a</i> ]anthracene
9,10-DMBA	9,10-Dimethylbenz[ <i>a</i> ]anthracene

\* Assuming  $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$ .

TABLE 4.2.2

Summary of selected physical-chemical properties of polynuclear aromatic hydrocarbons (PAHs) at 25°C

Compound	Selected properties		Solubility			Henry's law constant	
	Vapor pressure		S/(g/m³)	C <sup>S</sup> /(mmol/m³)	C <sub>L</sub> /(mmol/m³)	log K <sub>OW</sub>	H/(Pa·m³/mol)
	P <sup>S</sup> /Pa	P <sub>L</sub> /Pa					calculated P/C
Indan	197	197	100	846.2	846.2	3.33	232.8
Naphthalene	10.4	36.24	31	241.9	842.7	3.37	43.00
1-Methyl-	8.84	8.84	28	196.9	196.9	3.87	44.89
2-Methyl-	9.0	11.2	25	175.8	218.4	3.86	51.19
1,2-Dimethyl-	0.87	0.87				4.31	
1,3-Dimethyl-			8	51.21	51.21	4.42	
1,4-Dimethyl-	2.27	2.27	11.4	72.97	72.97	4.37	31.11
1,5-Dimethyl-			3.1	19.84	71.90	4.38	
2,3-Dimethyl-	1.0	6.10	2.5	16.00	97.58	4.40	62.49
2,6-Dimethyl-	1.4	10.0	1.7	10.88	77.73	4.31	128.7
1-Ethyl-	2.51	2.51	10.1	64.65	64.65	4.40	38.82
2-Ethyl-	4.0	4.0	8.0	51.21	51.21	4.38	78.11
1,4,5-Trimethyl-	0.681	1.61	2.1	12.33	29.09	5.00	55.21
Biphenyl	1.3	3.50	7.0	45.39	122.4	3.90	28.64
4-Methyl-			4.05	24.07	41.87	4.63	
4,4'-Dimethyl-			0.175	0.960	9.232	5.09	
Diphenylmethane	0.0885	0.0893	16	95.10	95.10	4.14	0.931
Bibenzyl	0.406	0.756	4.37	23.98	44.65	4.70	16.93
<i>trans</i> -Stilbene	0.065	0.613	0.29	1.609	15.18	4.81	40.40
Acenaphthylene	0.9	4.14	16.1	107.2	485.0	4.00	8.396
Acenaphthene	0.3	1.41	3.80	24.64	115.7	3.92	12.17
Fluorene	0.09	0.682	1.90	11.43	85.60	4.18	7.873
1-Methyl-			1.09	6.047	24.58	4.97	
Phenanthrene	0.02	0.107	1.10	6.172	33.00	4.57	3.240
1-Methyl-			0.27	1.404	12.88	5.14	
Anthracene	0.001	0.0746	0.045	0.252	18.84	4.54	3.961
2-Methyl-			0.03	0.156	9.939	5.15	
9-Methyl-	0.00224	0.00803	0.261	1.358	4.866	5.07	1.650
9,10-Dimethyl-	1.53 × 10 <sup>-4</sup>	5.50 × 10 <sup>-3</sup>	0.056	0.271	9.765	5.25	0.564
Pyrene	0.0006	0.0119	0.132	0.652	12.89	5.18	0.919
Fluoranthene	0.00123	8.42 × 10 <sup>-3</sup>	0.26	1.286	8.805	5.22	0.957
Benzo[ <i>a</i> ]fluorene			0.045	0.208	8.564	5.40	

Benzo[ <i>b</i> ]fluorene			0.002	0.00925	0.634	5.75	
Chrysene	$5.70 \times 10^{-7}$	$1.07 \times 10^{-4}$	0.002	0.00876	1.599	5.60	0.065
Triphenylene	$2.30 \times 10^{-9}$	$1.21 \times 10^{-4}$	0.043	0.188	9.325	5.49	0.012
<i>p</i> -Terphenyl	$4.86 \times 10^{-9}$	$3.47 \times 10^{-4}$	0.0180	0.0782	5.583	6.03	0.062
Naphthacene	$7.30 \times 10^{-9}$	$1.33 \times 10^{-5}$	0.0006	0.00263	4.779	5.76	$2.77 \times 10^{-3}$
Benz[ <i>a</i> ]anthracene	$2.80 \times 10^{-5}$	$5.98 \times 10^{-4}$	0.011	0.0482	1.030	5.91	0.581
Benzo[ <i>b</i> ]fluoranthene			0.0015	0.00595	0.150	5.80	
Benzo[ <i>j</i> ]fluoranthene			0.0025	0.0099	0.239		
Benzo[ <i>k</i> ]fluoranthene	$5.20 \times 10^{-8}$	$3.97 \times 10^{-9}$	0.0008	0.00317	0.242	6.00	0.016
Benzo[ <i>a</i> ]pyrene	$7.00 \times 10^{-7}$	$2.38 \times 10^{-5}$	0.0038	0.0151	0.512	6.04	0.046
Benzo[ <i>e</i> ]pyrene	$7.40 \times 10^{-7}$	$2.53 \times 10^{-5}$	0.004	0.0159	0.543		0.047
Perylene	$1.40 \times 10^{-8}$	$4.23 \times 10^{-9}$	0.0004	0.00159	0.479	6.25	$8.83 \times 10^{-3}$
7,12-DMBA	$3.84 \times 10^{-8}$	$3.45 \times 10^{-7}$	0.0500	0.195	1.757	6.00	$1.97 \times 10^{-4}$
9,10-DMBA	$3.73 \times 10^{-7}$	$3.33 \times 10^{-9}$	0.0435	0.170	1.543	6.00	$2.20 \times 10^{-3}$
3-MCA	$1.03 \times 10^{-9}$	$3.42 \times 10^{-5}$	0.0019	0.00708	0.235	6.42	0.145
Benzo[ <i>ghi</i> ]perylene		$2.25 \times 10^{-5}$	0.00026	0.000941	0.252	6.50	
Indeno[1,2,3- <i>c,d</i> ]pyrene							
Dibenz[ <i>a,c</i> ]anthracene	$1.30 \times 10^{-9}$	$7.84 \times 10^{-8}$	0.0016	0.00575	0.336		$2.26 \times 10^{-4}$
Dibenz[ <i>a,h</i> ]anthracene	$3.70 \times 10^{-10}$	$9.27 \times 10^{-8}$	0.0006	0.00216	0.540	6.75	$1.72 \times 10^{-4}$
Dibenz[ <i>a,j</i> ]anthracene			0.012	0.0431	2.210		
Pentacene	$1.0 \times 10^{-10}$						
Coronene	$2.0 \times 10^{-10}$	$2.22 \times 10^{-9}$	0.00014	0.000466	5.179	6.75	$4.29 \times 10^{-4}$

Abbreviations:

3-MCA	3-Methylcholanthrene
7,12-DMBA	7,12-Dimethylbenz[ <i>a</i> ]anthracene
9,10-DMBA	9,10-Dimethylbenz[ <i>a</i> ]anthracene

TABLE 4.2.3

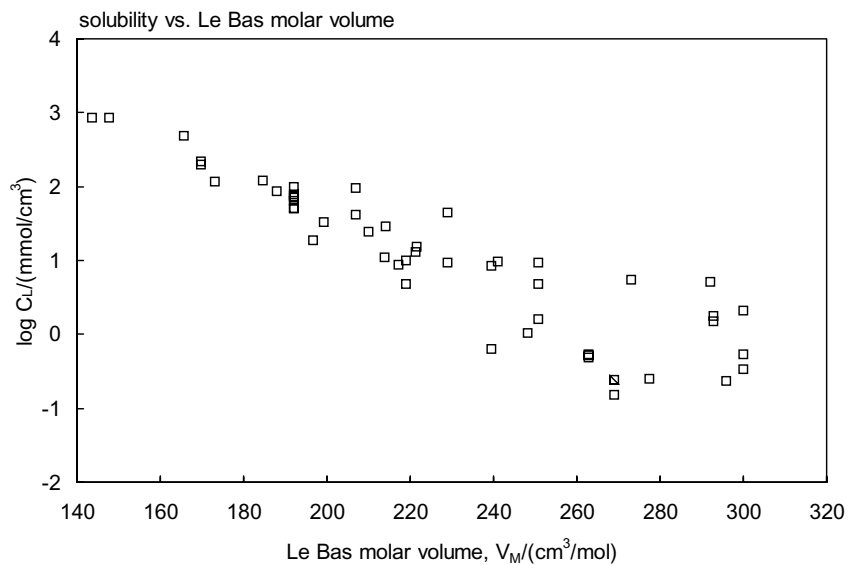
Suggested half-life classes of polynuclear aromatic hydrocarbons (PAHs) in various environment compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Indan	2	4	6	7
Naphthalene	2	4	6	7
1-Methyl-	2	4	6	7
2,3-Dimethyl-	2	4	6	7
1-Ethyl-	2	4	6	7
1,4,5-Trimethyl-	2	4	6	7
Biphenyl	3	4	5	6
Acenaphthene	3	5	7	8
Fluorene	3	5	7	8
Phenanthrene	3	5	7	8
Anthracene	3	5	7	8
Pyrene	4	6	8	9
Fluoranthene	4	6	8	9
Chrysene	4	6	8	9
Benz[ <i>a</i> ]anthracene	4	6	8	9
Benzo[ <i>k</i> ]fluoranthene	4	6	8	9
Benzo[ <i>a</i> ]pyrene	4	6	8	9
Perylene	4	6	8	9
Dibenz[ <i>a,h</i> ]anthracene	4	6	8	9

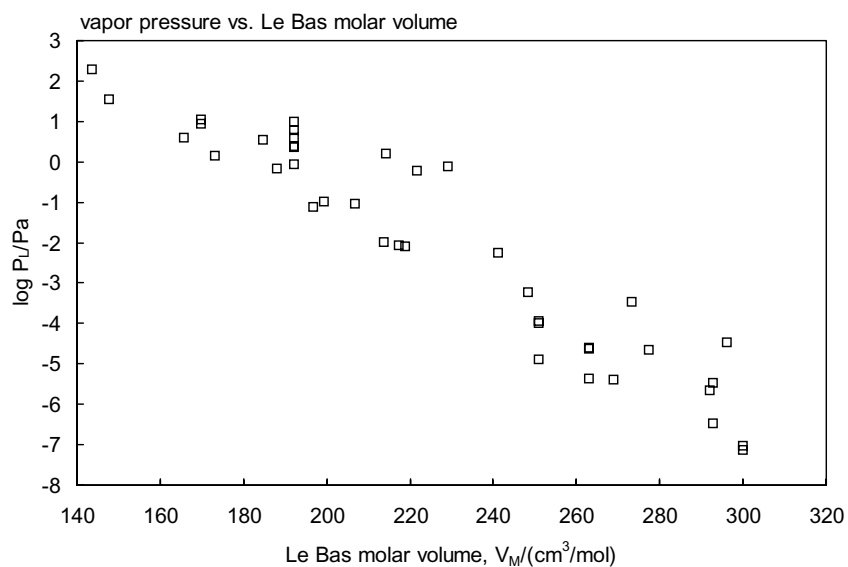
where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,00
9	55000 (~ 6 years)	> 30,000

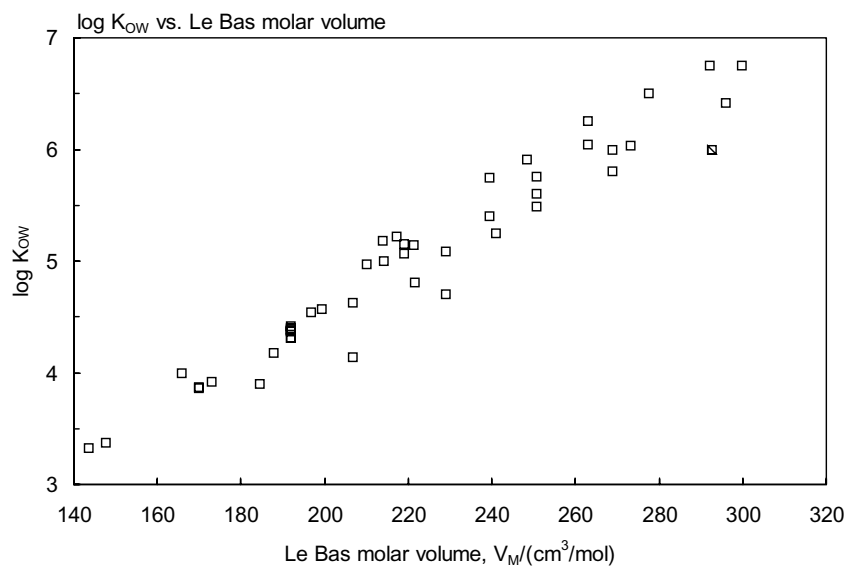




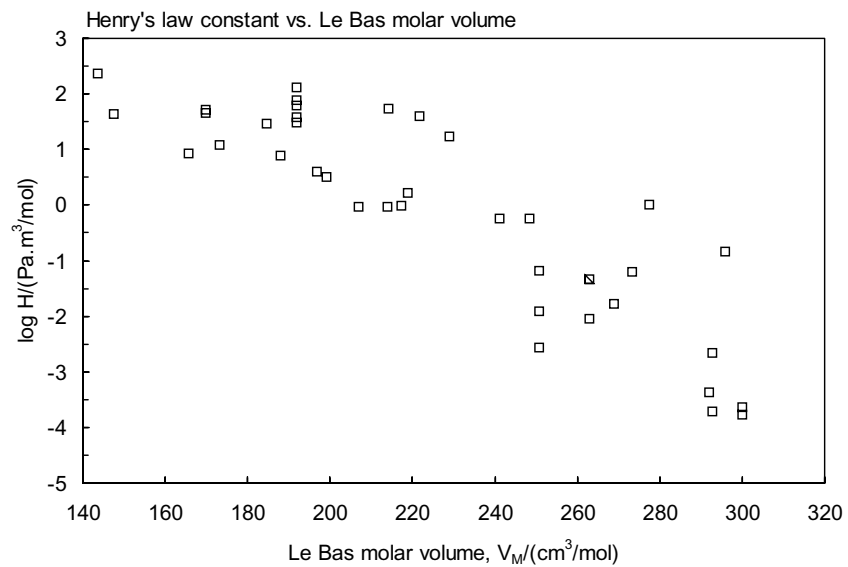
**FIGURE 4.2.1** Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polynuclear aromatic hydrocarbons.



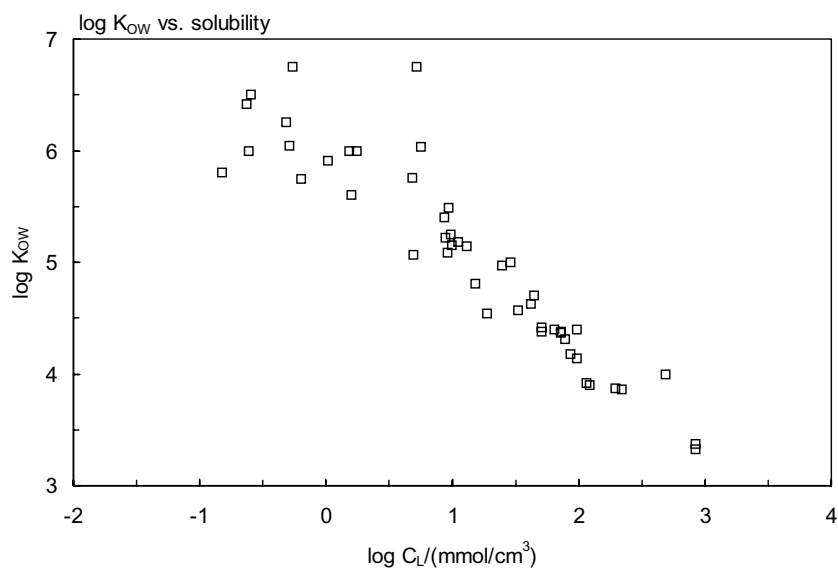
**FIGURE 4.2.2** Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polynuclear aromatic hydrocarbons.



**FIGURE 4.2.3** Octanol-water partition coefficient versus Le Bas molar volume for polynuclear aromatic hydrocarbons.



**FIGURE 4.2.4** Henry's law constant versus Le Bas molar volume for polynuclear aromatic hydrocarbons.



**FIGURE 4.2.5** Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polynuclear aromatic hydrocarbons.

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