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# 3 Mononuclear Aromatic Hydrocarbons

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### 3.1 LIST OF CHEMICALS AND DATA COMPILATIONS

#### 3.1.1 MONONUCLEAR AROMATIC HYDROCARBONS

##### 3.1.1.1 Benzene



Common Name: Benzene

Synonym: benzol, cyclohexatriene

Chemical Name: benzene

CAS Registry No: 71-43-2

Molecular Formula:  $C_6H_6$

Molecular Weight: 78.112

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

5.49 (Lide 2003)

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

80.09 (Lide 2003)

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

0.8765 (Weast 1982–1983)

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

89.1 ( $20^{\circ}C$ , calculated from density)

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

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

33.843, 30.726 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

9.916 (Tsonopoulos & Prausnitz 1971)

9.866 (Riddick et al. 1986)

9.87 (exptl., Chickos et al. 1999)

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

35.564 (Tsonopoulos & Prausnitz 1971)

35.4, 44.5 (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  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

1850 ( $30^{\circ}C$ , shake flask-interferometer, Gross & Saylor 1931)

1786 (shake flask-turbidimetric method, Stearns et al. 1947)

1402 (residue-volume method, Booth & Everson 1948)

1740 (shake flask-UV spec., Andrews & Keefer 1949)

1860 (shake flask-UV, Klevens 1950)

1790\* (shake flask-UV, Bohon & Claussen 1951)

1755 (shake flask-UV, McDevit & Long 1952)

1718 (shake flask-UV, Morrison & Billett 1952)

1796 (Hayashi & Sasaki 1956; quoted, Keeley et al. 1988)

1780, 1823 (selected, calculated-molar volume, Lindenburg 1956; quoted, Horvath 1982)

1760 (Brady & Huff 1958)

1740\* (shake flask-UV, measured range  $0.4$ – $45^{\circ}C$ , Arnold et al. 1958)

$S/(wt.\%) = 0.1806 - 0.001095 \cdot (t/^{\circ}C) + 3.170 \times 10^{-5} \cdot (t/^{\circ}C)^2$ ; temp range  $5$ – $45^{\circ}C$  (shake flask-UV, Arnold et al. 1958); or

$S/(wt.\%) = 0.1784 - 0.0007436 \cdot (t/^{\circ}C) + 1.1906 \times 10^{-5} \cdot (t/^{\circ}C)^2 + 1.217 \times 10^{-7} \cdot (t/^{\circ}C)^3$ ; temp range  $5$ – $45^{\circ}C$  (shake flask-UV, Arnold et al. 1958)

1800\* ( $24^{\circ}C$ , shake flask-UV, measured range  $0.8$ – $64.5^{\circ}C$ , Alexander 1959)

1890 ( $35^{\circ}C$ , shake flask-UV spectrophotometry, Hine et al. 1962)

1742\* (shake flask-UV, measured range  $17$ – $63^{\circ}C$ , Franks et al. 1963)

- 1780 (shake flask-GC, McAuliffe 1963, 1966)
- 2100\* (20°C, polythermic method, measured range 20–79.5°C, Udovenko & Aleksandrova 1963)
- 1778 (calculated-group contribution, Irmann 1965; quoted, Horvath 1982)
- 2167 (vapor saturation-UV, Worley 1967)
- 1740 (21°C, extraction by nonpolar resins/elution, Chey & Calder 1972)
- 1765\* (shake flask-GC, measured range 4–25°C, Leinonen 1972)
- 1830\* (shake flask-UV spectroscopy, measured range 25–55°C, Bradley et al. 1973)
- 1755 (shake flask-GC, Polak & Lu 1973)
- 1755\* (shake flask-GC, measured range 25–84.7°C, Price 1973)
- 1765 (shake flask-GC, Leinonen & Mackay 1973)
- 1760\* (shake flask-UV, measured range 4.5–20.1°C, Brown & Wasik 1974)
- 1906 (shake flask-UV, Vesala 1974)
- 1769 (shake flask-GC, Mackay et al. 1975)
- 1780 (shake flask-GC, Mackay & Shiu 1975)
- 1740 (shake flask-GC, Price 1976)
- 1791\* (generator column-HPLC/UV, May et al. 1978; May 1980)
- $S/(\mu\text{g/kg}) = [1833 + 0.3166 \cdot (t/^\circ\text{C})^2 - 0.6838 \cdot (t/^\circ\text{C})^3] \times 10^3$ ; temp range 0.2–25.8°C (generator column-HPLC/UV, May et al. 1978, 1980)
- $\log x = 424.544/(T/K)^2 - 2955.82/(T/K) + 1.6606$ ; temp range 0–55°C (Ueda et al. 1978)
- 1769 (shake flask-fluorescence spectrophotometry, Aqun-Yuen et al. 1979)
- 1734\* (20°C, shake flask-UV, Ben-Naim & Wilf 1979)
- 1790\* (20°C, shake flask-GC, Bittrich et al. 1979)
- 1820–1930 (elution chromatography-UV, Schwarz 1980)
- 1750 (shake flask-LSC, Banerjee et al. 1980)
- 1610\* (vapor saturation-UV spec., measured range 5–45°C, Sanemasa et al. 1981)
- 1787 (shake flask-GC, Chiou et al. 1982; 1983)
- 1620\* (vapor saturation-UV spec., measured range 5–45°C, Sanemasa et al. 1982)
- 1792\* (generator column-HPLC/UV, May et al. 1983)
- 1789 (generator column-HPLC, Wasik et al. 1983)
- 1809 (HPLC- $k'$  correlation, converted from reported  $\gamma_w$ , Hafkenscheid & Tomlinson 1983a)
- 1617 (vapor saturation-UV spec., Sanemasa et al. 1984)
- 1810 (shake flask-radiometric method, Lo et al. 1986)
- 1695 (shake flask-GC, Keeley et al. 1988)
- 1650 (shake flask-GC, Coutant & Keigley 1988)
- 1770\* (IUPAC recommended, temp range 0–70°C, Shaw 1989a)
- $S/(\text{g}/100 \text{ g soln}) = 5.5773 - 4.6067 \times 10^{-2} \cdot (T/K) + 1.2504 \times 10^{-4} \cdot (T/K)^2 - 1.0489 \times 10^{-7} \cdot (T/K)^3$ ; temp range 0–70°C (summary of literature data, Shaw 1989a)
- 1732\* (20°C, activity coefficient-GC, Cooling et al. 1992)
- 1840\* (30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen & Wagner 1994a)
- $\ln(1/x) = -6.191 + 14.03 \cdot [(T/K)/562.2]^{-1} - 3.511 \cdot [(T/K)/562.2]^{-2}$ ; temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994a)
- $\ln x = 6.191 - 14.03 \cdot (T_r/K)^{-1} + 3.511 \cdot (T_r/K)^{-2}$ ,  $T_r = T/T_c$ , the reduced temp, system temp  $T$  divided by critical temp  $T_c$  (Chen & Wagner 1994c)
- 1760 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
- $\ln x = -15.544647 - 1442.4276/(T/K) - 3.283 \times 10^{-5} \cdot (T/K)^2$ , temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
- $\ln x = -180.368 + 7524.83/(T/K) + 25.8585 \cdot \ln(T/K)$ ; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 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):

- 12654 (Hg manometer, Hovorka & Dreisbach 1934)
- 9960\* (20°C, manometer, measured range 0–50°C, Stuckey & Saylor 1940)
- $\log(P/\text{mmHg}) = 7.12491 - 1323.06/(T/K - 41.23)$ ; temp range 0–75°C (manometer, Stuckey & Saylor 1940)

- 11700\* (23.7°C, ebulliometry-manometer, measured range 14.5–80.9°C, Willingham et al. 1945)  
 $\log (P/\text{mmHg}) = 6.89324 - 1203.835/(219.924 + t/^\circ\text{C})$ ; temp range 14.5–80.9°C (ebulliometry-manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
- 13332\* (26.1°C, summary of literature data, Stull 1947)
- 11720\* (23.27°C, ebulliometry, measured range 10.9–80.9°C, Forziati et al. 1949)  
 $\log (P/\text{mmHg}) = 6.91210 - 1214.645/(221.205 + t/^\circ\text{C})$ ; temp range 10.9–80.9°C (ebulliometry-manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
- 12690 (interpolated-Antoine eq., Dreisbach 1955)  
 $\log (P/\text{mmHg}) = 6.90565 - 1211.033/(220.79 + t/^\circ\text{C})$ ; temp range 0–160°C (Antoine eq. for liquid state, Dreisbach 1955)
- 23450\* (39.093°C, summary of literature data, temp range 7.565–260°C, Bond & Thodos 1960)
- 545800\* (146.85°C, ebulliometry, measured range 146.85–286.85°C, Ambrose et al. 1967)
- 32045\* (46.85°C, summary of literature data, temp range 46.85–286.85°C, Ambrose et al. 1970)
- 12700\* (extrapolated-Antoine eq., Zwolinski & Wilhoit, 1971)  
 $\log (P/\text{mmHg}) = 6.90565 - 1211.033/(220.790 + t/^\circ\text{C})$ ; temp range –11.6 to 103.92°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 12680 (extrapolated, Antoine eq., Boublik et al. 1973; 1984)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 10254.2/(T/\text{K})] + 9.5560$ ; temp range –58 to –30°C (Antoine eq., Weast 1972–73)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 8146.5/(T/\text{K})] + 7.833714$ ; temp range –36.7 to 290.3°C (Antoine eq., Weast 1972–73)
- 12339\* (24.396°C, ebulliometry, measured range 19.071–32.467°C, Osborn & Scott 1978)
- 19933\* (32.182°C, ebulliometry, measured range 32.182–115.697°C, Scott & Osborn 1979)
- 12640\* (average, ebulliometry-bubble cap boilers, measured range 290–378 K, Ambrose 1981)
- 12100 (gas saturation-GC, Politzki et al. 1982)  
 $\log (P/\text{atm}) = (1 - 353.214/T) \times 10^{(0.832632 - 6.72598 \times 10^4 \cdot T + 6.38324 \times 10^7 \cdot T^2)}$ ; T in K, temp range 280.0–562.6 K (Cox vapor pressure eq., Chao et al. 1983)
- 12690, 12680 (interpolated-Antoine equations, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.01905 - 1204.637/(220.069 + t/^\circ\text{C})$ ; temp range 21.2–105°C (Antoine eq. from reported exptl. data of Ambrose 1981, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.01788 - 1203.677/(219.904 + t/^\circ\text{C})$ ; temp range 14.5–80.9°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
- 12690 (extrapolated, Antoine eq., Dean 1985, 1992)  
 $\log (P/\text{mmHg}) = 9.1064 - 1885.9/(244.2 + t/^\circ\text{C})$ ; temp range –12 to 3°C (Antoine eq., Dean 1985, 1992)  
 $\log (P/\text{mmHg}) = 6.90565 - 1211.033/(220.79 + t/^\circ\text{C})$ ; temp range 8–103°C (Antoine eq., Dean 1985, 1992)
- 12716 (headspace-GC, Hussam & Carr 1985)  
 $\log (P/\text{kPa}) = 6.02232 - 1206.33/(220.91 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)
- 12700 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log (P_s/\text{kPa}) = 10.0091 - 2836/(25.31 + T/\text{K})$ ; temp range 223–279 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)  
 $\log (P_s/\text{kPa}) = 8.45261 - 1986.69/(-23.089\text{C} + T/\text{K})$ ; temp range 218–279 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.01907 - 1204.682/(-53.072 + T/\text{K})$ ; temp range 279–377 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.06832 - 1236.034/(-48.99 + T/\text{K})$ ; temp range 353–422 K (Antoine eq.-IV, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.3607 - 1466.083/(-15.44 + T/\text{K})$ ; temp range 420–502 K (Antoine eq.-V, Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.51922 - 2809.514/(171.489 + T/\text{K})$ ; temp range 501–562 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- 13100\* (gas saturation, measured range –15.4 to 40°C, Liu & Dickhut 1994)  
 $\log (P/\text{mmHg}) = 31.7718 - 2.7254 \times 10^3/(T/\text{K}) - 8.4442 \cdot \log (T/\text{K}) - 5.3534 \times 10^{-9} \cdot (T/\text{K}) + 2.7187 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 279–562 K (vapor pressure eq., Yaws 1994)  
 $\log (P/\text{kPa}) = 6.02994 - 1211.033/[(T/\text{K}) - 52.36]$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

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

- 653 (30°C, concn ratio-UV, Saylor et al. 1938)  
 576 (Taha et al. 1966)  
 442\* (20.06°C, headspace-GC, Brown & Wasik 1974)  
 $\ln [H/(\text{Pa m}^3/\text{mol})] = 21.26071 - 4445.58/(T/K)$ ; temp range 4.5–20°C (regression eq. of exptl. data of Brown & Wasik 1974, Shiu & Ma 2000)  
 555, 530 (calculated as  $1/K_{AW}$ , calculated-bond contribution, Hine & Mookerjee 1975)  
 551 (headspace-GC, Vitenberg et al. 1975)  
 562, 556 (batch air stripping-GC, calculated-P/C, Mackay et al. 1979)  
 552\* (shake flask-concn. ratio-UV, measured range 10–30°C, Green & Frank 1979)  
 $\log (H/\text{atm}) = 8.58 - 1852.308/(T/K)$ ; temp range 10–30°C (shake flask-concn-UV, Green & Frank 1979)  
 $\ln (H/\text{atm}) = 8.58 - 1852.038/(T/K)$  (Kavanaugh & Trussell 1980)  
 554\* (equilibrium cell-concentration ratio-GC/FID, Leighton & Calo 1981)  
 $\ln (k_H/\text{atm}) = 19.02 - 3964/(T/K)$ ; temp range 1.0–27.2°C (equilibrium cell-concn ratio, Leighton & Calo 1981)  
 610\* (vapor-liquid equilibrium-GC, measured range 15–45°C, Sanemasa et al. 1981)  
 608\* (vapor-liquid equilibrium-GC, measured range 5–45°C, Sanemasa et al. 1982)  
 562 (gas stripping-GC, Warner et al. 1987)  
 740; 441 (20°C, EPICS-GC, calculated-P/C, Yurteri et al. 1987)  
 535; 588; 557; 554; 555 (EPICS-GC/FID; batch air stripping-GC; calculated P/C; direct concentration ratio; calculated-UNIFAC, Ashworth et al. 1988)  
 535\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm m}^3/\text{mol})] = 5.534 - 3194/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 586 (concentration ratio, Keeley et al. 1988)  
 555 (infinite activity coeff.  $\gamma^\infty$  from solubility measurement, Abraham et al. 1990)  
 564 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 570\* (extrapolated from equilibrium headspace-GC data, measured range 40–80°C, Ettre et al. 1993)  
 $\log (1/K_{AW}) = -2.1678537 + 836.2228/(T/K)$ ; temp range: 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)  
 569 (infinite activity coeff.  $\gamma^\infty$  in water determined by inert gas stripping-GC, Li et al. 1993)  
 604\* (equilibrium headspace-GC, measured range 10–30°C, Perlinger et al. 1993)  
 535\* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)  
 644 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)  
 488 (23°C, gas stripping-IR, Nielsen et al. 1994)  
 481\* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)  
 267, 612 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35‰, Dewulf et al. 1995)  
 $\ln K_{AW} = -3640/(T/K) + 0.00786 \cdot Z + 10.577$ ; with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)  
 552\* (25.4°C, gas stripping-HPLC/UV/fluorescence, Alaei et al. 1996)  
 $\ln [H/(\text{Pa m}^3/\text{mol})] = 21.87689 - 4672.28/(T/K)$ ; temp range: 4–34.9°C and enthalpy of volatilization  $\Delta H_{vol} = 32.2 \text{ kJ/mol}$  at 20°C; (gas stripping-HPLC/UV measurements, Alaei et al. 1996)  
 485 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 640\* (vapor-liquid equilibrium-GC, measured range 10–35°C, Turner et al. 1996)  
 $K_{AW} = 0.0763 + 0.00211 \cdot (T/K) + 0.000162 \cdot (T/K)^2$ ; temp range 0–50°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)  
 538\* (headspace equilibrium-GC, Peng & Wan 1997)  
 $\ln K_{AW} = 7.15 - 1397/(T/K)$ ; temp range 15–45°C (headspace equilibrium-GC, Peng & Wan 1997)  
 272 (gas stripping-GC, Altschuh et al. 1999)  
 439 (20°C, headspace equilibrium-GC, Peng & Wan 1998)  
 $\ln K_{AW} = 7.44 - 1448/(T/K)$ ; temp range 0–45°C (seawater with salinity of 36‰, headspace-GC, Peng & Wan 1998)  
 466 (21°C, headspace equilibrium-GC, de Wolf & Lieder 1998)  
 558 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 580.6 (modified EPICS method-GC, Ryu & Park 1999)  
 556 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)  
 466 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

- $\log K_{AW} = 5.053 - 1693/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)  
 538\* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)  
 $\ln K_{AW} = 8.1648 - 2889.4/(T/K)$ ; temp range 15–40°C (SPME-GC, Bierwagen & Keller 2001)  
 573.4\* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)  
 $\ln K_{AW} = 10.01 - 3430.4/(T/K)$ ; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)  
 514–606 (27°C, headspace equilibrium-GC, at different solute concn: 0.48–19.1 mg/L, measured temp range 300–315 K, Cheng et al. 2003)  
 558\* (headspace-GC, measured range 10–25°C, Bakierowska & Trzeszczyński 2003)  
 $\ln (1/K_{AW}) = 11.663 - 3920/(T/K)$ ; temp range 10–25°C, headspace-GC, Bakierowska & Trzeszczyński 2003)

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

- 2.13 (shake flask-UV, Fujita et al. 1964)  
 1.56, 1.65 (shake flask-UV, calculated-M.O. indices, Rogers & Cammarata 1969)  
 2.13 (calculated-fragment const., Rekker 1977)  
 2.13, 1.56, 2.15, 2.03, 2.04 (Hansch & Leo 1979)  
 2.39 (HPLC-RT correlation, Veith et al. 1979a)  
 2.12 (shake flask-LSC, Banerjee et al. 1980)  
 2.28 (HPLC- $k'$  correlation, Hanai et al. 1981)  
 2.11 (HPLC-RT correlation, McDuffie 1981)  
 2.43 (HPLC- $k'$  correlation, McDuffie 1981)  
 2.16 (HPLC- $k'$  correlation, D'Amboise & Hanai 1982)  
 2.13 (shake flask-GC, Watarai et al. 1982)  
 2.20 (shake flask-HPLC, Hammers et al. 1982)  
 2.18 (HPLC- $k'$  correlation, Miyake & Terada 1982)  
 2.02 (shake flask method, Eadsforth & Moser 1983)  
 2.38 (HPLC method, Eadsforth & Moser 1983)  
 2.10 (shake flask-GC, Platford 1983)  
 2.48 (HPLC-RT correlation, Swann et al. 1983)  
 2.10 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983b)  
 2.04 (HPLC-RV correlation, Garst 1984)  
 2.25 (RP-HPLC- $k'$  correlation, Rapaport & Eisenreich 1984)  
 2.13 (generator column-GC/ECD, Miller et al. 1984)  
 2.26 (HPLC- $k'$  correlation, De Kock & Lord 1987)  
 2.01 (generator column-reversed phase-LC, Schantz & Martire 1987)  
 2.16 (RP-HPLC-capacity factor correlation, Sherblom & Eganhouse 1988)  
 1.91 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)  
 2.13 (recommended, Sangster 1989, 1993)  
 2.186 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 2.21 (normal phase-HPLC- $k'$  correlation, Govers & Evers 1992)  
 2.13 (recommended, Hansch et al. 1995)  
 1.97\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

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

- 2.90\* (20.29°C, from GC-determined  $\gamma^\infty$  in octanol, measured range 20.290–50.28°C, Gruber et al. 1997)  
 2.80 (head-space GC-FID both phases, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 0.64 (pacific herring, Korn et al. 1977)  
 0.54 (eels, Ogata & Miyake 1978; Ogata et al. 1984)  
 1.10 (fathead minnow, Veith et al. 1980)  
 1.48, 1.0 (algae, fish, Freitag et al. 1984)  
 1.48 (algae, Geyer et al. 1984)  
 0.63 (gold fish, Ogata et al. 1984)

- < 1.0, 3.23 (fish, activated sludge, Freitag et al. 1985)  
 0.54, 0.64, 0.63; 1.38 (selected: eels, pacific herring, gold fish; calculated, Howard 1990)  
 1.63 (*S. capricornutum*, Herman et al. 1991)

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

- 1.92 (sediment, sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)  
 1.63; 1.82 (Hastings soil pH 5.6; Overton soil pH 7.8, batch equilibrium, Rogers et al. 1980)  
 1.78 (average of 17 sediments and soils, sorption isotherms by batch equilibrium, Karickhoff 1981)  
 1.58; 1.73; 1.64 (forest soil pH 5.6; forest soil pH 4.2; agricultural soil pH 7.4, Seip et al. 1986)  
 1.42 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)  
 1.34 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.08, 2.04 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.65, 2.59, 2.25 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.69, 2.66 (organic cations HDTMA treated soils: St. Clair soil B<sub>t</sub> horizon OC 3.25%; Oshtemo soil B<sub>t</sub> horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 1.89 (aquifer material with  $f_{OC}$  of 0.006 and measured partition coeff.  $K_p = 0.47$  mL/g., Abdul et al. 1990)  
 1.58, 1.49 (Riddles soil top layer, pH 5.0; below top layer pH 5.3, batch equilibrium, Boyd et al. 1990)  
 1.82, 1.87 (RP-HPLC- $k'$  correlation, humic acid-silica column, Szabo et al. 1990a,b)  
 1.74; 1.81 (Captina silt loam pH 4.97; McLaurin sandy loam pH 4.43, batch equilibrium, Walton et al. 1992)  
 1.75 (average of 5 soils, sorption isotherms by batch equilibrium method-GC, Xing et al. 1994)  
 1.96 (soil, calculated-molecular connectivity indices, Sabljic et al. 1995)  
 1.57, 1.62, 1.74 (RP-HPLC- $k'$  correlation on 3 different stationary phases, Szabo et al. 1995)  
 1.82, 1.84 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)  
 1.84, 1.86, 1.87, 1.88, 1.90, 1.87, 1.90 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)  
 2.76, 2.41 (natural zeolite modified with a cation surfactant HDTMA with surface coverage of 100, 200 mmol/kg at pH 7, batch equilibrium-sorption isotherm, Li et al. 2000)  
 1.64, 1.58, 1.78 (soils: organic carbon OC  $\geq 0.1\%$ , OC  $\geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)

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

- 1.26 (Woodburn silt loam soil, 1.9% organic matter, equilibrium isotherm-GC, Chiou et al. 1983)  
 1.04 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 1.89, 1.81 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.53, 2.46, 2.08 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil B<sub>t</sub> horizon OM 4.38%; Oshtemo soil B<sub>t</sub> horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 1.34; 1.14 (high-organic-content soils: Florida peat - 57.1% C; Michigan muck - 53.7% C, equilibrium isotherm-GC, Rutherford & Chiou 1992)

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

- Volatilization:  $t_{1/2} = 4.81$  h from water depth of 1 m (calculated, Mackay & Leinonen 1975; Haque et al. 1980);  
 $k = 0.03$  d<sup>-1</sup> with  $t_{1/2} = 23$  d in spring at 8–16°C,  $k = 0.22$  d<sup>-1</sup> with  $t_{1/2} = 31$  d in summer at 20–22°C,  $k = 0.054$  d<sup>-1</sup> with  $t_{1/2} = 13$  d in winter at 3–7°C during the periods when volatilization appears to dominate, and  $k = 0.101$  d<sup>-1</sup> with  $t_{1/2} = 6.9$  d with HgCl<sub>2</sub> in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983);  
 $t_{1/2} \sim 27$  h from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s is 2.7 h at 20°C (Lyman et al. 1982).



Photolysis: atmospheric photolysis  $t_{1/2} = 2808\text{--}16152$  h, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991);

aqueous photolysis  $t_{1/2} = 2808\text{--}16152$  h, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991);

reaction rate constants,  $k = 8.64 \times 10^{-4} \text{ h}^{-1}$  in air, and  $k = 1.8 \times 10^{-4} \text{ h}^{-1}$  in water (Mackay et al. 1985).

Oxidation: rate constant  $k$ ; and 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 are designated \*, see reference:

$k_{\text{OH}} = 1.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k_{\text{O}(^3\text{P})} = 0.24 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction of  $\text{O}(^3\text{P})$  atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{\text{OH}} \leq 2.3 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} \geq 5.1$  h;  $k_{\text{O}(^3\text{P})} = (0.144 \pm 0.2) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $\text{O}(^3\text{P})$  atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{\text{OH}} = 0.85 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ , with  $t_{1/2} = 2.4\text{--}24$  h (Darnall et al. 1976)

$k_{\text{OH}}^* = (1.20 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

photooxidation  $t_{1/2} = 8.021 \times 10^3\text{--}3.21 \times 10^5$  h in water, based on measured rate constant for reaction with OH radical in water (Güsten et al. 1981)

$k_{\text{OH}} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and residence time of 8.3 d, loss of 11.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = 28 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at 300 K (Lyman et al. 1982)

$k_{\text{OH}} = 0.82 \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 6.8$  d in the atmosphere (Mill 1982)

$k = (2.0 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 50–1000 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}} = (8.8 \pm 0.4) 1.45 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{\text{NO}_3} < 2.3 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 1.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson et al. 1985)

$k_{\text{OH}}^* = 1.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 1.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}} = 1.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K. (relative rate method, Ohta & Ohya 1985)

$k_{\text{OH}} = 1.26 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 23.8°C, with an atmospheric lifetime of 9.1 d (Edney et al. 1986)

$k_{\text{OH}}^* = 1.14 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp., measured range 239–354 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{\text{OH}}(\text{calc}) = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 1.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}}^* = (1.29 \pm 1.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k_{\text{OH}} = 1.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{\text{NO}_3} < 3.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson & Aschmann 1988)

$k_{\text{OH}}^* = 1.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 1.23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 1.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

$t_{1/2} = 6$  d in estuarine water (estimated, Lee & Ryan 1976)

$t_{1/2}(\text{aq. aerobic}) = 120\text{--}384$  h, based on seawater dieaway test data (Van der Linden 1978) and river dieaway data (Vaishnav & Babeu, 1987; Howard et al. 1991)

$k = 4.58 \times 10^{-3} \text{ h}^{-1}$  in water (Lee & Ryan 1979; Mackay et al. 1985)

$k = 0.2 \text{ yr}^{-1}$  with  $t_{1/2} = 110$  d (Zoeteman et al 1981; Olsen & Davis 1990)

$k = 0.5 \text{ d}^{-1}$  significant degradation in favourable aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2}(\text{aq. anaerobic}) = 2688\text{--}17280$  h, based on unacclimated aqueous anaerobic biodegradation screening test data (Horowitz et al. 1982; Howard et al. 1991)

$k = 0.12 \text{ d}^{-1}$  in river water (estimated, Bartholomew & Pfaender 1983; quoted, Battersby 1990)

$t_{1/2} = 8.6$  d in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991)

$k = 0.025 \text{ d}^{-1}$  with  $t_{1/2} = 28 \text{ d}$  in groundwater,  $k = 0.044 \text{ d}^{-1}$  with  $t_{1/2} = 16 \text{ d}$  in Lester River with nutrient and microbial addition, and  $k = 0.082 \text{ d}^{-1}$  with  $t_{1/2} = 8 \text{ d}$  in Superior harbor waters (Vaishnav & Babeu 1987)  
 $t_{1/2}(\text{aerobic}) = 5 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 110 \text{ d}$  in natural waters (Capel & Larson 1995)  
 $k = 0.58 \text{ d}^{-1}$  associated with microbial population growth initially followed by a slower second phase with  $k = 0.12 \text{ d}^{-1}$  degradation by *P. aeruginosa* is a two-stage process (Kim et al. 2003).

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

$t_{1/2} = 0.5 \text{ d}$  for elimination from eels,  $0.5 \text{ d}$  (Ogata & Miyake 1978).

#### Half-Lives in the Environment:

Air:  $t_{1/2} \geq 5.1 \text{ h}$ , based on a determined rate of disappearance in ambient LA basin air for reaction with OH radical at 300 K (Doyle et al. 1975);

$t_{1/2} = 2.4\text{--}24 \text{ h}$ , based on rate of disappearance for the reaction with OH radical (Darnall et al. 1976);  
 residence time of 8.3 d, loss of 11.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981);

$t_{1/2} = 50.1\text{--}501 \text{ h}$ , based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);  
 calculated lifetime of 9.1 d due to reaction with OH radical (Edney et al. 1986);  
 summer daylight lifetime of 115 h due to reaction with OH radical (Altshuller 1991);  
 calculated lifetimes of 9.4 d,  $> 4 \text{ yr}$  and  $> 4.5 \text{ yr}$  for reactions with OH radical,  $\text{NO}_3$  radical and  $\text{O}_3$ , respectively (Atkinson 2000).

#### Surface Water:

$t_{1/2} = 4.81 \text{ h}$ , based on evaporation loss at  $25^\circ\text{C}$  and 1 m depth of water (Mackay & Leinonen 1975)  
 biodegradation  $t_{1/2} \sim 6 \text{ d}$  in estuarine water (Lee & Ryan 1976)

$t_{1/2} = 120\text{--}384 \text{ h}$ , based on unacclimated aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991);

$t_{1/2} = 23 \text{ d}$  at  $8\text{--}16^\circ\text{C}$  in the spring,  $t_{1/2} = 3.1 \text{ d}$  at  $20\text{--}22^\circ\text{C}$  in the summer and  $t_{1/2} = 13 \text{ d}$  at  $3\text{--}7^\circ\text{C}$  in the winter, and  $t_{1/2} = 6.9 \text{ d}$  with  $\text{HgCl}_2$  in September 9–15 from mesocosm experiments (Wakeham et al. 1983).

Ground water:  $t_{1/2} \sim 1 \text{ yr}$  from persistence observed in the groundwater of Netherlands (Zoeteman et al. 1981),  
 $t_{1/2} = 240\text{--}17280 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991).

Soil:  $t_{1/2} = 120\text{--}384 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991);

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

$t_{1/2} = 365 \text{ d}$ , assumed first-order biological/chemical degradation in the soil (Jury et al. 1990);  
 disappearance  $t_{1/2} < 2 \text{ d}$  for test soils (Anderson et al. 1991).

#### Biota:

**TABLE 3.1.1.1.1**

**Reported aqueous solubilities of benzene at various temperatures and reported temperature dependence equations**

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

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

$$\ln x = A - B/T(K) \quad (3)$$

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_0, T_0 = 298.15 \text{ K} \quad (4)$$

1.

Bohon & Claussen 1951		Arnold et al. 1958		Alexander 1959		Franks 1963	
shake flask-UV		shake flask-UV		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>
0.4	1741	4.5	1720	0.8	1840	17	1714
5.2	1810	4.9	1770	9.4	1790	22	1723
10	1800	5.0	1740	16.8	1770	25	1742
14.9	1770	6.7	1740	24	1800	29	1745
21	1790	9.0	1730	31	1830	32	1788
25.6	1790	12.5	1720	38	1920	35	1823
30.2	1843	15	1730	44.7	2030	40.5	1905
34.9	1877	20	1710	51.5	2140	42	1910
42.8	1998	20.6	1720	65.4	2340	44	1931
		24.8	1710			46	1983
		24.9	1740			51	2075
		27.3	1745			56	2183
	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$						
25	2.42	30	1775			61	2305
12	-2.30	30.9	1884			63	2352
17	-0.25	45	1975				
18	0	49.8	2044				
22	1.34	54.5	2152				
27	3.01	59.8	2265				
32	4.435	64.8	2313				
37	5.86						
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.27$					
		at 25°C					

2.

Leinonen 1972		Udovenko & Aleksandrova 1963		Price 1973		Bradley et al. 1973	
shake flask-GC		polythermic method		shake flask-GC		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>
4	1710	20	2100	25	1755	25	1830
5	1737	40	2270	55.3	3980	45	2160
5.4	1746	40.5	2480	84.7	6468	55	2380
6.1	1735	44.5	2590				
7.0	1781	56.5	2880				
10.3	1748	60	3000				
13	1741	65	3190				
16	1730	79.5	3730				
19.1	1721						
22.1	1739						

(Continued)

TABLE 3.1.1.1.1 (Continued)

3.

Brown & Wasik 1974		May et al. 1980, 1983		Ben-Naim & Wiff 1979		Bittrich et al. 1979	
shake flask-UV		generator column-HPLC/UV		shake flask-UV		shake flask-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
4.5	1840	0.2	1836	10	1625	20	1790
6.3	1850	6.2	1804	20	1734	40	2025
7.1	1810	11	1799			69	2442
9.0	1810	13	1770				
11.8	1770	16.9	1762				
12.1	1770	18.6	1767				
15.1	1790	25.0	1790				
17.9	1790	25.8	1819				
20.1	1760						

temp dependence eq. 2  
given in May et al. 1978b and  
May 1980

S	mg/kg
a	0.0247
b	-0.6838
c	0.3166
d	1833

4.

Sanemasa et al. 1981		Shaw 1989a (IUPAC)		Cooling et al. 1992		Chen & Wagner 1994a	
vapor saturation-UV		recommended values		activity coefficient-GC		equilibrium flow cell-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
15	1540	0	1690	20	1732	30	1840
25	1610	5	1800	30	1688	40	2014
35	1770	10	1780	40	1712	50	2213
45	1870	15	1760	50	1760	60	2452
		20	1760			70	2713
		25	1770			80	3033
		30	1810			90	3472
		35	1860			100	4123
		40	1930				
		45	1990				
		50	2080				
		55	2190				
		60	2310				
		65	2410				
		70	2670				

Sanemasa et al. 1982  
vapor saturation-UV

t/°C	S/g·m <sup>-3</sup>
5	1620
15	1580
25	1620
35	1710
45	1800

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.07$   
at 25°C

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.69$   
25°C

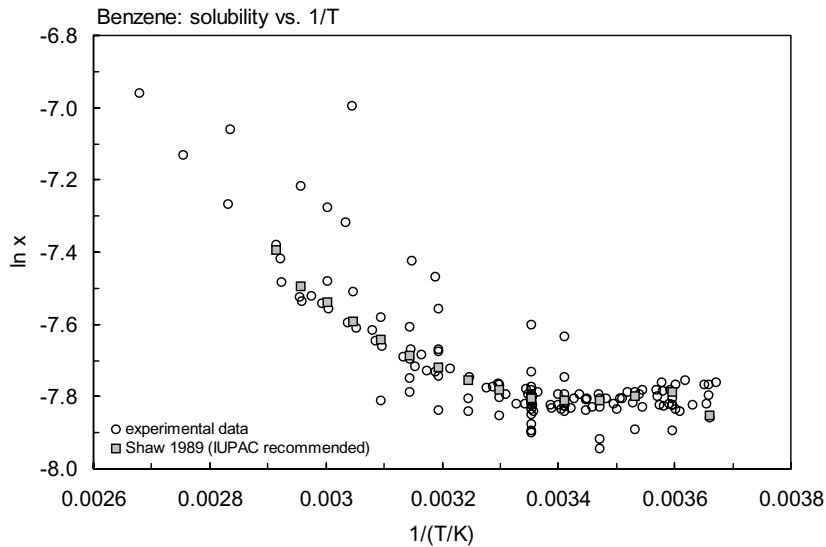


FIGURE 3.1.1.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzene.

TABLE 3.1.1.1.2  
Reported vapor pressures of benzene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)

log P = A – B/(C + t/°C)

log P = A – B/(C + T/K)

log P = A – B/(T/K) – C·log (T/K)

log P = A – B/(T/K) – C·log (T/K) + D·P/(T/K)<sup>2</sup>

(1)

(2)

(3)

(4)

(5)

ln P = A – B/(T/K)

ln P = A – B/(C + t/°C)

(1a)

(2a)

1.

Stuckey & Saylor 1940		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
mercury manometer		ebulliometry		summary of lit. data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	3509	14.548	7654	–36.7	133.3*	10.983	6397
12.5	6040	17.720	8962	–19.6	266.6*	14.575	7690
25	9960	20.504	10303	–11.5	1333*	17.697	8989
37.5	15800	23.270	11699	–2.60	2666*	20.028	11700
40	24240	26.886	13818	7.60	5333	23.271	11720
50	36050	31.004	16621	15.4	7999	26.908	13840
		35.191	19922	26.1	13332	31.013	16631
eq. 4	P/mmHg	30.078	23450	42.2	26664	35.207	19942
A	7.12491	44.284	28952	60.5	53323	39.095	23465
B	1323.06	49.066	34897	80.1	101325	44.294	28976
C	41.23	54.832	43320			49.084	34924
		60.784	53652		*solid	54.852	43358
bp/°C	80.06	67.135	66753	mp/°C	5.5	60.803	53697
		74.028	83717			67.148	66795
		78.891	97601			74.035	83746
		79.413	99197			78.903	97643
		79.898	100689			79.424	99230

(Continued)

TABLE 3.1.1.1.2 (Continued)

1.

Stuckey & Saylor 1940		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
mercury manometer		ebulliometry		summary of lit. data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		80.442	102384			79.090	100722
		80.922	106570			80.461	102460
						80.948	104000
		eq. 2	P/mmHg			eq. 2	P/mmHg
		A	6.89324			A	6.9210
		B	1203.835			B	1214.645
		C	219.924			B	221.205
		bp/°C	80.103			bp/°C	80.099

2.

Bond & Thodos 1960		Ambrose et al. 1967		Ambrose et al. 1970		Zwolinski & Wilhoit 1971	
compiled data		ebulliometry		compiled data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
7.565	5333	146.85	545800	46.85	32045	-11.6	1333*
39.093	23450	166.85	809200	66.85	66116	-2.60	2666*
67.15	66753	186.85	1156700	86.85	124180	3.0	4000*
95.713	159987	206.85	1603700	106.85	215960	7.55	5333
110.015	231848	226.85	2166700	126.85	352460	11.80	6666
150.015	577419	246.85	2864400	146.85	545760	15.39	7999
180.015	1017250	266.85	3719300	166.85	809050	21.293	10666
240.015	2589787	286.85	4771700	186.85	1156600	26.075	13332
260.015	3376922			206.85	1603800	35.266	19998
		eq. 5	P/mmHg	226.85	2166900	42.214	26664
eq. 5	P/mmHg	A	20.87440	246.85	2864000	47.868	33331
A	23.36128	B	2472.77	266.85	3718800	52.672	39997
B	2457.12	C	5.44671	286.85	4772600	60.611	53329
C	5.28840	D	1238			67.093	66661
D	1.56738					72.616	79993
bp/°C	80.115					77.454	93326
						78.354	95991
						79.236	98659
						80.100	101325
						25.0	12690
							*solid
						eq. 2	P/mmHg
						A	9.1064
						B	1885.9
						C	244.2
							for liquid
						eq. 2	P/mmHg
						A	6.90565
						B	1211.033
						C	220.790

TABLE 3.1.1.1.2 (Continued)

Bond & Thodos 1960		Ambrose et al. 1967		Ambrose et al. 1970		Zwolinski & Wilhoit 1971	
compiled data		ebulliometry		compiled data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						bp/°C	80.100
						$\Delta H_v/(\text{kJ mol}^{-1})$	
						at 25°C	33.85
						at bp	30.76

3.

Osborn & Scott 1978		Scott & Osborn 1979		Ambrose 1981			
ebulliometry		ebulliometry		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
				set 1		set 2	
19.071	9585	32.182	19933	290.076	8634	294.165	10527
21.728	10887	40.637	25023	302.392	15388	297.699	12431
24.396	12339	46.139	31177	311.186	22484	303.293	16017
27.0755	13955	51.684	38565	318.694	30464	306.060	18080
29.765	15748	57.276	47375	325.097	38953	314.942	26227
32.467	17735	62.991	57817	330.437	47571	318.971	30791
		68.591	70120	334.886	55511	323.246	36326
		74.319	84532	338.935	63815	328.325	43899
		80.092	101325	342.946	72985	334.125	54050
		85.911	120791	346.244	81275	338.779	63474
		91.777	143240	349.910	91346	348.400	87089
		97.689	169030	353.469	102043	352.356	98297
		103.645	198490	356.187	110854	353.212	101226
		109.648	232020	358.873	120137	353.802	103094
		115.697	270030	362.286	132779	357.611	115693
				365.234	144528	363.086	135887
				367.897	155797	367.789	155309
				370.527	167605	372.897	178812
				373.151	180059	378.152	205747
				375.844	193529		
				378.523	207939		
				381.325	223436		

4.

Ambrose 1981 (continued)				Liu & Dickhut 1994	
ebulliometry		ebulliometry		gas saturation-GC	
T/K	P/Pa	T/K	P/Pa	t/°C	P/Pa
set 3		set 4			
285.957	7014	297.769	12471	-15.4	880
292.893	9903	302.633	15553	-5.0	1750
298.684	13007	307.159	18957	10	6540
302.619	15545	308.384	19979	25	13100
304.302	16745	314.503	25716	40	26400
310.167	21539	319.907	31940		
314.406	25665	324.512	38019		
319.512	31444	329.473	45774		

(Continued)

TABLE 3.1.1.1.2 (Continued)

4.

Ambrose 1981 (continued)				Liu & Dickhut 1994	
ebulliometry		ebulliometry		gas saturation-GC	
T/K	P/Pa	T/K	P/Pa	t/°C	P/Pa
323.921	37264	333.842	53510		
329.536	45876	338.144	62115		
334.406	54580	342.687	77356		
339.063	64081	347.828	85511		
343.751	74940	352.112	97852		
348.357	86959	352.617	99394		
352.594	99320	352.955	100439		
353.078	100816	358.109	117426		
353.660	102633	362.258	132666		
358.727	119597	367.239	152938		
363.062	135783	372.175	175319		
367.554	154281	377.584	202669		
372.630	177510				
377.875	204219				
383.175	234260				

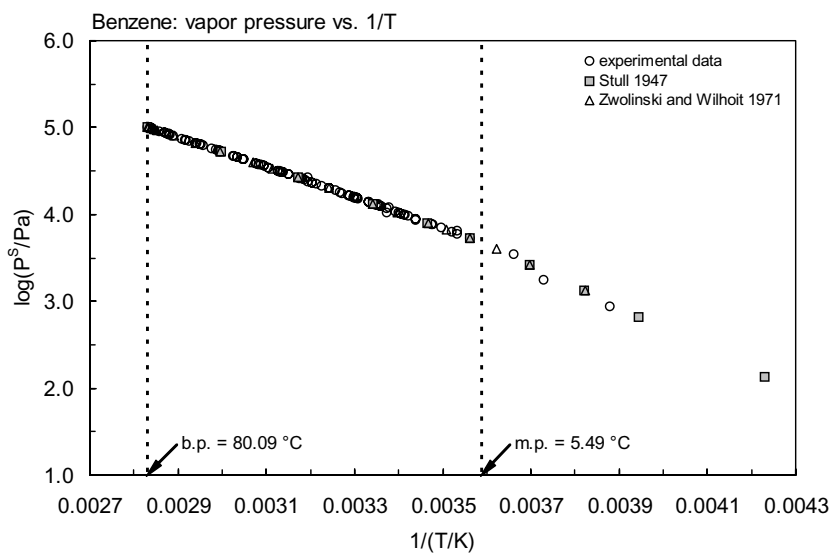


FIGURE 3.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for benzene.



TABLE 3.1.1.1.3

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

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

1.

Brown & Wasik 1974		Green & Frank 1979		Leighton & Calo 1981		Sanemasa et al. 1981	
headspace-GC		concentration ratio-UV		equilibrium cell-GC		vapor-liquid equilibrium	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
4.5	187.2	10	262	1.0	178	15	396
6.33	209.3	15	332	1.3	174	25	610
7.06	222.9	20	430	11	280	35	877
8.96	246.4	25	552	13	330	45	1267
11.75	289.9	30	688	21	470		
12.1	295.3			33	482		
15.1	346.8	eq. 3	k <sub>H</sub> /atm	27.2	597	Sanemasa et al. 1982	
17.93	391.6	A	8.58	25	554	vapor liquid-equilibrium	
20.06	442.4	B	1852.308			t/°C	H/(Pa m <sup>3</sup> /mol)
				eq. 3	k <sub>H</sub> /atm	5	225
				A	19.02	15	387
				B	3964	25	608
						35	905
						45	1321

2.

Ashworth et al. 1988		Robbins et al. 1993		Perlinger et al. 1993		Ettre et al. 1993	
EPICS-GC		static headspace-GC		headspace-GC		equil. headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
10	334	25	535	10	290	25	570
15	391	30	679	15	380	45	912
20	458	40	890	20	460	60	1220
25	535	45	1236	25	604	70	1668
30	730	50	1450	30	741	80	1767
eq. 4	H/(atm·m <sup>3</sup> /mol)					eq.2	1/K <sub>AW</sub>
A	5.534					A	-2.1678537
B	3194					B	836.2228

3.

Dewulf et al. 1995		Alaee et al. 1996		Turner et al. 1996		Peng & Wan 1997	
EPICS-GC		gas stripping-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
2.0	162	4	169	10	287	15	366
6.0	208	10	228	15	390	20	436
10	228	15	326	25	640	25	538

(Continued)

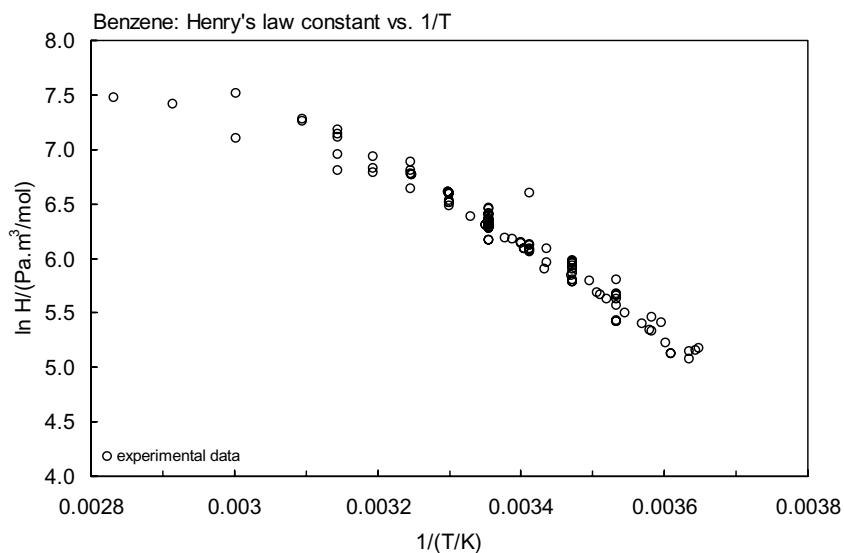
TABLE 3.1.1.1.3 (Continued)

3.

Dewulf et al. 1995		Alaee et al. 1996		Turner et al. 1996		Peng & Wan 1997	
EPICS-GC		gas stripping-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
18.2	366	20.6	441	35	986	30	675
25	481	25.4	552			35	766
		30.1	744			40	947
eq. 1	K <sub>AW</sub>	34.9	874	eq. 5	K <sub>AW</sub>	45	1053
A	10.577			A	0.0763		
B	3640			B	0.00211		
				C	0.000162		
		enthalpy of volatilization: $\Delta H_{vol}/(\text{kJ}\cdot\text{mol}^{-1}) = 32.2$ at 20°C				eq.1	K <sub>AW</sub>
		eq. 1	K <sub>AW</sub>			A	7.15
		A	11.5352			B	1397
		B	3873				

4.

Bierwagen & Keller 2001		Görgényi et al. 2002		Bakierowska & T. 2003	
SPME-GC		EPICS-SPME method		headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
15	376	2	172.2	10	294
25	538	6	235.6	15	353.5
30	675	10	279.2	20	440
40	893	18	441.3	25	558
		25	573.4		
eq. 1	K <sub>AW</sub>	30	740.0	Eq. 2	1/K <sub>AW</sub>
A	8.1648	40	1033	A	11.663
B	2889.4	50	1429	B	3920
		60	1844		
		eq. 1	K <sub>AW</sub>		
		A	10.01		
		B	3430.4		



**FIGURE 3.1.1.1.3** Logarithm of Henry's law constant versus reciprocal temperature for benzene.

**TABLE 3.1.1.1.4**

**Reported octanol-water partition coefficients and octanol-air partition coefficients of benzene at various temperatures**

$\log K_{OW}$		$\log K_{OA}$	
Dewulf et al. 1999		Gruber et al. 1997	
EPICS-GC, both phases		activity coefficient-GC	
t/°C	$\log K_{OW}$	t/°C	$\log K_{OA}$
2.2	1.973	20.29	2.9
6	1.961	30.3	2.71
10	2.053	40.4	2.56
14.1	2.01	50.28	2.42
18.7	2.04		
24.8	1.974		

change in enthalpy:  
 $\Delta H_{OW}/(\text{kJ mol}^{-1}) = 1.7$   
 (-8.3 to 11.8)  
 enthalpy of transfer  
 $\Delta H_{oct}/(\text{kJ mol}^{-1}) = 8.1$   
 (-1.9 to 18.2)

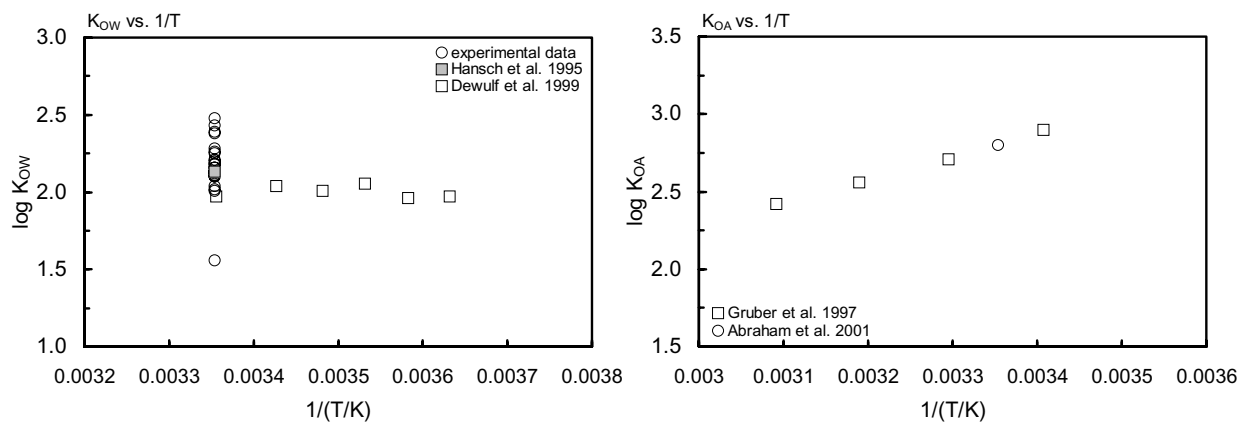
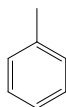


FIGURE 3.1.1.1.4 Logarithm of  $K_{OW}$  and  $K_{OA}$  versus reciprocal temperature for benzene.

## 3.1.1.2 Toluene



Common Name: Toluene

Synonym: methyl benzene, phenylmethane, toluol, methylbenzol, methacide

Chemical Name: toluene

CAS Registry No: 108-88-3

Molecular Formula:  $C_7H_8$ ,  $C_6H_5CH_3$

Molecular Weight: 92.139

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

−94.95 (Lide 2003)

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

110.63 (Lide 2003)

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

0.8669 (Weast 1982–83)

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

106.3 ( $20^{\circ}C$ , calculated from density)

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

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

37.99, 33.183 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

6.636 (Riddick et al. 1986)

6.62 (exptl., Chickos et al. 1999)

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

37.15, 45.0 (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  $25^{\circ}C$  or indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

470	( $16^{\circ}C$ , shake flask, Fühner, 1924)
570	( $30^{\circ}C$ , shake flask-interferometer, Gross & Saylor 1931)
347	(residue-volume method, Booth & Everson 1948)
530	(shake flask-UV, Andrews & Keffer 1949)
500	(flask flask-UV, Klevens 1950)
627*	(shake flask-UV, measured range $0.4$ – $45.3^{\circ}C$ , Bohon & Claussen 1951)
546	(shake flask-UV, Morrison & Billett 1952)
550	(Dreisbach 1955)
595	(quoted, Deno & Berkheimer 1960)
538	(shake flask-GC, McAuliffe 1963)
515	(shake flask-GC, McAuliffe 1966)
479	( $21^{\circ}C$ , shake flask-GC, Chey & Calder 1972)
530*	(shake flask-GC, measured range $5$ – $45^{\circ}C$ , Pierotti & Liabastre 1972)
547*	(shake flask-UV, measured $25$ – $55^{\circ}C$ , Bradley et al. 1973)
573*	(shake flask-GC, Polak & Lu 1973)
517	(shake flask-GC, Mackay & Wolkoff 1973)
573*	(headspace-GC, measured range $4.5$ – $20.1^{\circ}C$ , Brown & Wasik 1974)
627	(shake flask-UV, Vesala 1974)
520	(shake flask-GC, Mackay & Shiu 1975)
534.8	(shake flask-GC, Sutton & Calder 1975)
554	(shake flask-GC, Price 1976)
488; 563	(shake flask-titration, shake flask-cloud point, Sada et al. 1975)

- 534 (shake flask-fluorescence, Schwarz 1977)  
 554 (shake flask-GC, Krzyzanowska & Szeliga 1978)  
 $\log x = 626.526/(T/K)^2 - 4300.59/(T/K) + 3.3585$ , temp range 0–50°C (Ueda et al. 1978)  
 572, 587 (10, 20°C, shake flask-UV, Ben-Naim & Wiff 1979)  
 660 (elution chromatography, Schwarz 1980)  
 732\*, 739\* (20°C, exptl.-elution chromatography, shake flask-UV, Schwarz & Miller 1980)  
 155 (shake flask-LSC, Banerjee et al. 1980)  
 507 (shake flask-GC, Rossi & Thomas 1981)  
 557\* (vapor saturation-UV spec., measured range 15–45°C, Sanemasa et al. 1981)  
 526\* (vapor saturation-UV spec., measured range 15–45°C, Sanemasa et al. 1982)  
 585 (generator column-HPLC/UV, Tewari et al. 1982b)  
 578 (generator column-HPLC/UV, Tewari et al. 1982c)  
 580 (generator column-HPLC/UV, Wasik et al. 1983)  
 524 (shake flask-HPLC/UV, Banerjee 1984)  
 521 (vapor saturation-UV spec., Sanemasa et al. 1984)  
 $\ln x = -185.1695 + 7348.55/(T/K) + 26.34525 \cdot \ln (T/K)$ ; temp range 310–560 K (Heidman et al. 1985)  
 520 (shake flask-radiometry, Lo et al. 1986)  
 580 (shake flask-GC, Keeley et al. 1988)  
 538 (shake flask-GC, Coutant & Keigley 1988)  
 530\* (IUPAC recommended value, temp range 5–55°C, Shaw 1989a)  
 599\* (30°C, equilibrium flow cell-GC; measured range 30–100°C Chen & Wagner 1994b)  
 $\ln (1/x) = -12.21 + 21.39 \cdot [(T/K)/591.8]^{-1} - 3.572 \cdot [(T/K)/591.8]^{-2}$ ; temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994b)  
 $\ln x = 12.21 - 21.39 \cdot (T_r/K)^{-1} + 5.372 \cdot (T_r/K)^{-2}$ ,  $T_r = T/T_c$ , the reduced temp, system temp T divided by critical temp  $T_c$  (Chen & Wagner 1994c)  
 562.9 (shake flask-UV spectrophotometry, Poulson et al. 1999)  
 $\ln x = -46.05 - 7268.85/(T/K) - 1.411 \times 10^{-4} \cdot (T/K)^2$ ; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)  
 519\* (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)  
 556\* (vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)  
 558\* (shake flask-UV, measured range 0–50°C, Sawamura et al. 2001)  
 $\ln x = -221.739 + 9274.79/(T/K) + 31.8721 \cdot \ln (T/K)$ ; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

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

- 920\* (0°C, mercury manometer, measured range –9.70 to 0°C, Linder 1931)  
 3786\* (Hg manometer measurements, Pitzer & Scott 1943)  
 $\log (P/\text{mmHg}) = -2866.53/(T/K) - 6.7 \log (T/K) + 27.6470$ ; temp range: 0–50°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)  
 6357\* (35.366°C, ebulliometry, measured range 35.366–111.509°C, Willingham et al. 1945)  
 $\log (P/\text{mmHg}) = 6.95337 - 1343.943/(219.377 + t/^\circ\text{C})$ ; temp range 35.4–111.5°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)  
 2666\* (18.4°C, summary of literature data, temp range –16.7 to 110.6°C, Stull 1947)  
 6386\* (35.504°C, ebulliometry, measured range 35.504–111.545°C, Forziati et al. 1949)  
 $\log (P/\text{mmHg}) = 6.95508 - 1345.087/(219.516 + t/^\circ\text{C})$ ; temp range 35.5–111.5°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)  
 3792 (calculated from det. data, Dreisbach 1955)  
 $\log (P/\text{mmHg}) = 6.95334 - 1343.943/(219.377 + t/^\circ\text{C})$ ; temp range 20–200°C (Antoine eq. for liquid state, Dreisbach 1955)  
 1333\* (6.375°C, compiled data, temp range 6.375–136.435°C, Bond & Thodos 1960)  
 256200\* (146.85°C, ebulliometry, measured range 146.85–306.85°C, Ambrose et al. 1967)  
 48898\* (86.85°C, compiled data, temp range 86.85–306.85°C, Ambrose et al. 1970)  
 3792\* (interpolated, Antoine eq., Zwolinski & Wilhoit 1971)

- log (P/mmHg) =  $6.95464 - 1344.80/(219.482 + t/^{\circ}\text{C})$ ; temp range; 6.36–136.42°C (Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) =  $[-0.2185 \times 9368.5/(T/K)] + 8.3300$ ; temp range –92 to –15°C (Antoine eq., Weast 1972–73)
- log (P/mmHg) =  $[-0.2185 \times 8586.5/(T/K)] + 8.719392$ ; temp range –26.7 to 319°C (Antoine eq., Weast 1972–73)
- 2904\* (19.99°C, differential capacitance gauge, measured range 0–49.26°C, Munday et al. 1980)
- log (P/mmHg) =  $-5541.623/(T/K) + 25.08047 - 0.01055321(T/K)$ ; temp range 0–49.26°C (differential capacitance gauge, Munday et al. 1980)
- 3560 (gas saturation-GC, Politzki et al. 1982)
- log (P/atm) =  $(1 - 383.737/T) \times 10^{(0.837122 - 6.48791 \times 10^4/T + 5.91293 \times 10^7/T^2)}$ ; T in K, temp range 245.0–590.0 K (Cox vapor pressure eq., Chao et al. 1983)
- log (P/kPa) =  $6.08436 - 1347.62/(219.787 + t/^{\circ}\text{C})$ ; temp range 35.37–111.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- log (P/kPa) =  $6.37988 - 1575.007/(249.372 + t/^{\circ}\text{C})$ ; temp range 86.85–306.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 3786 (Daubert & Danner 1985)
- 3790 (interpolated-Antoine eq., Dean 1985, 1992)
- log (P/mmHg) =  $6.95464 - 1344.80/(219.48 + t/^{\circ}\text{C})$ ; temp range 6–137°C (Antoine eq., Dean 1985, 1992)
- 3790 (headspace-GC, Hussam & Carr 1985)
- log (P/kPa) =  $6.08540 - 1348.77/(219.976 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)
- 3800 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $6.08627 - 1349.122/(-53.154 + T/K)$ ; temp range 308–386 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $6.1258 - 1376.61/(-51.1 + T/K)$ ; temp range 210–219 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $6.12012 - 1374.901/(-49.657 + T/K)$ ; temp range 383–445 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $6.40815 - 1615.834/(-15.897 + T/K)$ ; temp range 440–531 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $7.65383 - 3153.235/(188.566 + T/K)$ ; temp range 530–592 K (liquid, Antoine eq.-V, Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $6.16273 - 1391.005/(-48.974 + T/K)$ ; temp range 273–295 K (liquid, Antoine eq.-VI, Stephenson & Malanowski 1987, selected, Shiu & Ma 2000)
- 3090\* (20.98°C, static method, measured range 199.22–402.21 K, Mokbel et al. 1998)

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

- 474\* (headspace-GC, Brown & Wasik 1974)
- 527 (headspace-GC, Vitenberg et al. 1975)
- 673 (batch air stripping-GC, Mackay et al. 1979)
- 625\* (23.0°C, equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
- ln (k<sub>H</sub>/atm) =  $18.46 - 3751/(T/K)$ ; temp range: 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
- 628\* (vapor-liquid equilibrium-GC., Sanemasa et al. 1981)
- 664\* (vapor-liquid equilibrium, Sanemasa et al. 1982)
- 647 (EPICS-GC, Garbarnini & Lion 1985)
- 634\* (20°C, headspace-GC, measured range 20–46°C, Schoene & Steinhanses 1985)
- 601 (gas stripping-GC, Warner et al. 1987)
- 594 (20°C, EPICS, Yurteri et al. 1987)
- 651\* (EPICS-GC, Ashworth et al. 1988)
- ln [H/(atm m<sup>3</sup>/mol)] =  $5.133 - 3024/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
- 652 (infinite activity coeff. γ<sup>∞</sup> from solubility measurement, Abraham et al. 1990)
- 644 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 933\* (40°C, static headspace-GC, measured range 40–80°C, Kolb et al. 1992)
- ln (1/K<sub>AW</sub>) =  $-6.03 + 2198/(T/K)$ ; temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
- 1116\* (45°C, headspace-GC, measured range 45–80°C, Ettre et al. 1993)

$\log (1/K_{AW}) = -2.5323790 + 928.3536/(T/K)$ ; temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)

631 (infinite activity coeff.  $\gamma^\infty$  in water determined by inert gas stripping-GC, Li et al. 1993)

660\* (equilibrium headspace-GC, Perlinger et al. 1993)

652\* (static headspace-GC, Robbins et al. 1993)

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

676 (23°C, gas stripping-IR, Nielsen et al. 1994)

555\* (EPICS-GC/FID, Dewulf et al. 1995)

699 (EPICS-GC/FID, natural seawater with salinity of 35‰ Dewulf et al. 1995)

$\ln K_{AW} = -4064/(T/K) + 0.00834 \cdot Z + 12.150$ ; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)

541 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

684\* (vapor-liquid equilibrium.-GC, Turner et al. 1996)

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

605\* (headspace equilibrium-GC, Peng & Wan 1997)

$\ln K_{AW} = 7.94 - 1621/(T/K)$ ; temp range 15–45°C (headspace equilibrium-GC, Peng & Wan 1997)

478 (headspace-GC, Peng & Wan 1998)

$\ln K_{AW} = 7.89 - 1565/(T/K)$ ; temp range 0–45°C (seawater with salinity of 36‰, headspace-GC, Peng & Wan 1998)

637.2 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

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

652 (EPICS-GC, David et al. 2000)

644 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

959 (EPICS-GC, Ayuttaya et al. 2001)

509 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 5.271 - 1745/(T/K)$  (van = t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

647.5\* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)

$\ln K_{AW} = 11.25 - 3770.4/(T/K)$ ; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

556–574 (27°C, solid-phase microextraction-GC, solute concn 0.47–19.21 mg/L, measured range 15–40°C, Cheng et al. 2003)

612\* (headspace-GC, measured range 10–25°C, Bakierowska & Trzeszczyński 2003)

$\ln (1/K_{AW}) = 11.926 - 3977/(T/K)$ ; temp range 10–25°C, headspace-GC, Bakierowska & Trzeszczyński 2003)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at 25°C or as indicated. Additional data at other temperatures designated

\* are compiled at the end of this section:

2.69 (shake flask-UV, Fujita et al. 1964; quoted, Hansch et al. 1968; Hansch et al. 1972)

2.11 (shake flask-UV, Rogers & Cammarata 1969)

2.69, 2.73, 2.11, 2.80 (Leo et al. 1971; Hansch & Leo 1979)

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

2.68 (shake flask-HPLC, Nahum & Horvath 1980)

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

2.97 (HPLC- $k'$  correlation, McDuffie 1981)

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

2.59 (HPLC- $k'$  correlation, D'Amboise & Hanai 1982)

2.65 (generator column-HPLC/UV, Tewari et al. 1982b,c)

2.62 (HPLC- $k'$  correlation, Miyake & Terada 1982)

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

2.74 (HPLC- $k'$  correlation, Hafkansch & Tomlinson 1983b)

2.11–2.80, 2.65 (range, mean; shake flask method, Eadsforth & Moser 1983)

2.51–3.06, 2.88 (range, mean; HPLC method, Eadsforth & Moser 1983)

2.10 (shake flask, Platford 1979, 1983)

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

2.89 (HPLC-RT correlation, Rapaport & Eisenreich 1984)

2.78 (HPLC/MS correlation, Burkhard et al. 1985)

3.00 (HPLC- $k'$  correlation, De Kock & Lord 1987)

2.65 (generator column-RP-LC, Schantz & Martire 1987)



- 2.62 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 2.73 (recommended, Sangster 1989, 1993)
- 2.66, 2.69 (RP-HPLC capacity factor correlations, Sherblom & Eganhouse 1988)
- 2.786 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
- 2.63 ± 0.05, 2.786 ± 0.005 (shake flask/slow stirring, interlaboratory studies, Brooke et al. 1990)
- 2.76 (normal phase HPLC-*k'* correlation, Govers & Evers 1992)
- 2.73 (recommended, Hansch et al. 1995)
- 2.77 ± 0.02 (HPLC-*k'* correlation, Poulson et al. 1997)
- 2.32\* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

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

- 3.42\* (20.29°C, from GC-determined  $\gamma^\infty$  in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
- 3.31 (head-space GC/FID both phases, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 1.12 (eels, Ogata & Miyake 1978)
- 0.22 (Manila clam, Nunes & Benville 1979)
- 0.62 (mussels, Geyer et al. 1982)
- 0.92 (goldfish, Ogata et al. 1984),
- 3.28, 2.58, 1.95 (activated sludge, algae, fish, Freitag et al. 1985)
- 1.99 (*S. capricornutum*, Herman et al. 1991)

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

- 2.39 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)
- 2.27, 1.89 (ICN humic acid, ICN HA coated  $Al_2O_3$ , headspace equilibrium, Garbarnini & Lion 1985)
- 2.28, 1.89 (Offutt AFB soil, Whitean AFB soil, headspace equilibrium, Garbarnini & Lion 1985)
- 1.91, 1.13, 1.19, 2.18, 2.09, -1.30, 1.94 (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, tannic acid, lignin, zein, cellulose, Aldrich humic acid, headspace equilibrium, Garbarnini & Lion 1986)
- 2.18, 2.21, 2.43, 2.54 (Sapsucker Woods S.W. soil, S.W. ethyl ether extracted soil, humin, oxidized humin, headspace equilibrium, Garbarnini & Lion 1986)
- 1.74, 2.13, 1.98 (forest soil pH 5.6, forest soil pH 4.2, agricultural soil pH 7.4, Seip et al. 1986)
- 2.0 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
- 1.70 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.50, 2.39 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.86, 2.86, 2.43 (organic cations treated Marlette soil B<sub>t</sub> horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 1.59 (untreated St Clair soil B<sub>t</sub> horizon, OC 0.44%, batch equilibrium, Lee et al. 1989)
- 3.03, 2.90 (organic cations HDTMA treated soils: St. Clair soil B<sub>t</sub> horizon OC 3.25%; Oshtemo soil B<sub>t</sub> horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.01 (aquifer material with  $f_{OC} = 0.006$  and measured partition coeff.  $K_p = 0.61$  mL/g., Abdul et al. 1990)
- 2.10, 2.26 (HPLC-*k'* correlation, humic acid-silica column, Szabo et al. 1990a,b)
- 2.22, 2.16 (Captina silt loam, McLaurin sandy loam, batch equilibrium, Walton et al. 1992)
- 2.10 (average of 5 soils, sorption isotherms by batch equilibrium method-GC, Xing et al. 1994)
- 2.21, 2.31, 2.21 (RP-HPLC-*k'* correlation on 3 different stationary phases, Szabo et al. 1995)
- 2.17, 2.18 (RP-HPLC-*k'* correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 2.12 (HPLC-screening method, Müller & Kördel 1996)
- 2.23, 2.31, 2.33, 2.34, 2.40, 2.31, 2.34 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)
- 1.89, 2.00, 1.79 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

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

- 1.39 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.30, 2.16 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.74, 2.72, 2.28 (organic cations treated Marlette soil B<sub>1</sub> horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 1.29 (untreated St Clair soil B<sub>1</sub> horizon, OM 0.88%, batch equilibrium, Lee et al. 1989)
- 2.89; 2.74 (organic cations HDTMA treated soils: St. Clair soil B<sub>1</sub> horizon OM 4.38%; Oshtemo soil B<sub>1</sub> horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

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

Volatilization:  $t_{1/2} = 5.18$  h from water depth of 1-m (Mackay & Leinonen 1975; Haque et al. 1980);

$k = 0.043$  d<sup>-1</sup> with  $t_{1/2} = 16$  d in spring at 8–16°C,  $k = 0.0463$  d<sup>-1</sup> with  $t_{1/2} = 1.5$  d in summer at 20–22°C,  $k = 0.053$  d<sup>-1</sup> with  $t_{1/2} = 13$  d in winter at 3–7°C for the periods when volatilization appears to dominate, and  $k = 0.088$  d<sup>-1</sup> with  $t_{1/2} = 7.6$  d with HgCl<sub>2</sub>, in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);

evaporation  $t_{1/2} \sim 2.9$  d from a river of 1-m depth with wind speed of 3 m/s and water current of 1 m/s at 20°C (Lyman et al. 1982);

estimated  $t_{1/2} = 1$  and 4 d for evaporation from a river and lake, respectively (Howard 1990).

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

$k = 3.39 \times 10^{-3}$  h<sup>-1</sup> with H<sub>2</sub>O<sub>2</sub> under photolysis at 25°C in F-113 solution and with HO· in the gas (Dilling et al. 1988);  $t_{1/2} < 0.25$  h on silica gel under indoor artificial UV-light “continuous” condition (Söderström et al. 2004).

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

$k_{OH} = (2.5 \pm 0.9) \times 10^9$  L mol<sup>-1</sup> s<sup>-1</sup> with  $t_{1/2} = 4.6$  h;  $k_{O(3P)} = (0.450 \pm 0.045) \times 10^8$  L mol<sup>-1</sup> s<sup>-1</sup> with O(3P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = 5.78 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>;  $k_{O_3} = 0.75 \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for the reaction of O(3P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 3.6 \times 10^9$  L mol<sup>-1</sup> s<sup>-1</sup>, with  $t_{1/2} = 2.4$ –24 h at room temp. (Darnall et al. 1976)

$k_{OH}^* = (6.40 \pm 0.64) \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH} = 6 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{NO_3} \leq 3 \times 10^{-14}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at  $300 \pm 1$  K (Carter et al. 1981)

$k_{OH} = 6.0 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> and residence time of 1.9 d, loss of 40.9% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360$  M<sup>-1</sup> h<sup>-1</sup> for singlet oxygen and  $k = 144$  M<sup>-1</sup> h<sup>-1</sup> for RO<sub>2</sub> radical (Mabey et al. 1982)

$k_{O_3} = 160$  cm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup> at 300 K (Lyman et al. 1982)

$k_{OH} = 3.5 \times 10^9$  M<sup>-1</sup> s<sup>-1</sup> with  $t_{1/2} = 1.6$  d in the atmosphere (Mill 1982)

$k = (14 \pm 3)$  M<sup>-1</sup> s<sup>-1</sup> for the reaction with ozone in water at pH 1.7 and 20–23°C (Hoigné & Bader 1983)

$k_{O_3} < 1.0 \times 10^{-20}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a loss rate of  $< 0.0006$  d<sup>-1</sup>;  $k_{OH} = 6.4 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a loss rate of 0.6 d<sup>-1</sup> and  $k_{NO_3} = 3.7 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a loss rate of 0.0007 d<sup>-1</sup> at room temp. (review, Atkinson & Carter 1984)

$k_{NO_3} = 1.8 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296 K (Atkinson et al. 1984)

$k_{OH}^* = 6.19 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K (recommended, Atkinson 1985)

$k_{OH}(\text{calc}) = 5.9 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}(\text{obs.}) = 5.7 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH} = 5.7 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with  $t_{1/2} = 10$ –104 h (Atkinson 1985; Howard 1991)

$k_{O_3} < 1.0 \times 10^{-20}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a loss rate of  $< 0.0006$  d<sup>-1</sup>;  $k_{OH} = 6.2 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a loss rate of 0.27 d<sup>-1</sup> and  $k_{NO_3} = 3.6 \times 10^{-17}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with a loss rate of 0.0007 d<sup>-1</sup> at room temp. (review, Atkinson 1985)

$k_{OH} = 6.03 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K (relative rate method, Ohta & Ohya 1985)

$k_{OH} = 5.35 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 24.2°C, with a calculated atmospheric lifetime  $\tau = 2.2$  d (Edney et al. 1986)

$k_{\text{OH}}(\text{calc}) = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{NO}_3} = 6.46 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}} = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ;  $k_{\text{OH}} = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{\text{NO}_3} = (7.8 \pm 1.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (relative rate method, Atkinson & Aschmann 1988)

$k_{\text{OH}}^* = 5.96 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

photooxidation  $t_{1/2} = 10\text{--}104 \text{ h}$ , based on measured rate data for the vapor phase reaction with OH radicals in air;  $t_{1/2}(\text{aq.}) = 321\text{--}1284 \text{ h}$ , based on measured rate data for hydroxyl radicals in aqueous solution (Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 5.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 4.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (based on molecular orbital calculations, Klamt 1993)

Hydrolysis: not aquatically significant (Callahan et al. 1979);

no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of  $2.22 \times 10^{-6} \text{ L/L}$  (Jamison et al. 1976)

$t_{1/2} \approx 90 \text{ d}$  in uncontaminated estuarine water; and  $t_{1/2} \approx 30 \text{ d}$  in oil polluted water (Lee 1977)

$k = 0.5 \text{ d}^{-1}$ , significant degradation in aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$k = 0.07 \text{ yr}^{-1}$  with  $t_{1/2} = 39 \text{ d}$  (Zoeteman et al. 1981; Olsen & Davis 1990)

$t_{1/2}(\text{aq. anaerobic}) = 1344\text{--}5040 \text{ h}$ , based on anaerobic screening test data and anaerobic sediment grab sample data (Horowitz et al. 1982; Howard et al. 1991)

$t_{1/2} = 9.5 \text{ d}$  in activated sludge (estimated, Freitag et al. 1985; quoted, Anderson et al. 1991)

$t_{1/2}(\text{aq. aerobic}) = 96\text{--}528 \text{ h}$ , based on an acclimated seawater dieaway test (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 4 \text{ d}$ ,  $t_{1/2}(\text{anaerobic}) = 56 \text{ d}$  in natural waters (Capel & Larson 1995)

$t_{1/2} = 31\text{--}220 \text{ h}$  for toluene concn range from 0.5–200  $\mu\text{g/g}$  in sandy loam soil and degradation rate  $k = 1.76 \times 10^{-2}$  and  $0.42 \mu\text{g g}^{-1} \text{ h}^{-1}$  of soil for 0.5 and 5.0  $\mu\text{g/g}$ , respectively;  $t_{1/2} = 172$  and  $165 \text{ h}$  in sand and degradation rate  $k = 1.05 \times 10^{-2}$  and  $0.22 \mu\text{g g}^{-1} \text{ h}^{-1}$  of soil for toluene concn 0.5 and 5  $\mu\text{g/g}$  respectively in sand (Davis & Madsen 1996)

Biotransformation:  $1.0 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$  (Mabey et al. 1982).

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

$t_{1/2} \sim 1.4 \text{ d}$  elimination from eels in seawater (Ogata & Miyake 1978).

Half-Lives in the Environment:

Air:  $t_{1/2} = 4.6 \text{ h}$  in ambient air based on reaction with OH radical at  $\sim 300\text{K}$  (Doyle et al. 1975);

$t_{1/2} = 2.4\text{--}24 \text{ h}$  based on rate of disappearance for the reaction with hydroxyl radicals (Darnall et al. 1976)

photodecomposition  $t_{1/2} = 6.8 \text{ h}$  under simulated atmospheric conditions, with NO (Dilling et al. 1976)

residence time of 1.9 d, loss of 40.9% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

calculated lifetime  $\tau = 2.2 \text{ d}$  due to reaction with OH radical (Edney et al. 1986)

summer daylight lifetime of 23 h due to reaction with OH radical (Altshuller 1991)

$t_{1/2} = 10\text{--}104 \text{ h}$ , based on photooxidation in air (Howard et al. 1991)

calculated lifetimes,  $\tau = 1.9 \text{ d}$ ,  $1.9 \text{ yr}$  and  $> 4.5 \text{ yr}$  for reactions with OH radical,  $\text{NO}_3$  radical and  $\text{O}_3$  respectively (Atkinson 2000).

Surface Water:  $t_{1/2} = 5.55 \text{ h}$ , based on evaporative loss at 25°C and 1-m depth of water (calculated, Mackay & Leinonen 1975; Haque et al. 1980)

photooxidation  $t_{1/2} = 321\text{--}1284 \text{ h}$  in water, based on measured rate data for hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)

$t_{1/2} = 16 \text{ d}$  in spring at 6–16°C,  $t_{1/2} = 1.5 \text{ d}$  in summer at 20–22°C,  $t_{1/2} = 13 \text{ d}$  in winter at 3–7°C when volatilization dominates and  $t_{1/2} = 7.9 \text{ d}$  with  $\text{HgCl}_2$  in marine mesocosm experiments (Wakeham et al. 1983)

$t_{1/2} = 96\text{--}528 \text{ h}$ , based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water:  $t_{1/2} \approx 0.3 \text{ yr}$  from observed persistence in groundwater of Netherlands (Zoeteman et al. 1981);

$t_{1/2} = 168\text{--}672 \text{ h}$ , based on unacclimated grab sample data of aerobic soil from groundwater aquifers (Wilson et al. 1983; Swindoll et al. 1987; Howard et al. 1991).

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

$t_{1/2} = 5 \text{ d}$  assumed first-order biological/chemical degradation in soil (Jury et al. 1990);

reported lit.  $t_{1/2} = 0.1 - 1.7$  d and 7 d in soil, measured disappearance  $t_{1/2} < 2.0$  d from test soils (Anderson et al. 1991)

$t_{1/2} = 96-528$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} = 31, 57, 96$  and 220 h with toluene concn range from 0.5, 5, 50 and 200  $\mu\text{g/g}$  in sandy loam soil,  $t_{1/2} = 172$  and 165 h with toluene concn 0.5 and 5  $\mu\text{g/g}$ , respectively, in sand (Davis & Madsen 1996).

Biota:  $t_{1/2} = 10$  h clearance from fish (Neely 1980).

**TABLE 3.1.1.2.1**

**Reported aqueous solubilities of toluene at various temperatures and reported enthalpy of solution**

**1.**

Bohon & Claussen 1951		Pierotti & Liabastre 1972		Bradley et al. 1973		Brown & Wasik 1974	
shake flask-UV		shake flask-GC		shake flask-UV		headspace-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0.4	658	5	634	25	547	25	573
3.6	646	10	632	45	722	4.5	612
10	628	20	661	55	860	6.3	601
11.2	624	25	630			7.1	586
14.9	623	35	672			9	587
15.9	621	45	672			11.8	573
25	627			<b>Polak &amp; Lu 1973</b>		12.1	575
25.6	625			shake flask-GC		15.1	569
30	640			t/°C	S/g·m <sup>-3</sup>	17.9	577
30.2	642			0	724	20.1	566
35.2	657			25	573		
42.8	701						
45.3	717						
	$\Delta_{\text{sol}}H/(\text{kJ mol}^{-1})$						
25°C	2.3						
2°C	-3.93						
7°C	-3.01						
12°C	-1.38						
17°C	0						
22°C	0.962						
27°C	3.22						
32°C	4.435						
37°C	5.73						
42°C	7.15						

**2.**

Ben-Naim & Wiff 1979		Schwarz & Miller 1980		Sanemasa et al. 1981		Shaw 1989a (IUPAC)	
shake flask-UV		shake flask-UV		vapor saturation-UV		recommended values	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
10	572	10	777	15	533	0	690
20	587	20	739	25	557	5	630
		30	754	35	587	10	590
				45	635	20	570
						25	530
						30	590
						40	640
						45	660
		<b>Elution chromatography</b>					
		t/°C	S/g·m <sup>-3</sup>				
		10	758				

TABLE 3.1.1.2.1 (Continued)

Ben-Naim & Wiff 1979		Schwarz & Miller 1980		Sanemasa et al. 1981		Shaw 1989 (IUPAC)	
shake flask-UV		shake flask-UV		vapor saturation-UV		recommended values	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
		20	732	Sanemasa et al. 1982		55	860
		30	920	vapor saturation-UV		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.70$ at 25°C	
				15	514		
				25	526		
				35	545		
				45	584		
				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.10$ at 25°C			
3.							
Chen & Wagner 1994b		Ma et al. 2001		Dohányosová et al.2001		Sawamura et al. 2001	
equilibrium flow cell-GC		shake flask-GC/FID		vapor absorption-HPLC/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>
30	599	5	540	0.5	563	0	583.5
40	609	15	516	5	552	5	670
50	650	25	519	15	542	10	558
60	737	35	555	25	556	15	553
70	875	45	632	35	590	20	553
80	1013			45	632	25	558
90	1187			55	704	30	573.8
100	1371					35	589.1
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 0.37$ at 25°C				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.0$ at 25°C		40	614.7
						45	640.3
						50	676.6

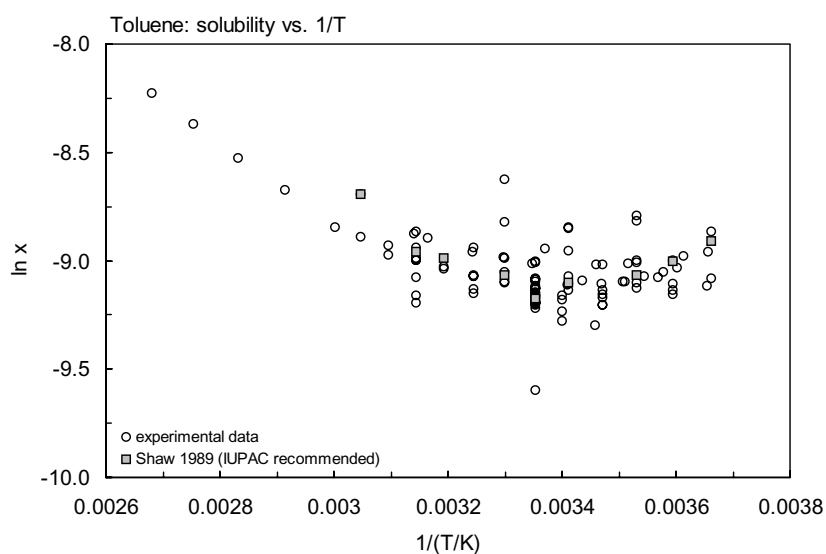
FIGURE 3.1.1.2.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for toluene.





TABLE 3.1.1.2.3

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

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

1.

Brown & Wasik 1974		Leighton & Calo 1981		Sanemasa et al. 1981		Schoene & S. 1985	
head space-GC		equilibrium cell-GC		vapor liquid-equilibrium		headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
4.5	179	1.0	222	15	382	20	634
6.33	204	1.3	236	25	628	36.9	670
7.06	218	12.4	373	35	979	41.5	680
8.96	244	12.5	361	45	1404	46	690
11.75	294	17.9	459				
12.1	299	19.1	525			eq. 1	K <sub>AW</sub>
15.1	259	22.7	565	Sanemasa et al. 1982		A	6.90
17.93	414	23	625	vapor-liquid equilibrium		B	2194
20.06	474			t/°C	H/Pa m <sup>3</sup> /mol		
		eq. 3	k <sub>H</sub> /atm				
		A	18.46	15	396		
		B	3751	25	664		
				35	1060		
				45	1571		

2.

Ashworth et al. 1988		Kolb et al. 1992		Ettre et al. 1993		Perlinger et al. 1993	
EPICS-GC		static headspace-GC		headspace-GC		equil. headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
10	386	40	933	45	1116	10	293
15	499	60	1565	60	1489	15	390
20	562	70	1915	70	1877	20	499
25	651	80	2312	80	2427	25	660
30	819					30	838
		eq. 2	1/K <sub>AW</sub>	eq. 2	1/K <sub>AW</sub>		
eq 4a	H/(atm m <sup>3</sup> /mol)	A	7.61	A	-2.532379		
A	5.133	B	2647	B	928.3536		
B	3024						

3.

Robbins et al. 1993		Dewulf et al. 1995		Turner et al. 1996		Peng & Wan 1997	
static headspace-GC		EPICS-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
25	652	2.0	175	11	376	15	391
30	835	6.0	203	15	460	20	475
40	1086	10	250	25	684	25	605



TABLE 3.1.1.2.3 (Continued)

Robbins et al. 1993		Dewulf et al. 1995		Turner et al. 1996		Peng & Wan 1997	
static headspace-GC		EPICS-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
45	1351	18.2	424	35	1202	30	774
50	1450	25	555			35	984
eq. 4a	H/(atm m <sup>3</sup> /mol)	eq. 1	K <sub>AW</sub>	eq. 5	K <sub>AW</sub>	40	1104
A	7.14	A	12.40	A	0.115	45	1309
B	3689	B	4064	B	0.00474		
				C	0.000466	eq. 1	K <sub>AW</sub>
						A	7.94
						B	1621

4.

Görgényi et al. 2002		Bakierowska & T. 2003	
EPICS-SPME method		headspace-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
2.0	169.3	10	288
6.0	238.2	15	358
10	304.9	20	467
18	476.9	25	612
25	647.5		
30	822.4	eq. 2	1/K <sub>AW</sub>
40	1214	A	11.926
50	1758	B	3977
60	2286		
eq. 1	K <sub>AW</sub>		
A	11.25		
B	3770.4		

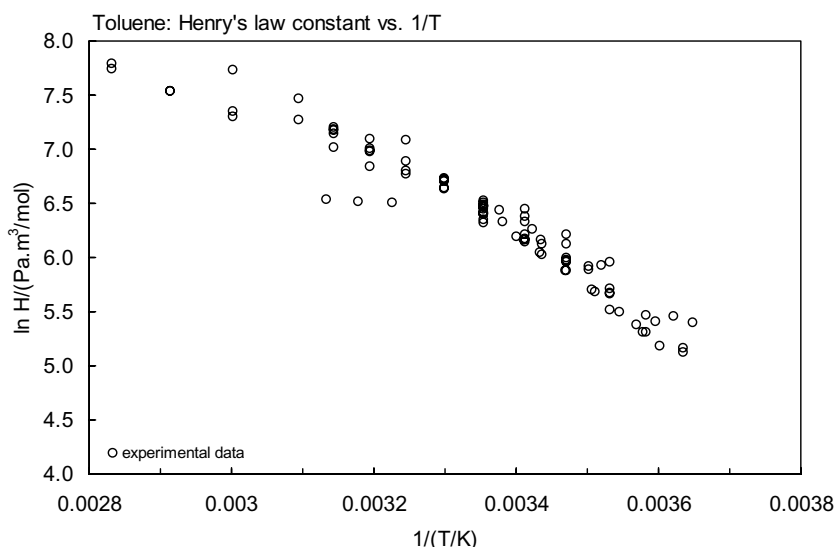


FIGURE 3.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for toluene.

TABLE 3.1.1.2.4

Reported octanol/water partition coefficients and octanol-air partition coefficients of toluene at various temperatures

log K <sub>OW</sub>		log K <sub>OA</sub>	
Dewulf et al. 1999		Gruber et al. 1997	
EPICS-GC, both phases		GC det'd activity coeff.	
t/°C	log K <sub>OW</sub>	t/°C	log K <sub>OA</sub>
2.2	2.316	20.29	3.42
6	2.405	30.3	3.2
10	2.464	40.4	3.03
14.1	2.38	50.28	2.86
18.7	2.41		
24.8	2.32		
enthalpy change $\Delta H/(\text{kJ mol}^{-1}) = -1.0$ (-16 to 13.9)			

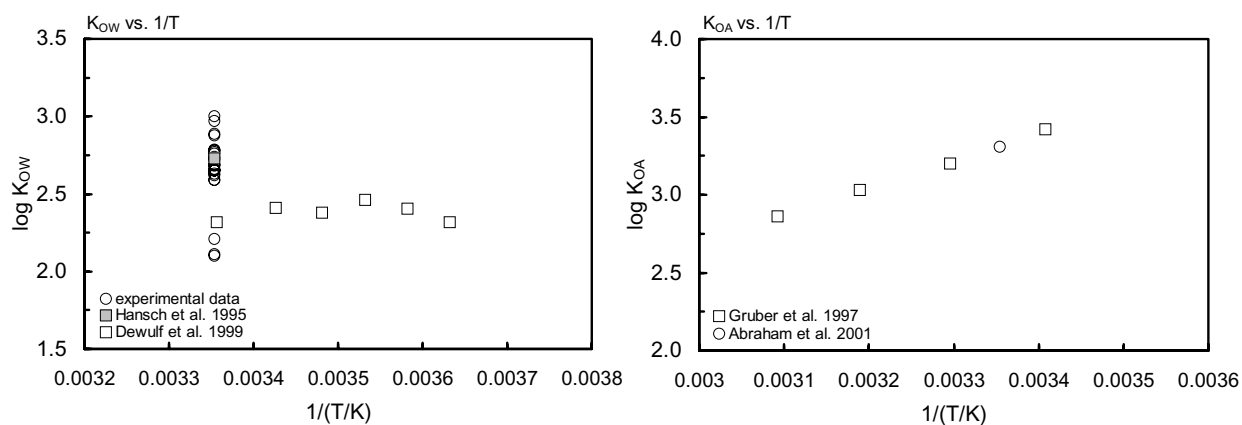
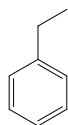


FIGURE 3.1.1.2.4 Logarithm of K<sub>OW</sub> and K<sub>OA</sub> versus reciprocal temperature for toluene.

## 3.1.1.3 Ethylbenzene



Common Name: Ethylbenzene

Synonym: phenylethane, ethylbenzol

Chemical Name: ethylbenzene

CAS Registry No: 100-41-4

Molecular Formula:  $C_8H_{10}$ ,  $C_2H_5C_6H_5$

Molecular Weight: 106.165

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

−94.96 (Lide 2003)

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

136.2 (Weast 1982–83; Lide 2003)

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

0.867 (Weast 1982–83)

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

122.4 ( $20^{\circ}C$ , calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

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

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

42.25, 35.2 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

9.184 (Riddick et al. 1986)

9.16 (Chickos et al. 1999)

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

51.43, 52.2 (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  $25^{\circ}C$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

140 ( $15^{\circ}C$ , shake flask, Fühner 1924)

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

175 (shake flask-UV, Klevens 1950)

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

165 (shake flask-UV, Morrison & Billett 1952)

159 (shake flask-GC, McAuliffe 1963)

152 (shake flask-GC, McAuliffe 1966)

177\* (shake flask-GC, Polak & Lu 1973)

180\* (shake flask-GC, measured range  $4.5$ – $20.1^{\circ}C$ , Brown & Wasik 1974)

203 (shake flask-UV, Vesala 1974)

161 (shake flask-GC, Sutton & Calder 1975)

131 (shake flask-GC, Price 1976)

131 (shake flask-GC, Krzyzanowska & Szeliga 1978)

203, 212 ( $10$ ,  $20^{\circ}C$ , shake flask-UV, Ben-Naim & Wiff 1979)

208\*, 184\* ( $20^{\circ}C$ , elution chromatography, shake flask-UV, measured range  $10$ – $30^{\circ}C$ , Schwarz & Miller 1980)

181\* (vapor saturation-UV, measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1981)

169\* (vapor saturation-UV, measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)

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

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

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

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

172 (vapor saturation-UV, Sanemasa et al. 1984)

- 192\* (generator column-HPLC/UV, measured range 10–45°C, Owens et al. 1986)
- 172 (shake flask-purge and trap-GC, Coutant & Keigley 1988)
- 169\* (IUPAC recommended value, temp range 0–100°C, Shaw 1989b)
- 170\* (30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen & Wagner 1994c)
- $\ln x = 11.59 - 20.52 \cdot (T_r/K)^{-1} + 4.750 \cdot (T_r/K)^{-2}$ ;  $T_r = T/T_c$ , the reduced temp, system temp  $T$  divided by critical temp  $T_c$ , temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994c)
- $\ln x = -30.799 + 3986.26/(T/K) + 7.9095 \times 10^{-5} \cdot (T/K)^2$ ; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
- 170\* (vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)
- 170\* (shake flask-UV, measured range 0–50°C, Sawamura et al. 2001)
- $\ln x = -263.220 + 11024.75/(T/K) + 37.8858 \cdot \ln (T/K)$ ; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 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):

- 209.3\* (0°C, mercury manometer, measured range –11.6 to 0°C, Linder 1931)
- 1546\* (30°C, Hg manometer, measured range 10–50°C, Rintelen 1937)
- $\log (P/\text{mmHg}) = 22.90283 - 2847.75/(T/K) - 5 \cdot \log (T/K)$ ; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)
- 6277\* (56.589°C, ebulliometry, measured range 56.589–137.124°C, Willingham et al. 1945)
- $\log (P/\text{mmHg}) = 6.94998 - 1419.315/(212.611 + t/^\circ\text{C})$ ; temp range 56.6–137.1°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
- 1333\* (25.9°C, summary of literature data, Stull 1947)
- 8399\* (63.3°C, static-Hg manometer, measured range 63.3–135.9°C, Buck et al. 1949)
- 6398\* (56.689°C, ebulliometry, measured range 56.689–137.16°C, Forziati et al. 1949)
- $\log (P/\text{mmHg}) = 6.95904 - 1425.464/(213.345 + t/^\circ\text{C})$ ; temp range 56.7–137.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
- $\log (P/\text{mmHg}) = -3225/(T/K) - 7.553 \cdot \log (T/K) + 30.49$ ; temp range 80–120°C (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
- 1276(extrapolated-Antoine eq., Dreisbach 1955)
- $\log (P/\text{mmHg}) = 6.95719 - 1424.255/(213.206 + t/^\circ\text{C})$ , temp range: 45–190°C (Antoine eq. for liquid state, Dreisbach 1955)
- 133800\* (146.85°C, ebulliometry, measured range 146.85–326.85°C, Ambrose et al. 1967)
- 1270\* (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
- $\log (P/\text{mmHg}) = 6.95719 - 1424.255/(213.206 + t/^\circ\text{C})$ ; temp range 25.88–163.47°C (Antoine eq., Zwolinski & Wilhoit 1971)
- $\log (P/\text{mmHg}) = [-0.2185 \times 9303.3/(T/K)] + 7.809470$ ; temp range –9.8 to 326.5°C, (Antoine eq., Weast 1972–73)
- 9585\* (66.031°C, comparative ebulliometry, measured range 66.031–176.953°C, Osborn & Scott 1980)
- $\log (P/\text{atm}) = (1 - 409.229/T) \times 10^{(0.859833 - 6.85948 \times 10^{-4} \cdot T + 5.94439 \times 10^{-7} \cdot T^2)}$ ;  $T$  in K, temp range 243.2–615.0 K (Cox vapor pressure eq., Chao et al. 1983)
- 1270, 1265 (extrapolated-Antoine eq., Boublik et al. 1984; quoted, Howard 1989)
- $\log (P/\text{kPa}) = 6.08206 - 1425.305/(213.415 + t/^\circ\text{C})$ , temp range: 25.88–92.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.0785 - 1421.653/(212.816 + t/^\circ\text{C})$ ; temp range 56.6–137.12°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
- 1268 (interpolated-Antoine eq., Dean 1985, 1992)
- $\log (P/\text{mmHg}) = 6.95719 - 1424.255/(213.21 + t/^\circ\text{C})$ ; temp range 26–164°C (Antoine eq., Dean 1985, 1992)
- 1300 (selected value., Riddick et al. 1986)
- $\log (P/\text{kPa}) = 6.09280 - 1431.71/(214.099 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)
- 1266 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.06991 - 1416.922/(-69.716 + T/K)$ ; temp range 298–420 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.10898 - 1445.262/(-57.128 + T/K)$ ; temp range 409–459 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.36656 - 1665.991/(-26.716 + T/\text{K})$ ; temp range 457–554 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.49119 - 3056.747/(159.496 + T/\text{K})$ ; temp range 549–617 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

1280, 283 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 36.1998 - 3.3402 \times 10^3/(T/\text{K}) - 9.7970 \cdot \log (T/\text{K}) - 1.1467 \times 10^{-11} \cdot (T/\text{K}) + 2.5758 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 178–617 K (vapor pressure eq., Yaws 1994)

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

559.1\* (20.06°C, headspace-GC, Brown & Wasik 1974)

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

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

854 (batch stripping-GC, Mackay et al. 1979; quoted, Howard 1989)

734\* (vapor-liquid equilibrium-GC, Sanemasa et al. 1981)

797\* (vapor-liquid equilibrium.-GC, Sanemasa et al. 1982)

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

798\* (EPICS-GC/FID, Ashworth et al. 1988)

$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 11.92 - 4994/(T/\text{K})$ , temp range 10–30°C, EPICS measurements, Ashworth et al. 1988)

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

756 (infinite activity coeff.  $\gamma^\infty$  in water determined by inert gas stripping-GC, Li et al. 1993)

660\* (equilibrium headspace-GC, Perlinger et al. 1993)

788\* (static headspace-GC, Robbins et al. 1993)

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

669\* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)

302, 838 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35‰, Dewulf et al. 1995)

$\ln K_{AW} = -4567/(T/\text{K}) + 0.01047 \cdot Z + 14.001$ ; with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)

602 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

895 (vapor-liquid equilibrium.-GC, Turner et al. 1996)

629 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

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

583 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 6.541 - 2100/(T/\text{K})$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

1173–1273 (27°C, equilibrium headspace-GC, solute concn 0.43–18.66 mg/L, measured range 300–315 K, Cheng et al. 2003)

Octanol/Water Partition Coefficient,  $\log K_{OW}$  at  $25^\circ\text{C}$ :

3.15 (shake flask-UV, Hansch et al. 1968; Hansch & Leo 1979; Hansch & Leo 1985)

3.13 (calculated-fragment const., Rekker 1977)

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

3.12 (HPLC- $k'$  correlation, D'Amboise & Hanai 1982)

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

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

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

3.16 (HPLC- $k'$  correlation, Miyake & Terada 1982)

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

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

3.13 (generator column-RP-LC, Schantz & Martire 1987)

3.13, 3.21 (RP-HPLC capacity factor correlations, Sherblom & Eganhouse 1988)

3.15 (recommended, Sangster 1989, 1993)

3.15 (recommended, Hansch et al. 1995)

3.32, 3.32, 3.53, 3.51 (HPLC- $k'$  correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovsakya et al. 1995)

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

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

- 3.85, 3.62, 3.41, 3.24 (20.29, 30.3, 40.4, 50.28°C, from GC-determined  $\gamma^\infty$  in octanol, Gruber et al. 1997)  
 3.72, 3.698 (interpolated value from exptl value of Gruber et al. 1997, calculated using measured  $\gamma^\infty$  in pure octanol by Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 0.67 (clams, exposed to water-soluble fraction of crude oil, Nunes & Benville 1979; selected, Howard 1989)  
 2.16 (fish, calculated, Lyman et al. 1982; quoted, Howard 1989)  
 2.67 (microorganisms-water, calculated- $K_{OW}$ , Mabey et al., 1982)  
 1.19 (goldfish, Ogata et al. 1984)  
 1.20, 1.19 (fish: calculated, correlated, Sabljic 1987b)  
 2.31 (*S. capricornutum*, Herman et al. 1991)

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

- 1.98 (soil, sorption isotherm, Chiou et al. 1983)  
 2.41 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)  
 2.30 (RP-HPLC- $k'$  correlation, cyanopropyl column, Hodson & Williams 1988)  
 2.03 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.83, 2.61 (organic cations treated Marlette soil A horizon: HDTMA treated OC 10.03%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.13 (untreated Marlette soil  $B_t$  horizon, organic carbon OC 0.30%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 3.23, 3.12, 2.58 (organic cations treated Marlette soil  $B_t$  horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.26, 2.38 (untreated soils: St. Clair soil  $B_t$  horizon OC 0.44%; Oshtemo soil  $B_t$  horizon OC 0.11%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 3.37, 3.19 (organic cations HDTMA treated soils: St. Clair soil  $B_t$  horizon OC 3.25%; Oshtemo soil  $B_t$  horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.27, 2.05 (Riddles soil: top layer pH 5.0, below top layer pH 5.3, batch equilibrium, Boyd et al. 1990)  
 2.52, 2.47 (RP-HPLC- $k'$  correlation, humic acid-silica column, Szabo et al. 1990a,b)  
 2.35, 2.40, 2.42 (RP-HPLC- $k'$  correlation on 3 different stationary phases, Szabo et al. 1995)  
 2.51, 2.51 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)  
 2.32 (HPLC-screening method, Müller & Kördel 1996)  
 2.49, 2.73, 2.65, 2.73, 2.77, 2.73 2.74 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon  $f_{OC}$  = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)  
 2.04, 2.18, 1.90 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%,  $0.1 \leq$  OC < 0.5%, average, Delle Site 2001)

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

- 1.98 (Woodburn silt loam soil, 1.9% organic matter, equilibrium isotherm-GC, Chiou et al. 1983)  
 1.04 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 1.89, 1.81 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.53, 2.46, 2.08 (organic cations treated Marlette soil  $B_t$  horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)  
 2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil  $B_t$  horizon OM 4.38%; Oshtemo soil  $B_t$  horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

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

- Volatilization: rate constants:  $k$  = 0.035 d<sup>-1</sup> with  $t_{1/2}$  = 20 d in spring at 8–16°C,  $k$  = 0.331 d<sup>-1</sup> with  $t_{1/2}$  = 2.1 d in summer at 20–22°C,  $k$  = 0.054 d<sup>-1</sup> with  $t_{1/2}$  = 13 d in winter at 3–7°C for the periods when volatilization

appears to dominate, and  $k = 0.097 \text{ d}^{-1}$  with  $t_{1/2} = 7.1 \text{ d}$  with  $\text{HgCl}_2$  in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);

$t_{1/2} \sim 3.1 \text{ h}$  of evaporation from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s at  $20^\circ\text{C}$  (Lyman et al. 1982; quoted, Howard 1989).

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

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 are designated \*, see reference:

$k_{\text{OH}} = (4.8 \pm 1.0) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  at  $305 \pm 2 \text{ K}$  (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 4.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.24\text{--}24 \text{ h}$  (Darnall et al. 1976)

$t_{1/2} \approx 15 \text{ h}$  in water, probably not important as aquatic fate (Callahan et al. 1979)

$k_{\text{OH}} = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and residence time of 1.4 d, loss of 51% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$  for singlet oxygen and  $720 \text{ M}^{-1} \text{ h}^{-1}$  for  $\text{RO}_2$  radical (Mabey et al. 1982)

$k_{\text{OH}} = 4.4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 1.3 \text{ d}$  in the atmosphere (Mill 1982)

$k_{\text{O}_3} = 340 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at 300 K (Lyman et al. 1982)

$k = (14 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 100 mM *t*-BuOH as scavenger at pH 2.0 and  $20\text{--}23^\circ\text{C}$  (Hoigné & Bader 1983)

$k_{\text{OH}} = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 8.56\text{--}85.6 \text{ h}$  (Atkinson 1985)

$k_{\text{OH}} = 6.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (relative rate method, Ohta & Ohshima 1985)

$k_{\text{OH}}(\text{calc}) = 6.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}} = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $\sim 298 \text{ K}$  (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 6.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis: not aquatically significant (Callahan et al. 1979);

no hydrolyzable functional groups (Mabey et al. 1982)

Biodegradation:

100% biodegraded after 192 h at  $13^\circ\text{C}$  with an initial concn of  $1.36 \times 10^{-6} \text{ L/L}$  (Jamison et al. 1976)

$t_{1/2}(\text{aq. aerobic}) = 72\text{--}240 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 4224\text{--}5472 \text{ h}$ , based on anaerobic groundwater die-away test data (Wilson et al. 1986; Howard et al. 1991)

$k = 0.5 \text{ d}^{-1}$ , significant degradation under favourable conditions in an aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2} \sim 2 \text{ d}$  degradation by established microorganisms depending on body of water and its temperature (Howard 1989)

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

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 0.24\text{--}24 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976); photodecomposition  $t_{1/2} = 5.0 \text{ h}$  under simulated atmospheric conditions, with NO (Dilling et al. 1976); residence time of 1.4 d, loss of 51% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

summer daylight lifetime  $\tau = 20 \text{ h}$  due to reaction with OH radical (Altshuller 1991);

$t_{1/2} = 8.56\text{--}85.6 \text{ h}$ , based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991).

Surface Water:  $t_{1/2} = 5\text{--}6 \text{ h}$  (Callahan et al. 1979), based on the estimated evaporative loss of toluene at  $25^\circ\text{C}$  and 1 m depth of water (Mackay & Leinonen 1975);

$t_{1/2} = 20 \text{ d}$  in spring at  $6\text{--}16^\circ\text{C}$ ,  $t_{1/2} = 2.1 \text{ d}$  in summer at  $20\text{--}22^\circ\text{C}$ ,  $t_{1/2} = 13 \text{ d}$  in winter at  $3\text{--}7^\circ\text{C}$  and  $t_{1/2} = 7.1 \text{ d}$  with  $\text{HgCl}_2$  in marine mesocosm experiments (Wakeham et al. 1983);

$t_{1/2} = 72\text{--}240 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991).

Ground water:  $t_{1/2} = 144\text{--}5472 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991);

$t_{1/2} \sim 0.3 \text{ yr}$  from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981).

Soil:  $t_{1/2} = 72\text{--}240$  h, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991);  
 $t_{1/2} < 10$  d (Ryan et al. 1988).

Biota:

**TABLE 3.1.1.3.1**  
**Reported aqueous solubilities of ethylbenzene at various temperatures**

1.

Bohon & Claussen 1951		Polak & Lu 1973		Brown & Wasik 1974		Ben-Naim & Wiffb 1979	
shake flask-UV		shake flask-GC		headspace-GC		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>
0.4	219	0	197	4.5	196	10	203
5.2	213	25	177	6.3	192	20	212
20.7	207			7.1	186		
21.2	207			9	187		
25	208			11.8	181		
25.6	209			12.1	183		
30.2	211			15.1	180		
34.9	221			17.9	184		
42.8	231			20.1	180		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 11.9$			
25°C	1.6			at 25°C			
2°C	-3.98						
7°C	-2.74						
12°C	-1.63						
17°C	-0.343						
22°C	-0.167						
27°C	1.97						
32°C	3.615						
37°C	7.36						

2.

Schwarz & Miller 1980		Sanemasa et al. 1981		Owens et al. 1986		Shaw 1989b (IUPAC)	
shake flask-UV		vapor saturation-UV		generator column-HPLC/UV		recommended values	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
10	180	15	176	10	197	0	200
20	184	25	181	14	192	10	180
		35	194	17	189	20	181
elution chromatography		45	215	18	183	25	169
10	211			19	178	30	190
20	208	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.60$		20	188	40	200
		at 25°C		21	183	50	220
				22	182	60	250
		<b>Sanemasa et al. 1982</b>		23.5	186	70	280
		<b>vapor saturation-UV</b>		25	192	80	330
		<b>t/°C S/g·m<sup>-3</sup></b>		25.8	186	90	390
				28	185.5	100	460
				30	188.7		
				35	193		
		15	160			$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.1$	
		25	169				



TABLE 3.1.1.3.1 (Continued)

Schwarz & Miller 1980		Sanemasa et al. 1981		Owens et al. 1986		Shaw 1989b (IUPAC)	
shake flask-UV		vapor saturation-UV		generator column-HPLC/UV		recommended values	
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>
		35	176	40	205	at 25°C	
		45	196	45	211.4		
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.90$ at 25°C		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.30$ 25°C			
3.							
Chen & Wagner 1994c		Dohányosová et al. 2001		Sawamura et al. 2001			
equil. flow cell-GC		vapor abs-HPLC/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>		
30	170	0.5	169	0	190.8		
40	172	5	167	5	182		
50	198	15	167	10	175		
60	240	25	170	15	170		
70	291	35	177	20	169		
80	353	45	188	25	170		
90	410	55	213.5	30	173.8		
100	504			35	179.8		
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.0$		40	188.1		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.30$		at 25°C		45	196.9		
at 25°C				50	208		

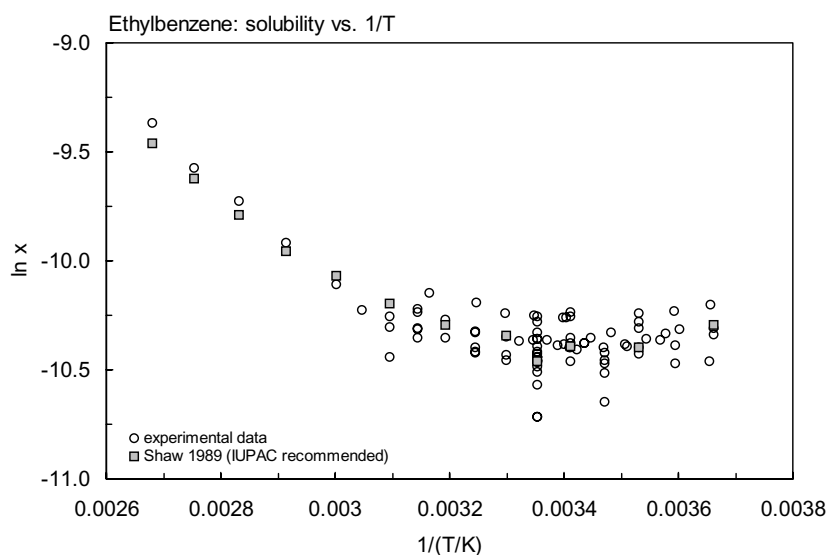
FIGURE 3.1.1.3.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for ethylbenzene.

TABLE 3.1.1.3.2

Reported vapor pressures of ethylbenzene 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.

Linder 1931		Willingham et al. 1945		Stull 1947		Buck et al. 1949	
mercury manometer		ebulliometry		summary of literature data		static-Hg manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-11.6	74.7	56.589	6277	-9.8	133.3	63.3	8399
-1.20	184	60.796	7654	13.9	266.6	67.7	10133
0	209.3	64.463	8962	25.9	1333	75.2	13999
		67.775	10303	38.6	2666	82.6	18665
		70.862	11699	52.8	5333	91.6	25998
		75.027	13919	61.8	7999	99	33864
		79.777	16608	74.1	13332	108.1	45596
		84.599	19924	92.7	26664	112.7	52662
<b>Rintelin et al. 1937</b>		89.071	23450	113.8	53323	117.6	60928
mercury manometer		95.056	28954	136.2	101325	120.5	66128
t/°C	P/Pa					125.6	75460
10	387	100.561	34897			129.3	85060
30	1546	107.183	43320	mp/°C	-94.9	135.9	100792
50	4613	114.02	53654				
		121.312	66755				
		129.221	83717			eq. 4	P/mmHg
		134.8	97603			A	3225
		135.399	99199			B	7.553
		135.954	100690			C	30.49
<b>Stuckey &amp; Saylor 1940</b>		136.574	102385				temp range:
static-Hg manometer		137.124	103903				80–120°C
t/°C	P/Pa						
measured 4–75°C		eq. 2	P/mmHg				
eq. 4	P/mmHg	A	6.94998				
A	22.9028	B	1419.315				
B	2857.75	C	212.611				
C	5						
		bp/°C	136.187				
bp/°C	136.32						

2.

Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971		Osborn & Scott 1980	
ebulliometry		ebulliometry		selected values		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
56.689	6398	146.85	133800	25.88	1333	66.031	9585
60.887	7690	166.85	216100	38.6	2666	69.091	10887
64.51	8990	186.85	332500	46.69	4000	72.167	12339
67.827	10330	206.85	492000	52.75	5333	75.258	13956
70.891	11720	226.85	703300	57.657	6666	78.254	15748
75.054	13840	246.85	976500	61.789	7999	81.465	17734

TABLE 3.1.1.3.2 (Continued)

Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971		Osborn & Scott 1980	
ebulliometry		ebulliometry		selected values		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
79.791	16633	266.85	1321500	68.596	10666	84.587	19933
83.619	19944	286.85	1751100	74.105	13332	90.869	25023
89.09	23474	306.85	2279100	84.687	19998	97.199	31177
95.074	28978	326.85	2924900	92.68	26664	103.575	38565
100.675	34925			99.182	33331	110.001	47375
107.21	43360	eq. 5	P/bar	104.703	39997	116.474	57817
114.046	53698	A	21.956	113.823	53329	122.998	70120
121.331	66796	B	2923.84	121.266	66661	129.571	84532
129.234	83749	C	5.67301	127.603	79993	136.193	101325
134.815	97645	D	1772	133.152	93326	142.863	120790
135.413	99235			134.185	95991	149.587	143240
135.969	100725			135.196	98659	156.356	169020
136.602	102462			135.164	101325	163.174	198490
137.16	103999			25	1266.6	170.038	232020
						176.953	270030
eq. 2	P/mmHg			eq. 2	P/mmHg		
A	6.959			A	6.95719	data fitted to 4-constant vapor pressure eq.	
B	1425.46			B	1424.255		
C	213.345			C	213.206		
bp/°C	136.186			bp/°C	136.186		
				$\Delta H_v / (\text{kJ mol}^{-1})$			
				at 25°C		42.25	
				at bp		35.56	

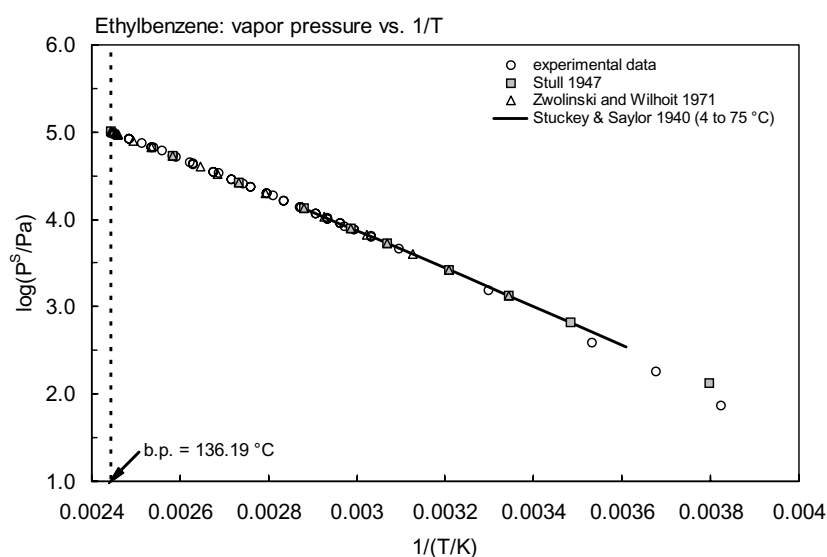


FIGURE 3.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for ethylbenzene.

TABLE 3.1.1.3.3

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

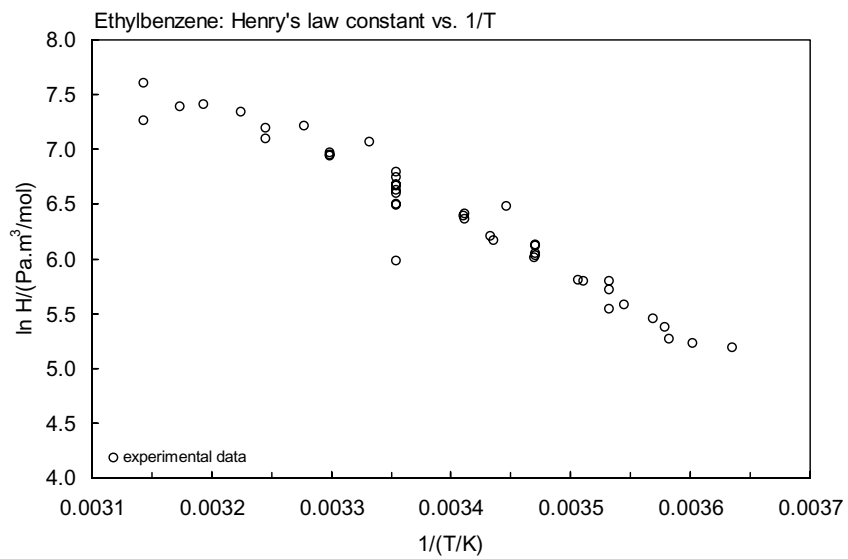
$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})]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

1.

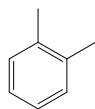
Brown & Wasik 1974		Sanemasa et al. 1981		Sanemasa et al. 1982		Ashworth et al. 1988	
head space-GC		vapor-liquid equilibrium		vapor-liquid equilibrium		EPICS-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
4.5	187.5	15	459	15	418	10	330
6.33	217.2	25	797	25	734	15	457
7.06	235.1	35	1339	35	1211	20	609
8.96	265	45	1436	45	1436	25	798
11.75	329					30	1064
12.1	333.6						
15.1	409.7					eq. 4a	H/(atm m <sup>3</sup> /mol)
17.93	480.2					A	11.92
20.06	559.1					B	4994

2.

Robbins et al. 1993		Perlinger et al. 1993		Dewulf et al. 1995	
static headspace-GC		equilibrium headspace-GC		EPICS-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
25	788	10	306	2	180
30	1034	15	428	6	194
40	1662	20	583	10	257
		25	660	18.2	497
eq. 4	H/(Pa m <sup>3</sup> /mol)	30	1044	25	669
A	7.14				
B	3689			eq 1	K <sub>AW</sub>
				A	14.001
				B	4567



**FIGURE 3.1.1.3.3** Logarithm of Henry's law constant versus reciprocal temperature for ethylbenzene.

3.1.1.4 *o*-Xylene

Common Name: *o*-Xylene

Synonym: 1,2-dimethylbenzene, *o*-xylol, 2-methyltoluene

Chemical Name: *o*-xylene

CAS Registry No: 95-47-6

Molecular Formula:  $C_8H_{10}$ ,  $C_6H_4(CH_3)_2$

Molecular Weight: 106.165

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

−25.2 (Weast 1982–83; Lide 2003)

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

144.5 (Lide 2003)

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

0.8802 (Weast 1982–83)

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

120.6 ( $20^{\circ}C$ , calculated-density)

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

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

43.434, 36.82 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

13.6 (Chickos et al. 1999)

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

55.23 (Yalkowsky & Valvani 1980)

54.9, 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  $25^{\circ}C$  or as indicated. Additional data at other temperatures designated \*, are compiled at the end of this section):

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

175 (shake flask-GC, McAuliffe 1963)

175 (shake flask-GC, McAuliffe 1966)

176 (shake flask-GC, Hermann 1972)

213\* (shake flask-GC, Polak & Lu 1973)

170.5 (shake flask-GC, Sutton & Calder 1975)

167 (shake flask-GC, Price 1976)

167 (shake flask-GC, Krzyzanowska & Szeliga 1978)

240\* ( $20^{\circ}C$ , shake flask-UV, Ben-Naim & Wiff 1979)

179\* (vapor saturation-UV spec., measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)

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

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

176 (shake flask-purge and trap-GC, Coutant & Keigley 1988)

173\* (IUPAC recommended value, temp range  $0$ – $45^{\circ}C$ , Shaw 1989b)

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):

146.7\* ( $0.60^{\circ}C$ , mercury manometer, measured range  $-17$  to  $0.60^{\circ}C$ , Linder 1931)

767\* ( $20^{\circ}C$ , Hg manometer, Kassel 1936)

$\log (P/mmHg) = -2830.0/(T/K) - 5 \cdot \log (T/K) + 22.7480$ ; temp range  $0$ – $80^{\circ}C$  (vapor pressure eq. from Hg manometer measurements, Kassel 1936)

987\* ( $30^{\circ}C$ , Hg manometer, measured range  $10$ – $50^{\circ}C$ , Rintelen et al. 1937)

$\log (P/\text{mmHg}) = -2908.07/(T/K) - 5 \cdot \log (T/K) + 22.95279$ ; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)

880\* (Hg manometer measurements, Pitzer & Scott 1943)

$\log (P/\text{mmHg}) = -3327.16/(T/K) - 8.0 \log (T/K) + 31.7771$ ; temp range 0–60°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)

6354\* (63.460°C, ebulliometry, measured range 63.460–145.367°C, Willingham et al. 1945)

6401\* (63.608°C, ebulliometry, measured range 63.608–145.400°C, Forziati et al. 1949)

$\log (P/\text{mmHg}) = 6.99937 - 1474.969/(213.714 + t/^\circ\text{C})$ ; temp range 63.5–145.4°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

266.6\* (20.2°C, summary of literature data, Stull 1947)

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t/^\circ\text{C})$ ; temp range 63.6–145.4°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

892 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t/^\circ\text{C})$ ; temp range 50–200°C (Antoine eq. for liquid state, Dreisbach 1955)

1333\* (32.155°C, compiled data, temp range 32.155–172.095°C, Bond & Thodos 1960)

108000\* (146.85°C, ebulliometry, measured range 146.85–346.85°C, Ambrose et al. 1967)

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

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t/^\circ\text{C})$ ; temp range 32.14–172.07°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 9998.5/(T/K)] + 8.147551$ ; temp range –3.8 to 144.4°C (Antoine eq., Weast 1972–73)

$\log (P/\text{atm}) = (1 - 417.496/T) \times 10^{(0.855257 - 6.48662 \times 10^4 \cdot T + 5.53883 \times 10^7 \cdot T^2)}$ ; T in K, temp range: 253.2–631.64 K (Cox vapor pressure eq., Chao et al. 1983)

882, 885 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.12699 - 1476.753/(213.911 + t/^\circ\text{C})$ ; temp range 63.46–145.4°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.9422 - 1387.336/(206.409 + t/^\circ\text{C})$ ; temp range 0–50°C (Antoine eq. from reported exptl. data of Pitzer & Scott 1943, Boublik et al. 1984)

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

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.69 + t/^\circ\text{C})$ ; temp range 32–172°C (Antoine eq., Dean 1985, 1992)

880 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.13072 - 1479.82/(214.315 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

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

$\log (P_L/\text{kPa}) = 6.13132 - 1480.155/(-58.804 + T/K)$ ; temp range 333–419 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15921 - 1502.949/(-55.725 + T/K)$ ; temp range 416–473 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.46119 - 1772.963/(-18.84 + T/K)$ ; temp range 471–571 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.91427 - 3735.582/(229.953 + T/K)$ ; temp range 567–630 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 37.2413 - 3.4573 \times 10^3/(T/K) - 10.126 \cdot \log (T/K) + 9.0676 \times 10^{-11} \cdot (T/K) + 2.6123 \times 10^{-6} \cdot (T/K)^2$ , temp range 248–630 K (vapor pressure eq., Yaws 1994)

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

542, 506 (calculated as  $1/K_{AW}$ , calculated-bond contribution, Hine & Mookerjee 1975)

647 (vapor liquid equilibrium-concentration ratio, Leighton & Calo 1981)

526\* (vapor-liquid equilibrium, Sanemasa et al. 1982)

594 (20°C, EPICS-GC, Yurteri et al. 1987)

493\* (EPICS-GC/FID, Ashworth et al. 1988)

$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.541 - 3220/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

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

592 (concentration ratio, Anderson 1992)

1067\* (40°C, equilibrium headspace-GC, Kolb et al. 1992)

$\ln (1/K_{AW}) = -7.61 + 2647/(T/K)$ , temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

485 (infinite activity coeff.  $\gamma^\infty$  in water determined by inert gas stripping-GC, Li et al. 1993)

506\* (static headspace-GC, Robbins et al. 1993)

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

429\* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)

189, 496 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35‰ Dewulf et al. 1995)

$\ln K_{AW} = -4232/(T/K) + 0.01115 \cdot Z + 12.400$ ; with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)

412 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

731 (vapor-liquid equilibrium-GC, Turner et al. 1996)

464.4 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

390 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 5.064 - 1719/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

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

3.15 (calculated- $\pi$  substituent constant, Hansch et al. 1968)

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

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

3.13 (generator column-HPLC/UV, Tewari et al. 1982b,c)

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

3.13; 3.14, 3.14, 3.06, 3.16, 3.42 (quoted exptl.; calculated- $\pi$  const., f const., MW, MCI  $\chi$ , TSA, Doucette & Andren 1988)

3.25, 3.35 (RP-HPLC- $k'$  capacity factor correlations, Sherblom & Eganhouse 1988)

3.12 (recommended, Sangster 1989)

3.18 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)

3.12 (recommended, Hansch et al. 1995)

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

3.80\* (30.3°C, from GC-determined  $\gamma^\infty$  in octanol, measured range 30.3–50.28°C, Gruber et al. 1997)

3.72 (calculated-measured  $\gamma^\infty$  in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

1.33 (eels, Ogata & Miyake 1978)

0.79 (clams, Nunes & Benville 1979)

1.15 (goldfish, Ogata et al. 1984)

2.34 (*S. capricornutum*, Herman et al. 1991)

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

1.68–1.83 (Nathwani & Philip 1977)

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

2.73 (HPLC- $k'$  correlation, cyanopropyl column, Hodson & Williams 1988)

2.37, 2.40 (RP-HPLC- $k'$  correlation, humic acid-silica column, Szabo et al. 1990a,b)

3.13 (average of 5 soils, sorption isotherms by batch equilibrium method, Xing et al. 1994)

2.36, 2.65, 2.65 (RP-HPLC- $k'$  correlation on 3 different stationary phases, Szabo et al. 1995)

2.45, 2.45 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

2.40, 2.70, 2.58, 2.68, 2.73, 2.69, 2.68 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)

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

Volatilization:  $t_{1/2} = 5.61$  h from water depth of 1 m (Mackay & Leinonen 1975; Haque et al. 1980);

$t_{1/2} \sim 3.2$  h of evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s (Lyman et al. 1982);



$t_{1/2} \sim 31\text{--}125$  h of evaporation from a typical river or pond (Howard 1990).

Photolysis:  $k = 7.46 \times 10^{-3} \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  under photolysis at  $25^\circ\text{C}$  in F-113 solution and with  $\text{HO}^-$  in the gas (Dilling et al. 1988).

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

$k_{\text{OH}} = (7.7 \pm 2.3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ ;  $k_{\text{O(}^3\text{P)}} = (1.05 \pm 0.11) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $\text{O(}^3\text{P)}$  atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{\text{OH}} = (15.3 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{O(}^3\text{P)}} = (1.74 \pm 0.18) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction of  $\text{O(}^3\text{P)}$  atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{\text{OH}} = 8.4 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.24\text{--}24$  h (Darnall et al. 1976)

$k_{\text{OH}}^* = (14.3 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp., measured over temp range  $296\text{--}473$  K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{\text{OH}} = (12.9, 13.0, 12.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with different dilute gas, Ar or He at  $298$  K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{\text{OH}} = 13.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and residence time of  $0.8$  d, loss of  $71.3\%$  in one day or  $12$  sunlit hours at  $300$  K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 2$  K with a calculated lifetime  $\tau > 2300$  d, and a calculated lifetime of  $0.8$  d due to reaction with OH radical at room temp. (Atkinson et al. 1982)

$k_{\text{O}_3} = 950 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  at  $300$  K (Lyman et al. 1982)

$k_{\text{OH}} = (5.9\text{--}12) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.47\text{--}1.0$  d (Mill 1982)

$k = (90 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water at pH  $1.7\text{--}5.0$  and  $20\text{--}23^\circ\text{C}$  (Hoigné & Bader 1983)

$k_{\text{NO}_3} = 1.1 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296$  K (Atkinson et al. 1984)

$k_{\text{OH}} = 13.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 4.4\text{--}44$  h (Atkinson 1985)

$k_{\text{OH}} = 12.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298$  K (relative rate method, Ohta & Ohyama 1985)

$k_{\text{OH}} = 12.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $24.2^\circ\text{C}$ , with a calculated atmospheric lifetime of  $0.93$  d (Edney et al. 1986)

$k_{\text{OH}}(\text{calc}) = 6.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 14.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship] Atkinson 1987)

$k_{\text{OH}} = 1.47 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{NO}_3} = 3.74 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298$  K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}} = 1.47 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{NO}_3} = 3.7 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson & Aschmann 1988)

$k_{\text{OH}}^* = 1.37 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  independent over  $296\text{--}320$  K (recommended, Atkinson 1989)

$k_{\text{OH}} = 13.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298$  K (Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 6.92 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298$  K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 14.75 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}}(\text{calc}) = 6.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{exptl}) = 13.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298$  K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

$100\%$  biodegraded after  $192$  h at  $13^\circ\text{C}$  with an initial concn of  $1.62 \times 10^{-6} \text{ L/L}$  (Jamison et al. 1976);

$t_{1/2}(\text{aq. Aerobic}) = 168\text{--}672$  h, estimated based on aqueous screening test data (Bridie et al. 1979; Howard et al. 1991) and soil column study simulating an aerobic river/ground-water infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 4320\text{--}8640$  h, estimated based on acclimated grab sample data for anaerobic soil from a groundwater aquifer receiving landfill leachate (Wilson et al. 1986) and a soil column study simulating an anaerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$k = 0.06 \text{ yr}^{-1}$  with  $t_{1/2} = 32$  d (Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 7$  d,  $t_{1/2}(\text{anaerobic}) = 180$  d in natural waters (Capel & Larson 1995)

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.24\text{--}2.4$  h, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976);

residence time of 0.8 d, loss of 71.3% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

calculated lifetimes  $\tau > 2300$  d and 0.8 d due to reactions with  $O_3$  and OH radical respectively at room temp. (Atkinson et al. 1982);

$t_{1/2} = 4.4\text{--}44$  h, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);

summer daylight lifetime  $\tau = 10$  h due to reaction with OH radical (Altshuller 1991);

calculated lifetime  $\tau = 0.93$  d due to reaction with OH radical (Edney et al. 1986).

Surface Water: photooxidation  $t_{1/2} = 3.9 \times 10^5\text{--}2.7 \times 10^8$  h in water, based on estimated rate data for alkoxy radical in aqueous solution (Hendry et al. 1974);

$t_{1/2} = 5.18$  h, based on evaporative loss at 25°C and 1 m depth of water (Mackay & Leinonen 1975; Haque et al. 1980);

$t_{1/2} = 168\text{--}672$  h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

$t_{1/2} = 1\text{--}5$  d, volatilization to be the dominant removal process (Howard 1990).

$t_{1/2}(\text{aerobic}) = 7$  d,  $t_{1/2}(\text{anaerobic}) = 180$  d in natural waters (Capel & Larson 1995)

Ground water:  $t_{1/2} = 336\text{--}8640$  h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Wilson et al. 1986; Howard et al. 1991);

$t_{1/2} \sim 0.3$  yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981).

Soil:  $t_{1/2} = 168\text{--}672$  h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).

Biota:  $t_{1/2} = 2$  d to eliminate from eels in seawater (Ogata & Miyake 1978).

TABLE 3.1.1.4.1

Reported aqueous solubilities of *o*-xylene at various temperatures

Polak & Lu 1973		Ben-Naim & Wiff 1979		Sanemasa 1982		Shaw 1989b (IUPAC)	
shake flask-GC		shake flask-UV		vapor saturation-UV		recommended values	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	142	10	212.4	15	168	0	140
25	213	20	240	25	179	15	170
				35	198	25	173
				45	214	35	200
						45	210

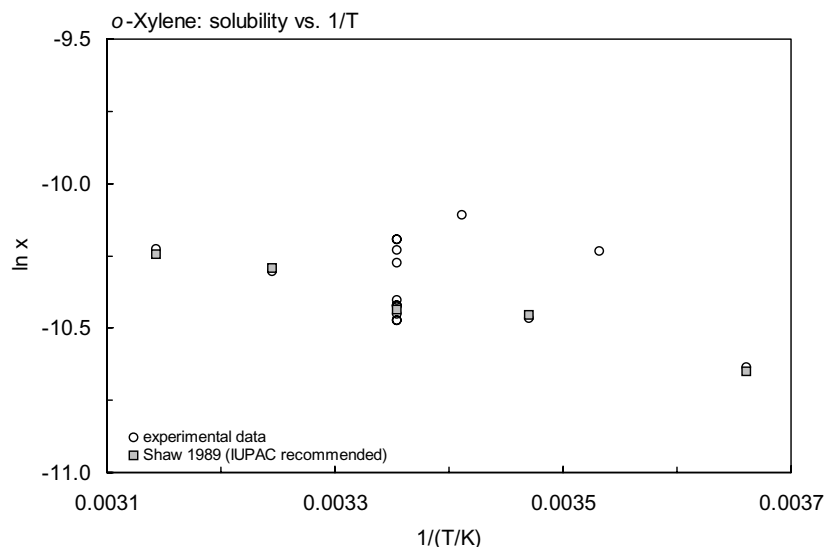


FIGURE 3.1.1.4.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *o*-xylene.

TABLE 3.1.1.4.2

Reported vapor pressures of *o*-xylene at various temperatures and the coefficients for the vapor pressure equations

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

1.

Kassel 1936		Rintelen et al. 1937		Stuckey & Saylor 1940		Pitzer & Scott 1943	
mercury manometer		mercury manometer		mercury manometer		mercury manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	215	10	213	measured 4–75°C		0	173
10	417	30	987	eq. 4	P/mmHg	12.5	400
20	767	50	3346	A	22.95279	25.0	880
30	1347			B	908.07	37.5	1800
40	2280	bp 144.0–144.1°C		C	5.0	50	3400
50	3680					60	5413
60	5826	Linder 1931		bp/°C	144.39–144.41		
70	8892	mercury manometer				eq. 4	P/mmHg
80	13186	t/°C	P/Pa			A	31.7771
		–17	26.66			B	3327.16
		–10.7	56.0			C	8.0
eq. 4	P/mmHg						
A	23.7480	0	141.3				
B	2830.06	0.60	146.7				
C	5.0						
						$\Delta H_v/(\text{kJ mol}^{-1}) = 43.806$ at 25°C	

2.

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Bond & Thodos 1960	
ebulliometry		summary of literature data		ebulliometry		compiled data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
63.460	6354	–3.80	133.3	63.608	6401	32.155	1333
67.746	7654	20.2	266.6	67.852	7693	63.48	6354
71.481	8963	32.1	1333	71.548	8991	74.87	10303
74.857	10303	45.1	2666	74.916	10331	112.46	39997
77.993	11699	59.5	5333	78.048	11722	141.35	93326
82.242	13819	68.8	7999	82.285	13843	172.095	199984
87.081	16621	81.3	13332	87.101	16635	eq. 5 P/mmHg	
91.987	19924	100.2	26664	92.015	19945	A	25.82849
96.541	23450	121.7	53329	96.568	23475	B	3040.72
102.632	28954	144.4	101325	102.657	28979	C	5.94175
108.227	34897	mp/°C –25.2		198.250	34926	D	2.61456
114.965	43322			114.988	43362	bp/°C 144.426	
121.909	53654			121.935	53700		
129.318	66756			129.333	66797		
137.346	83717			137.356	83750		
143.007	97604			143.619	97647		
143.614	99200			143.626	99236		
144.176	100692			144.190	87395		
144.809	102385			144.832	90465		

(Continued)

TABLE 3.1.1.4.2 (Continued)

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Bond & Thodos 1960	
ebulliometry		summary of literature data		ebulliometry		compiled data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
145.367	103905			145.400	104000		
eq. 2	P/mmHg			eq. 2	P/mmHg		
A	6.99937			A	6.99891		
B	1474.967			B	1474.679		
C	144.414			C	213.686		
bp/°C	144.414			bp/°C	144.411		

## 3.

Ambrose et al. 1967		Zwolinski & Wilhoit 1971			
ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
146.85	108000	32.14	1333	145.395	103991
166.85	177200	45.13	2666	146.359	106658
186.85	276700	53.38	4000	150.912	119990
206.85	413900	59.56	5333	155.08	13322
226.85	598300	64.558	6666	162.53	159987
246.85	839100	68.778	7999	172.07	199984
266.85	1146500	75.704	10666	25.0	879.9
286.85	1532100	81.314	13332		
306.85	2009000	92.085	19998	eq. 2	P/mmHg
326.85	2592500	100.217	26664	A	6.99891
346.85	3304100	106.829	33331	B	1474.679
		112.441	39997	C	213.686
eq. 5	P/bar	121.708	53329		
A	20.79970	129.267	66661	bp/°C	144.411
B	2921.11	135.700	79993		
C	5.26888	141.332	93326	$\Delta H_v$ /(kJ mol <sup>-1</sup> )	
D	1672	142.380	95991	at 25°C	43.43
		143.407	98659	at bp	36.82
1 bar = 1×10 <sup>5</sup> Pa		144.411	101325		

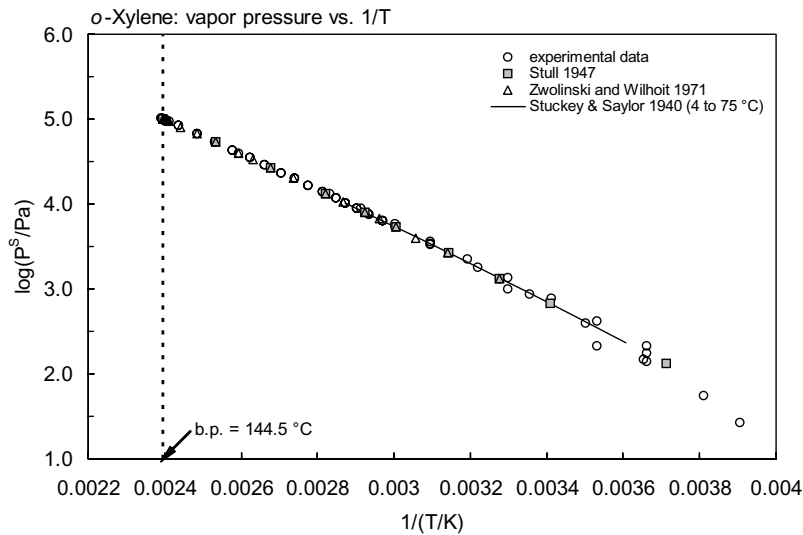
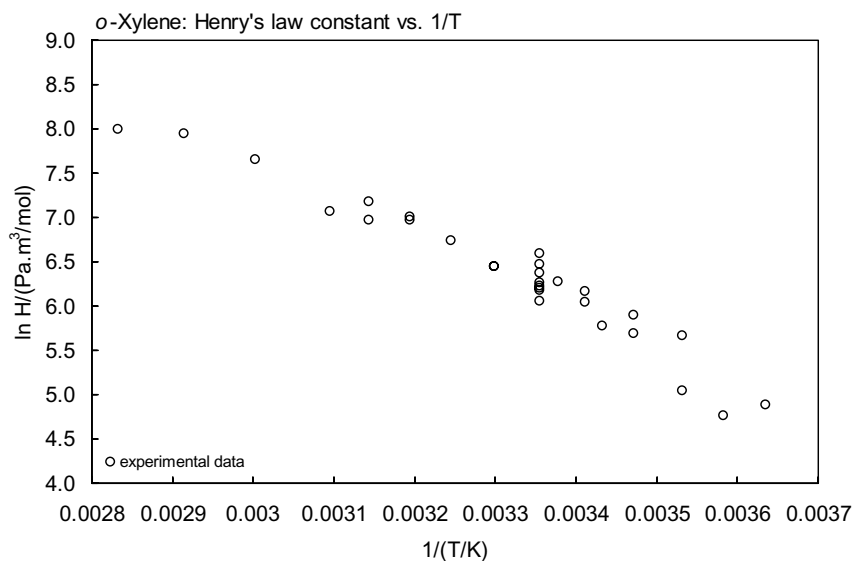


FIGURE 3.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for *o*-xylene.

TABLE 3.1.1.4.3  
Reported Henry’s law constants of *o*-xylene 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)				
$K_{AW} = A - B (T/K) + C (T/K)^2$		(5)							
Sanemasa et al. 1982		Ashworth et al. 1988		Kolb et al. 1992		Robbins et al. 1993		Dewulf et al. 1995	
vapor-liquid equilibrium		EPICS-GC		headspace-GC		static headspace-GC		EPICS-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
15	299	10	289	40	1067	25	506	2	133
25	526	15	366	60	2114	30	637	6	118
35	844	20	480	70	2825	40	1104	10	155
45	1323	25	493	80	2966	45	1074	18	325
		30	634			50	1175	25	429
		eq. 4a		eq. 2	K <sub>AW</sub>	eq. 4		eq 1	K <sub>AW</sub>
		H/(atm m <sup>3</sup> /mol)		A	761	H/(Pa m <sup>3</sup> /mol)		A	12.4
		A	5.541	B	2647/R	A	17.67818	B	4243
		B	3220			B	3397.97		

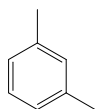


**FIGURE 3.1.1.4.3** Logarithm of Henry's law constant versus reciprocal temperature for *o*-xylene.

**TABLE 3.1.1.4.4**  
Reported octanol-air partition coefficients of *o*-xylene at various temperatures

Gruber et al. 1997

GC det'd activity coefficient	
$t/^{\circ}\text{C}$	$\log K_{\text{OA}}$
20.29	-
30.3	3.80
40.4	3.59
50.28	3.38

3.1.1.5 *m*-Xylene

Common Name: *m*-Xylene

Synonym: 1,3-dimethylbenzene, *m*-xylol, 3-methyltoluene

Chemical Name: *m*-xylene

CAS Registry No: 108-38-3

Molecular Formula:  $C_8H_{10}$ ,  $C_6H_4(CH_3)_2$

Molecular Weight: 106.165

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

−47.8 (Lide 2003)

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

139.12 (Lide 2003)

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

0.8842 (Weast 1982–83)

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

120.1 ( $20^{\circ}C$ , calculated-density)

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

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

42.656, 36.36 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

11.57 (Chickos et al. 1999)

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

51.88 (Yalkowsky & Valvani 1980)

51.4, 45.6 (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  $25^{\circ}C$ , or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

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

196\* (shake flask-UV, measured range  $0.4$ – $39.6^{\circ}C$ , Bohon & Claussen 1951)

157 (shake flask-GC, Hermann 1972)

162\* (shake flask-GC, Polak & Lu 1973)

206 (shake flask-UV, Vesala 1974)

146 (shake flask-GC, Sutton & Calder 1975)

160\* (synthetic method-GC, measured range  $20$ – $70^{\circ}C$ , Chernoglazova & Simulin 1976)

134 (shake flask-GC, Price 1976)

134 (shake flask-GC, Krzyzanowska & Szeliga 1978)

162\* (vapor saturation-UV spec., measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)

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

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

160\* (IUPAC recommended value, temp range  $0$ – $70^{\circ}C$ , Shaw 1989b)

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):

1812.7\* ( $-2.80^{\circ}C$ , mercury manometer, measured range  $-8.40$  to  $-2.80^{\circ}C$ , Linder 1931)

833\* ( $20^{\circ}C$ , Hg manometer, Kassel 1936)

$\log (P/mmHg) = -2876.3/(T/K) - 5 \cdot \log (T/K) + 22.9425$ ; temp range  $0$ – $80^{\circ}C$  (vapor pressure eq. from Hg manometer measurements, Kassel 1936)

1213\* ( $30^{\circ}C$ , Hg manometer, measured range  $10$ – $50^{\circ}C$ , Rintelen et al. 1937)

$\log (P/\text{mmHg}) = -2870.38/(T/K) - 5 \cdot \log (T/K) + 22.92341$ ; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)

1113\* (Hg manometer, measured range 0–60°C, Pitzer & Scott 1943)

$\log (P/\text{mmHg}) = -2871.66/(T/K) - 5.0 \log (T/K) + 22.9270$ ; temp range 0–60°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)

6355\* (59.203°C, ebulliometry, measured range 59.203–140.041°C, Willingham et al. 1945)

$\log (P/\text{mmHg}) = 7.00343 - 1458.214/(214.609 + t/^\circ\text{C})$ ; temp range 59.2–140.0°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

266.6\* (16.8°C, summary of literature data, temp range –6.9 to 139.1°C, Stull 1947)

6400\* (59.335°C, ebulliometry, measured range 59.335–140.078°C, Forziati et al. 1949)

$\log (P/\text{mmHg}) = 8.00849 - 1461.925/(215.073 + t/^\circ\text{C})$ ; temp range 59.3–140.1°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

1115 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/\text{mmHg}) = 7.00908 - 1462.266/(215.105 + t/^\circ\text{C})$ ; temp range 45–195°C (Antoine eq. for liquid state, Dreisbach 1955)

124200\* (146.85°C, ebulliometry, measured range 146.85–316.85°C, Ambrose et al. 1967)

1100\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 7.00908 - 1462.266/(215.105 + t/^\circ\text{C})$ ; temp range 28.24–166.39°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 9904.2/(T/K)] + 8.167049$ ; temp range –6.9 to 139.1°C (Antoine eq., Weast 1972–73)

$\log (P/\text{atm}) = (1 - 3412.335/T) \times 10^{(0.859841 - 6.73249 \times 10^4 \cdot T + 5.87438 \times 10^7 \cdot T^2)}$ ; T in K, temp range 243.2–619.2 K (Cox vapor pressure eq., Chao et al. 1983)

1104, 1142 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.13232 - 1460.805/(214.895 + t/^\circ\text{C})$ ; temp range 59.2–140.4°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.4729 - 1641.628/(230.899 + t/^\circ\text{C})$ ; temp range: 0–60°C (Antoine eq. from reported exptl. data of Pitzer & Scott 1943, Boublik et al. 1984)

1106 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.00908 - 1462.266/(215.11 + t/^\circ\text{C})$ ; temp range: 28–166°C (Antoine eq., Dean 1985, 1992)

1100 (selected lit. value., Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.13785 - 1465.39/(215.512 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

1110 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14083 - 1457.244/(-57.442 + T/K)$ ; temp range 331–414 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.76037 - 1292.22/(-72.052 + T/K)$ ; temp range 267–301 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.17035 - 1490.184/(-54.184 + T/K)$ ; temp range 412–462 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.42535 - 1710.901/(-24.591 + T/K)$ ; temp range 461–554 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.59221 - 3163.74/(165.278 + T/K)$ ; temp range 550–617 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 34.6803 - 3.2981 \times 10^3/(T/K) - 9.2570 \cdot \log (T/K) - 4.3563 \times 10^{-10} \cdot (T/K) + 2.4103 \times 10^{-6} \cdot (T/K)^2$ , temp range 226–617 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):

731\* (vapor-liquid equilibrium, Sanemasa et al. 1982)

754\* (EPICS-GC/FID, Ashworth et al. 1988)

$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 6.280 - 3337/(T/K)$ ; temp range: 10–30°C (EPICS measurements, Ashworth et al. 1988)

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

665 (infinite activity coeff.  $\gamma^\infty$  in water determined by inert gas stripping-GC, Li et al. 1993)

739\* (static headspace-GC, same as *p*-xylene, Robbins et al. 1993)

615\* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)



- 297, 771 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35%, Dewulf et al. 1995)  
 $\ln K_{AW} = -4026/(T/K) + 0.00846 \cdot Z + 12.123$ ; with Z salinity 0–35.5%, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)  
 590 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 658.5 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 561 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)  
 $\log K_{AW} = 5.204 - 1713/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

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

- 3.20 (Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)  
 3.18 (generator column-HPLC/UV, Wasik et al. 1981)  
 3.29 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 3.13 (generator column-HPLC/UV, Tewari et al. 1982b,c)  
 3.20 (generator column-HPLC/UV, Wasik et al. 1983)  
 3.28 (HPLC-RV retention volume correlation, Garst & Wilson 1984)  
 3.37 (HPLC- $k'$  correlation, Haky & Young 1984)  
 3.33, 3.45 (RP-HPLC- $k'$  capacity factor correlations, Sherblom & Eganhouse 1988)  
 3.20 (recommended, Sangster 1989, 1993)  
 3.31 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)  
 3.20 (recommended, Hansch et al. 1995)

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

- 3.69\* (30.3°C, from GC-determined  $\gamma^\infty$  in octanol, measured range 30.3–50.28°C, Gruber et al. 1997)  
 3.79 (calculated-measured  $\gamma^\infty$  in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

- 1.37 (eels, Ogata & Miyake 1978)  
 0.78 (clams, Nunes & Benville 1979)  
 1.17 (goldfish, Ogata et al. 1984)  
 2.40 (*S. capricornutum*, Herman et al. 1991)

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

- 2.11, 2.48, 2.20 (forest soil pH 5.6, forest soil pH 4.2, agricultural soil pH 7.4, Seip et al. 1986)  
 2.37, 2.40 (RP-HPLC- $k'$  correlation, Szabo et al. 1990a,b)  
 2.62, 2.63 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)  
 2.06, 2.33 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ , average, Delle Site 2001)

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

Volatilization:  $t_{1/2} \sim 3.1$  h for evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s (Lyman et al. 1982);  
 $t_{1/2} \sim 27$ –135 h for evaporation from a typical river or pond (Howard 1990).

Photolysis:

Oxidation: rate constant  $k$ ; for gas-phase second-order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with  $NO_3$  radical and  $k_{O_3}$  with  $O_3$  or as indicated. Data at other temperatures and/or the Arrhenius expression are designated \*, see reference:

photooxidation  $t_{1/2} = 4.8 \times 10^6 - 2.4 \times 10^8$  h in water, based on estimated rate data for alkoxy radical in aqueous solution (Hendry et al. 1974)

$k_{OH} = (14 \pm 1) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.83$  h;  $k_{O(3P)} = (2.12 \pm 0.21) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$  with O(<sup>3</sup>P) atom at room temp. (relative rate method, Doyle et al. 1975)

$k_{OH} = 1.4 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$  with an initial concn of  $2.0 \times 10^{-10} \text{ mol L}^{-1}$  at 300 K (Doyle et al. 1975)

$k_{OH} = (23.6 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $k_{O(3P)} = (3.52 \pm 0.35) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction of O(<sup>3</sup>P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = (12.9 \pm 2.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  at  $305 \pm 2$  K (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 14.1 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  (Darnall et al. 1976)

$k_{\text{OH}}^* = (24.0 \pm 2.5) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{\text{OH}} = (15.6 - 21.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishanakara et al. 1978)

$k_{\text{OH}} = 23.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and residence time of 0.5 d, loss of 86.5% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} < 0.005 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a calculated lifetime  $\tau > 1150 \text{ d}$  and a lifetime  $\tau = 0.5 \text{ d}$  due to reaction with OH radical at room temp. (Atkinson et al. 1982)

$k_{\text{O}_3} = 780 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  for the reaction with ozone at 300 K (Lyman et al. 1982)

$k_{\text{OH}} = (5.9\text{--}12) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.47\text{--}1.0 \text{ d}$  for xylenes (Mill 1982)

$k = (94 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{NO}_3} = 7.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 23.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 2.6\text{--}26 \text{ h}$  in air (Atkinson 1985; Howard et al. 1991)

$k_{\text{OH}} = 22.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Ohta & Ohyama 1985)

$k_{\text{OH}} = 22.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  23.5°C, with a calculated atmospheric lifetime  $\tau = 0.51 \text{ d}$  (Edney et al. 1986)

$k_{\text{OH}}(\text{calc}) = 14 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 24.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 2.49 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}} = 2.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{OH}}^* = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 1.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 17.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}} = (1.81 \pm 0.40) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $(2.03 \pm 0.10) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $298 \pm 2 \text{ K}$  (relative rate method, Phoussongphouang & Arey 2002)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of  $3.28 \times 10^{-6} \text{ L/L}$  (Jamison et al. 1976)

$t_{1/2}(\text{aq. aerobic}) = 168\text{--}672 \text{ h}$ , based on aqueous screening test data (Bridie et al. 1979; Howard et al. 1991) and soil column study simulating an aerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2} = 0.03 \text{ d}$  (Olsen & Davis 1990)

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.83 \text{ h}$ , based on rate of disappearance for the reaction with OH radical in ambient LA basin air at 300 K (Doyle et al. 1975);

photodecomposition  $t_{1/2} = 2.9 \text{ h}$  under simulated atmospheric conditions, with NO (Dilling et al. 1976); estimated lifetime  $\tau = 1.5 \text{ h}$  under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Perry et al. 1977);

residence time of 0.5 d, loss of 86.5% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

calculated lifetimes  $\tau > 1150 \text{ d}$  and 0.5 d due to reactions with  $\text{O}_3$  and OH radical, respectively, at room temp. (Atkinson et al. 1982);

$t_{1/2} = 2.6\text{--}26 \text{ h}$ , based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);

calculated atmospheric lifetime  $\tau = 0.51 \text{ d}$  due to reaction with OH radical (Edney et al. 1986);

summer daylight lifetime  $\tau = 5.9 \text{ h}$  due to reaction with OH radical (Altshuller 1991);

calculated lifetimes of 5.9 h, 200 d and  $> 4.5 \text{ yr}$  for reactions with OH radical,  $\text{NO}_3$  radical and  $\text{O}_3$ , respectively (Atkinson 2000).

Surface Water:  $t_{1/2} = 168\text{--}672 \text{ h}$ , based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

volatilization appears to be dominant removal process with  $t_{1/2} = 1\text{--}5.5 \text{ d}$  (Howard 1990).

Ground water:  $t_{1/2} = 336\text{--}8640$  h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

$t_{1/2} \sim 0.3$  yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981);

abiotic hydrolysis or dehydro-halogenation  $t_{1/2} = 377$  months (Olsen & Davis 1990).

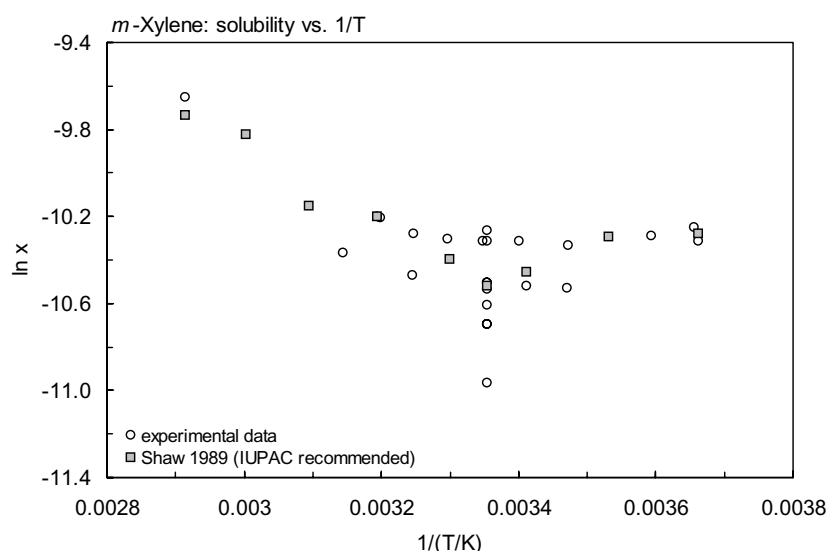
Soil:  $t_{1/2} = 168\text{--}672$  h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).

Biota:  $t_{1/2} = 2$  d, half-life to eliminate from eels in seawater (Ogata & Miyake 1978).

TABLE 3.1.1.5.1

Reported aqueous solubilities of *m*-xylene at various temperatures

Bohon & Claussen 1951		Polak & Lu 1973		Sanemasa et al. 1982		Shaw 1989b (IUPAC)	
shake flask-UV		shake flask-GC		vapor saturation-UV		recommended values	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0.4	209	0	196	15	158	0	203
5.2	201	25	162	25	162	10	200
14.9	192			35	168	20	170
21	196			45	186	25	160
25	196					30	180
25.6	196					40	220
30.3	198					50	230
34.9	203					60	320
39.6	218					70	350
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$		<b>Chernoglazova &amp; Simulin</b>		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.60$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.9$	
		<b>1976</b>		at $25^{\circ}\text{C}$			
		<b>synthetic method-GC</b>				(calc from Van't Hoff eq.)	
		$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$				
25 $^{\circ}\text{C}$	2.8						
2 $^{\circ}\text{C}$	-5.506						
7 $^{\circ}\text{C}$	-3.828						
12 $^{\circ}\text{C}$	-1.59	20	160				
17 $^{\circ}\text{C}$	0	40	220				
22 $^{\circ}\text{C}$	1.22	70	380				
27 $^{\circ}\text{C}$	1.99						
32 $^{\circ}\text{C}$	3.92						
37 $^{\circ}\text{C}$	8.87						
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 11.9$					
		between 127–239 $^{\circ}\text{C}$					

FIGURE 3.1.1.5.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *m*-xylene.

**Reported vapor pressures of *m*-xylene at various temperatures and the coefficients for the vapor pressure equations**

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

[illegible]

Stull 1947		Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−6.9	133.3	59.335	6400	146.85	124200	28.24	1333
16.8	266.6	63.518	7692	166.85	202100	41.07	2666
28.3	1333	67.157	8991	186.85	313700	49.23	4000
41.1	2666	70.506	10330	206.85	467000	56.33	5333

TABLE 3.1.1.5.2 (Continued)

Stull 1947		Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
55.3	5333	73.601	11720	226.85	671500	60.269	6666
64.4	7999	77.778	13842	246.85	937400	64.437	7999
76.8	13332	81.527	16633	266.85	1276300	71.277	10666
95.5	26664	87.387	19945	268.86	1700900	76.818	13332
116.7	53329	91.874	23474	306.85	2226600	87.454	19998
139.1	101325	97.887	28979	316.85	2872100	95.483	26664
		103.412	34925			102.01	33331
mp/°C	-47.9	110.067	43360	eq. 5	P/bar	107.55	39997
		116.923	53700	A	21.9924	116.69	53329
		124.226	66796	B	2957.79	124.15	66661
		132.144	83749	C	5.66789	130.58	79993
		137.731	97647	D	1776	136.06	93326
		138.329	99235			137.1	95991
		138.887	100726			138.112	98659
		129.52	102464			138.1	101325
		140.078	104000			25	1106.6
		eq. 2	P/mmHg			eq. 2	p/mmHg
		A	7.00849			A	7.00908
		B	1461.925			B	1462.266
		C	215.073			C	215.105
		bp/°C	139.104			bp/°C	139.103
						$\Delta H_v/(kJ\ mol^{-1}) =$	
						at 25°C	42.66
						at bp	36.36

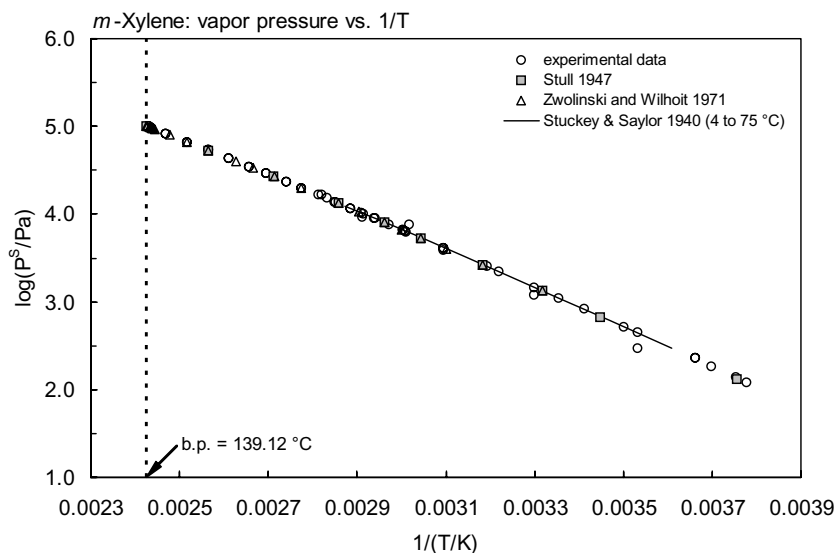
FIGURE 3.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for *m*-xylene.

TABLE 3.1.1.5.3

Reported Henry's law constants of *m*-xylene at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$

$$\ln (1/K_{AW}) = A - B/(T/K)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$

$$\log (1/K_{AW}) = A - B/(T/K)$$

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

(1)
(2)
(3)
(4)
(5)
(1a)
(2a)
(4a)

Sanemasa et al. 1982		Ashworth et al. 1988		Robbins et al. 1993		Dewulf et al. 1995	
vapor-liquid equilibrium		EPICS-GC		static headspace-GC		EPICS-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)
15	405	10	416	25	739	2	209
25	731	15	503	30	900	6	204
35	1329	20	606	40	1489	10	264
45	1872	25	754	45	1591	18.2	472
		30	899	50	1652	25	615
		eq. 4a	H/(atm m <sup>3</sup> /mol)	eq. 4	H/(Pa m <sup>3</sup> /mol)	eq 1	K <sub>AW</sub>
		A	6.28	A	17.83472	A	12.13
		B	3337	B	3337.45	B	4026

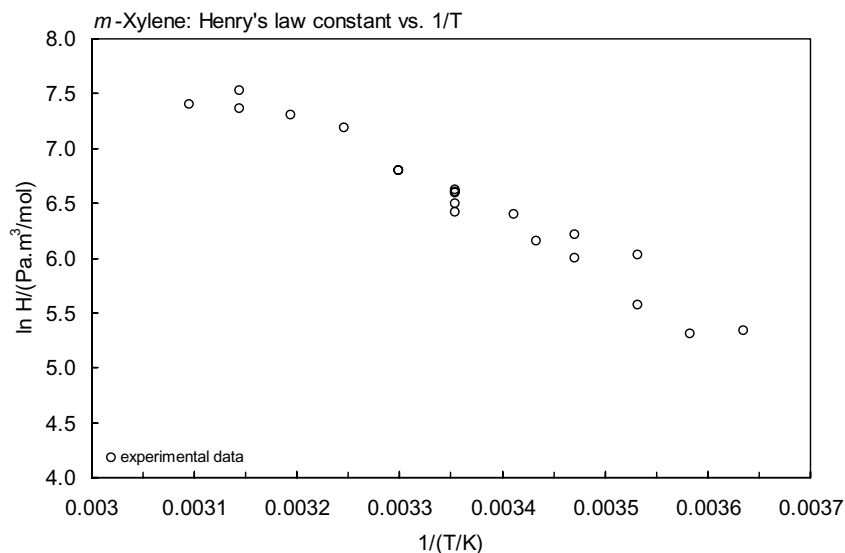


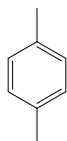
FIGURE 3.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for *m*-xylene.

TABLE 3.1.1.5.4

Reported octanol-air partition coefficients of *m*-xylene at various temperatures

Gruber et al. 1997

GC det'd activity coefficient	
t/°C	log K <sub>OA</sub>
20.29	-
30.3	3.69
40.4	3.51
50.28	3.30

3.1.1.6 *p*-XyleneCommon Name: *p*-XyleneSynonym: 1,4-dimethylbenzene, *p*-xylol, 4-methyltolueneChemical Name: *p*-xylene

CAS Registry No: 106-42-3

Molecular Formula:  $C_8H_{10}$ ,  $C_6H_4(CH_3)_2$ 

Molecular Weight: 106.165

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

13.25 (Lide 2003)

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

138.37 (Lide 2003)

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

0.8611 (Weast 1982–83)

Molar Volume ( $cm^3/mol$ ):123.3 ( $20^{\circ}C$ , calculated-density)

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

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):42.376, 35.98 ( $25^{\circ}C$ , bp, Riddick et al. 1986)Enthalpy of Fusion  $\Delta H_{fus}$  ( $kJ/mol$ ):

17.113 (Tsonopoulos &amp; Prausnitz 1971; Riddick et al. 1986)

17.11 (Chickos et al. 1999)

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

59.413 (Tsonopoulos &amp; Prausnitz 1971; Yalkowsky &amp; Valvani 1980)

59.77, 45.6 (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  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

200 (shake flask-UV, Andrews &amp; Keefer 1949)

198\* (shake flask-UV, measured range  $0.4$ – $85^{\circ}C$ , Bohon & Claussen 1951)

185\* (shake flask-GC, Polak &amp; Lu 1973)

156 (shake flask-GC, Sutton &amp; Calder 1975)

163 (shake flask-GC, Hermann 1972)

157 (shake flask-GC, Price 1976)

157 (shake flask-GC, Krzyzanowska &amp; Szeliga 1978)

191\* ( $20^{\circ}C$ , shake flask-UV, Ben-Naim & Wiff 1979)163\* (vapor saturation-UV spec., measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)

214.5 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)

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

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

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

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

180\* (IUPAC recommended value, temp range  $0$ – $90^{\circ}C$ , Shaw 1989b)169\* ( $30^{\circ}C$ , equilibrium flow cell-GC, measured range  $30$ – $100^{\circ}C$ , Chen & Wagner 1994c)

$\ln x = 11.79 - 20.89 \cdot (T/K)^{-1} + 4.892 \cdot (T/K)^{-2}$ ;  $T_r = T/T_c$ , the reduced temp, system temp  $T$  divided by critical temp  $T_c$ , temp range  $303.15$ – $373.15\ K$  (equilibrium flow cell-GC, Chen & Wagner 1994c)

$\ln x = -27.937 + 3230.3/(T/K) + 7.595 \times 10^{-5} \cdot (T/K)^2$ ; 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):

154.7\* (0.2°C, mercury manometer, Linder 1931)

787\* (20°C, Hg manometer, Kassel 1936)

$\log (P/\text{mmHg}) = -2930.0/(T/K) - 5 \cdot \log (T/K) + 23.1000$ ; temp range 0–80°C (vapor pressure eq. from Hg manometer measurements, Kassel 1936)

1437\* (30°C, Hg manometer, measured range 10–50°C, Rintelen et al. 1937)

$\log (P/\text{mmHg}) = -2851.90/(T/K) - 5 \cdot \log (T/K) + 22.88436$ ; temp range 4–75°C (vapor pressure eq. from manometer measurement, Stuckey & Saylor 1940)

1187\* (Hg manometer, Pitzer & Scott 1943)

$\log (P_s/\text{mmHg}) = -3141.33/(T/K) + 11.6092$ ; temp range 0–13.23°C (manometer, solid, two-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)

$\log (P_L/\text{mmHg}) = -3080.31/(T/K) - 6.7 \log (T/K) + 27.8581$ ; temp range 13.23–60°C (manometer, liquid, three-constant eq. from exptl. data, Pitzer & Scott 1943)

6354\* (58.288°C, ebulliometry, measured range 58.288–139.289°C, Willingham et al. 1945)

$\log (P/\text{mmHg}) = 6.98648 - 1491.548/(207.171 + t/^\circ\text{C})$ ; temp range 58.3–139.8°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

1333\* (27.3°C, summary of literature data, Stull 1947)

6398\* (58.419°C, ebulliometry, measured range 58.419–139.329°C, Forziati et al. 1949)

$\log (P/\text{mmHg}) = 6.99184 - 1454.328/(215.411 + t/^\circ\text{C})$ ; temp range 58.4–139.3°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

1175 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/\text{mmHg}) = 6.99052 - 1453.430/(215.307 + t/^\circ\text{C})$ ; temp range 45–190°C (Antoine eq. for liquid state, Dreisbach 1955)

126500\* (146.85°C, ebulliometry, measured range 146.85–316.85°C, Ambrose et al. 1967)

1170\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 6.9052 - 1453.430/(215.307 + t/^\circ\text{C})$ ; temp range 27.32–165.73°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 9809.9/(T/K)] + 8.124805$ ; temp range –8.1 to 138.3°C (Antoine eq., Weast 1972–73)

880.3\* (20.015 °C, inclined-piston gauge, measured range –26.043 to 20.015, Osborn & Douslin 1974)

$\log (P/\text{atm}) = (1 - 411.503/T) \times 10^4(0.847730 - 6.39489 \times 10^4 \cdot T + 5.59094 \times 10^7 \cdot T^2)$ ; T in K, temp range 290.0–618.2 K (Cox vapor pressure eq., Chao et al. 1983)

1170 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.11376 - 1452.215/(215.518 + t/^\circ\text{C})$ , temp range 58.3–139.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.11513 - 1453.812/(215.242 + t/^\circ\text{C})$ ; temp range 99.17–179.23°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1974, Boublik et al. 1984)

1167 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.90052 - 1453.430/(215.31 + t/^\circ\text{C})$ ; temp range 27–166°C (Antoine eq., Dean 1985, 1992)

1200; 1160 (quoted lit.; calculated-Antoine eq., Riddick et al. 1986; quoted, Howard 1990)

$\log (P/\text{kPa}) = 6.11140 - 1451.39/(215.148 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)

1180 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 15.50091 - 6327.014/(115.724 + T/K)$ ; temp range 247–286 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14779 - 1475.767/(-55.241 + T/K)$ ; temp range 286–453 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14049 - 1472.773/(-55.342 + T/K)$ ; temp range 411–463 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.44333 - 1735.196/(-19.846 + T/K)$ ; temp range 460–553 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.84182 - 3543.356/(208.522 + T/K)$ ; temp range 551–616 K (liquid, Antoine eq.-V, Stephenson & Malanowski 1987)

1165\* (McLeod gauge, measured range 20.0–50.07, Smith 1990)

$\log (P/\text{mmHg}) = 60.0531 - 4.1059 \times 10^3/(T/K) - 19.441 \cdot \log (T/K) + 8.2881 \times 10^{-3} \cdot (T/K) - 2.3647 \times 10^{-12} \cdot (T/K)^2$ , temp range 286–616 K (vapor pressure eq., Yaws 1994)



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

- 762\* (vapor-liquid equilibrium, measured range  $15\text{--}45^\circ\text{C}$ , Sanemasa et al. 1982)  
 754\*; 752 (EPICS-GC/FID; batch air stripping-GC, Ashworth et al. 1988)  
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 6.931 - 3520/(T/K)$ ; temp range  $10\text{--}30^\circ\text{C}$  (EPICS measurements, Ashworth et al. 1988)  
 614 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 856, 1189, 1576 ( $27, 35.8, 46^\circ\text{C}$ , EPICS-GC, Hansen et al. 1993)  
 $\ln [H/(\text{kPa}\cdot\text{m}^3/\text{mol})] = -3072/(T/K) + 10.0$ ; temp range  $27\text{--}46^\circ\text{C}$  (EPICS measurements, Hansen et al. 1993)  
 696 (infinite activity coeff.  $\gamma^\infty$  in water determined by inert gas stripping-GC, Li et al. 1993)  
 739\* (static headspace-GC, same as *m*-xylene, Robbins et al. 1993)  
 595 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)  
 575\* (EPICS-GC/FID, measured range  $2\text{--}25^\circ\text{C}$ , Dewulf et al. 1995)  
 318, 763 ( $6.0, 25^\circ\text{C}$ , EPICS-GC/FID, natural seawater with salinity of  $35\text{‰}$ , Dewulf et al. 1995)  
 $\ln K_{\text{AW}} = -4479/(T/K) + 0.01196\cdot Z + 13.597$ ; with *Z* salinity  $0\text{--}35.5\text{‰}$ , temp range  $2\text{--}25^\circ\text{C}$  (EPICS-GC/FID, Dewulf et al. 1995)  
 641 ( $20^\circ\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 1996)  
 678.6 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 669.1 (modified EPICS method-GC, Ryu & Park 1999)  
 604 ( $20^\circ\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 2001)  
 $\log K_{\text{AW}} = 4.900 - 1615/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient,  $\log K_{\text{OW}}$  at  $25^\circ\text{C}$ :

- 3.15 (Leo et al. 1971; Hansch & Leo 1985)  
 3.20 (Hansch & Leo 1979)  
 3.10 (HPLC- $k'$  correlation, Hanai et al. 1981)  
 3.28 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 3.18 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982b,c)  
 3.29 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983b)  
 3.18 (generator column-HPLC/UV, Wasik et al. 1983)  
 3.29 (HPLC-RV correlation, Garst 1984)  
 3.36, 3.48 (RP-HPLC- $k'$  capacity factor correlations; Sherblom & Eganhouse 1988)  
 3.15 (recommended, Sangster 1989, 1993)  
 3.35 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)  
 3.15 (recommended, Hansch et al. 1995)

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

- 3.68\* ( $30.3^\circ\text{C}$ , from GC-determined  $\gamma^\infty$  in octanol, measured range  $30.3\text{--}50.28^\circ\text{C}$ , Gruber et al. 1997)  
 3.79 (calculated-measured  $\gamma^\infty$  in pure octanol of Gruber et al. 1997, Abraham et al. 2001)

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

- 1.37 (eels, Ogata & Miyake 1978)  
 1.17 (goldfish, Ogata et al. 1984)  
 2.41 (*S. capricornutum*, Herman et al. 1991)

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

- 2.52 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)  
 2.42 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)  
 2.24 (aquifer material with  $f_{\text{OC}}$  of 0.006 and measured partition coeff.  $K_p = 1.04 \text{ mL/g.}$ , Abdul et al. 1990)  
 1.87, 2.22 (Webster soil, Webster soil HP, batch equilibrium, Pennell et al. 1992)  
 3.53, 2.63 (sorbent: Silica gel, kaolinite, batch equilibrium, Pennell et al. 1992)  
 2.72, 2.17 (Captina silt loam pH 4.97, McLaurin sandy loam pH 4.43, Walton et al. 1992)  
 2.43, 2.44 (RP-HPLC- $k'$  correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

- 2.37 (HPLC-screening method, Müller & Kördel 1996)  
 2.49, 2.75, 2.65, 2.76, 2.79, 2.76, 2.78 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon  $f_{OC} = 4.12\%$ , EPICS-GC/FID, Dewulf et al. 1999)  
 2.27, 2.31, 2.21 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)

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

Volatilization:  $t_{1/2} \sim 3.1$  h for evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s h (Lyman et al. 1982);  
 $t_{1/2} \sim 27\text{--}135$  h for evaporation from a typical river or pond (Howard 1990).

#### Photolysis:

Oxidation: rate constant  $k$  for gas-phase second order rate constants,  $k_{OH}$  for reaction with OH radical,  $k_{NO_3}$  with  $NO_3$  radical and  $k_{O_3}$  with  $O_3$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section:

photooxidation  $t_{1/2} = 2.8 \times 10^6\text{--}1.4 \times 10^8$  h, based on estimated rate data for alkoxy radical in aqueous solution (Hendry 1974)

$k_{OH} = (7.4 \pm 1.5) \times 10^9$  L mol<sup>-1</sup> s<sup>-1</sup>;  $k_{O(3P)} = (1.09 \pm 0.11) \times 10^8$  L mol<sup>-1</sup> s<sup>-1</sup> with O(<sup>3</sup>P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (12.2 \pm 1.2) \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>;  $k_{O(3P)} = (1.81 \pm 0.18) \times 10^{-13}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for the reaction of O(<sup>3</sup>P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 7.45 \times 10^9$  L mol<sup>-1</sup> s<sup>-1</sup> with  $t_{1/2} = 0.24\text{--}2.4$  h (Darnall et al. 1976)

$k_{OH}^* = (15.3 \pm 1.7) \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH} = (8.8\text{--}10.5) \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{OH} = 12.3 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> and residence time of 0.9 d, loss of 67% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH} = 950$  cm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup> at 300 K (Lyman et al. 1982)

$k_{OH} = (5.9\text{--}12) \times 10^9$  M<sup>-1</sup> s<sup>-1</sup> with  $t_{1/2} = 0.47\text{--}1.0$  d for xylenes (Mill 1982)

$k = (140 \pm 30)$  M<sup>-1</sup> s<sup>-1</sup> for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{NO_3} = 1.4 \times 10^{-16}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296 K (Atkinson et al. 1984)

$k_{OH} = 14.1 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with half-life of 4.2–42 h (Atkinson 1985; Howard et al. 1991)

$k_{OH} = 12.9 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 25°C (Ohta & Ohya 1985)

$k_{OH} = 13.6 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 22.8°C, with a calculated atmospheric lifetime  $\tau = 0.84$  d (Edney et al. 1986)

$k_{OH}(\text{calc}) = 6.9 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}(\text{obs.}) = 15.2 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{NO_3} = 4.50 \times 10^{-16}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH} = 1.52 \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{OH}^* = 1.43 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> over temp range at 296–335 K (recommended, Atkinson 1989)

$k_{OH} = 14.3 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K (Atkinson 1990)

$k_{OH}(\text{calc}) = 6.92 \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{OH}(\text{calc}) = 17.40 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> (molecular orbital calculations, Klamt 1993)

$k_{OH}(\text{calc}) = 6.51 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,  $k_{OH}(\text{exptl}) = 14.3 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982)

$t_{1/2} = 1150$  months, abiotic hydrolysis or dehydro-halogenation half-life (Olsen & Davis 1990).

#### Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of  $1.03 \times 10^{-6}$  L/L (Jamison et al. 1976)

$t_{1/2}(\text{aq. aqueous}) = 168\text{--}672$  h, based on aqueous screening test data (Bridie et al. 1979) and soil column study simulating an aerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688$  h, based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2} = 0.03$  d (Olsen & Davis 1990).

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

## Half-Lives in the Environment:

Air:  $t_{1/2}$  = 0.24–2.4 h, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976)  
residence time of 0.9 d, loss of 67% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photodecomposition  $t_{1/2}$  = 3.1 h under simulated atmospheric conditions, with NO (Dilling et al. 1976)

$t_{1/2}$  = 4.2–42 h, based on photooxidation half-life (Howard et al. 1991);

calculated atmospheric lifetime  $\tau$  = 0.84 d due to reaction with OH radical (Edney et al. 1986);

summer daylight lifetime  $\tau$  = 10 h due to reaction with OH radical (Altshuller 1991).

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

Ground water:  $t_{1/2}$  = 336–8640 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991);

$t_{1/2}$  ~ 0.3 yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981);

abiotic hydrolysis or dehydro-halogenation  $t_{1/2}$  = 1150 months (Olsen & Davis 1990).

Soil:  $t_{1/2}$  = 168–672 h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

disappearance  $t_{1/2}$  = 2.2 d from test soils (Anderson et al. 1991).

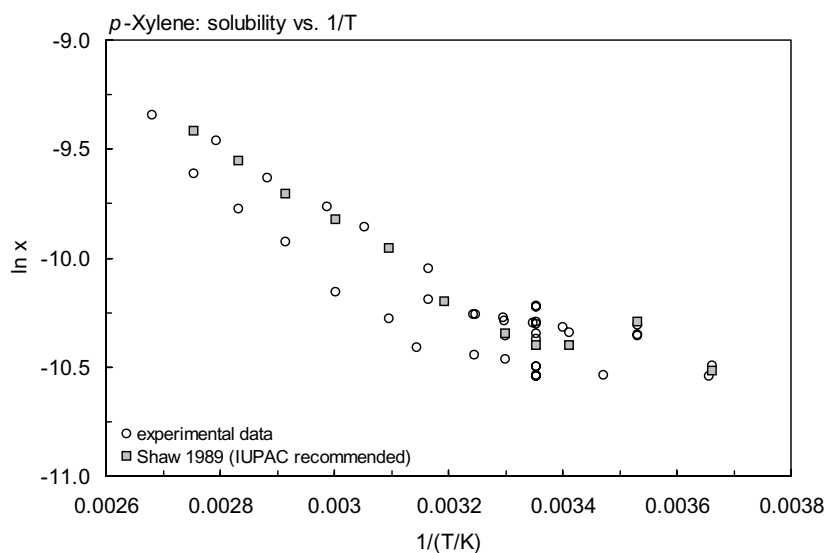
Biota:  $t_{1/2}$  = 2.6 d, half-life to eliminate from eels in seawater (Ogata & Miyake 1978).

TABLE 3.1.1.6.1

Reported aqueous solubilities of *p*-xylene at various temperatures

1.

Bohon & Claussen 1951		Polak & Lu 1973		Shaw 1989b (IUPAC)		Chen & Wagner 1994c	
shake flask-UV		shake flask-GC		recommended values		equilibrium flow cell-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0.4	156	0	164	0	160	30	169
10	188	25	185	10	200	30	188
10	197			20	180	50	102
21	195			25	180	60	230
25	198			30	190	70	289
25.6	199	<b>Ben-Naim &amp; Wiff 1979</b>		40	220	80	337
30.2	201	shake flask-UV		50	280	90	395
30.3	204	t/°C S/g·m <sup>-3</sup>		60	320	100	516
34.9	207	10	189	70	360		
35.2	207	20	191	80	420	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.48$	
42.8	222			90	480	at 25°C	
42.8	256						
54.4	310			$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.90$			
61.7	340	<b>Sanemasa et al. 1982</b>		at 25°C			
73.9	387	vapor saturation-UV					
85	459	t/°C S/g·m <sup>-3</sup>					
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$		15	157				
25°C	3.9	25	163				
7°C	-0.422	35	176				
12°C	-1.34	45	178				
17°C	0.515						
22°C	1.36						
27°C	2.29	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.20$					
32°C	4.23	at 25°C					
37°C	7.36						



**FIGURE 3.1.1.6.1** Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *p*-xylene.

**TABLE 3.1.1.6.2**

Reported vapor pressures of *p*-xylene at various temperatures and the coefficients for the vapor pressure equations

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

1.

Kassel 1936		Rintelen et al. 1937		Pitzer & Scott 1943		Willingham et al. 1945		
mercury manometer		mercury manometer		mercury manometer		ebulliometry		
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	
0	208	10	307	0	178	58.288	6354	
10	415	30	1427	12.5	540	62.523	7657	
20	787	50	4306	25	1187	66.216	8966	
30	1427	bp 138.27–138.37°C		37.7	2333	69.549	10306	
40	2453			50	4346	72.657	11696	
50	4093			60	6846	76.832	13822	
60	6573					81.636	16623	
70	10226					86.488	18725	
80	15452							
					0–13.23°C solid		90.990	23454
					eq. 1	P/mmHg	97.013	28956
eq. 4	P/mmHg				A	11.6092	102.546	34901
A	23.100				B	3141.33	109.211	43326
B	2930.0						116.083	53656
C	5.0				13.23–60°C liquid		123.049	66756
					eq. 4	P/mmHg	131.355	83717
					A	27.8581	136.956	97605
				B	3080.31	137.558	99201	

TABLE 3.1.1.6.2 (Continued)

Kassel 1936		Rintelen et al. 1937		Pitzer & Scott 1943		Willingham et al. 1945	
mercury manometer		mercury manometer		mercury manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
Linder 1931		Stuckey & Saylor 1940		C	6.7	138.114	100694
mercury manometer		mercury manometer		$\Delta H_v/(\text{kJ mol}^{-1}) = 42.30$ at 298 K		138.742	102392
t/°C	P/Pa	t/°C	P/Pa			139.289	103906
–9.5	44.0	measured 4–75°C				eq. 2	P/mmHg
–2.5	116	eq. 4	P/mmHg			A	6.98648
0	126.7	A	22.88436			B	1450.688
0.2	154.7	B	2851.90			C	214.990
		C	5.0				
		bp/°C 138.33–138.38				bp/°C	138.348
		mp/°C 13.20–12.95					

2.

Stull 1947		Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–8.10	133.3	58.419	6398	146.85	126500	27.32	1333
15.5	266.6	62.419	7690	166.85	205200	40.15	2666
27.3	1333	66.280	8990	186.85	317100	48.31	4000
40.1	2666	69.605	10330	206.85	470900	54.42	5333
54.4	5333	72.684	11720	226.85	675800	59.363	6666
63.5	7999	76.885	13842	246.85	941900	63.535	7999
75.9	13332	81.658	16633	266.85	1280800	70.383	10666
94.6	26664	86.506	19944	286.85	1705700	75.931	13332
115.9	53323	91.017	23474	306.85	2232400	86.583	19998
138.3	101325	97.032	28978	316.85	2880400	94.626	26664
		102.573	34925			101.167	33331
mp/°C	13.3	109.240	43360	eq. 5	P/bar	106.719	39997
		123.431	66796	A	21.14250	115.887	53329
		131.371	83749	B	2892.27	123.366	66661
		137.574	99235	C	5.40051	129.372	79993
		138.132	100726	D	1759	135.304	93326
		138.768	102462			136.341	95991
		139.329	104000			137.347	98659
						138.351	101325
		eq. 2	P/mmHg			25.0	1173.2
		A	6.99184				
		B	1454.328			eq. 2	P/mmHg
		C	215.411			A	6.99052
						B	1453.430
						C	215.307
		bp/°C	138.351			bp/°C	138.351
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	42.38
						at bp	35.98

(Continued)

TABLE 3.1.1.6.2 (Continued)

3.

Osborn & Douslin 1974				Smith 1990	
inclined-piston gauge		ebulliometry		McLeod gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−26.043	11.60	67.795	9590	20.0	865.3
−21.164	19.60	70.881	10892	25.0	1165
−16.277	33.20	73.978	12344	30.0	1541
−10.403	60.79	77.086	13960	35.24	2075
−4.995	103.86	80.206	15752	40.0	2645
−0.006	170.5	83.339	17737	44.27	3306
4.912	272.4	86.483	19933	50.07	4374
9.838	429.2	92.804	25023		
12.483	544.4				
13.285	581.7			eq. 2a	P/mmHg
15.004	648.9			A	16.19136
17.474	755.4			B	3371.18
20.015	880.3			C	215.367
				$\Delta H_v/(kJ\ mol^{-1}) = 42.98$	
				at 25°C	
				$\Delta S_v/(J\ mol^{-1}\ K^{-1}) = 107.0$	
				at 25°C	

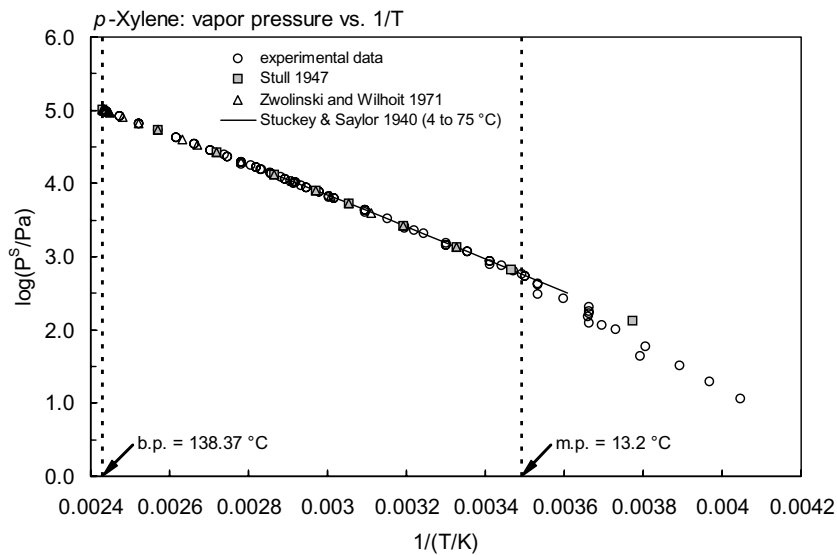


FIGURE 3.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for *p*-xylene.

TABLE 3.1.1.6.3

Reported Henry's law constants of *p*-xylene 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)							
Sanemasa et al. 1982		Ashworth et al. 1988		Robbins et al. 1993		Hansen et al. 1993		Dewulf et al. 1995	
vapor-liquid equil		EPICS-GC		static headspace-GC		EPICS-GC		EPICS-GC	
t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol
15	430	10	426	25	739	27	856	2	176
25	762	15	489	30	900	35.8	1189	6	158
35	1265	20	654	40	1489	46	1576	10	252
45	2052	25	754	45	1591			18.2	468
		30	958	50	1652			25	575
		eq. 4a		eq. 4		eq. 4		eq 1	
		H/(atm m³/mol)		H/(Pa m³/mol)		H/(kPa m³/mol)		A	
		A	6.931	A	17.83472	A	10.1	B	13.597
		B	3520	B	3337.45	B	3072		4479

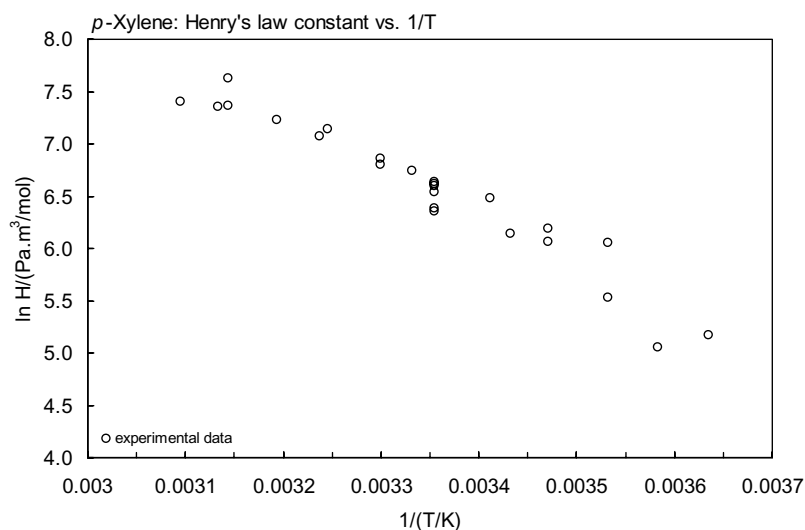
FIGURE 3.1.1.6.3 Logarithm of Henry's law constant versus reciprocal temperature for *p*-xylene.

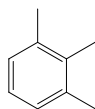
TABLE 3.1.1.6.4

Reported octanol-air partition coefficients of *p*-xylene at various temperatures

Gruber et al. 1997

GC det'd activity coefficient	
t/°C	log $K_{OA}$
20.29	-
30.3	3.68
40.4	3.48
50.28	3.29

## 3.1.1.7 1,2,3-Trimethylbenzene



Common Name: 1,2,3-Trimethylbenzene

Synonym: hemimellitene

Chemical Name: 1,2,3-trimethylbenzene

CAS Registry No: 526-73-8

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_3(CH_3)_3$

Molecular Weight: 120.191

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

−25.4 (Weast 1982–83; Lide 2003)

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

176.1 (Weast 1982–83; Lide 2003)

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

0.8944 (Weast 1982–83)

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

134.4 ( $20^{\circ}C$ , calculated-density)

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

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

0.66, 1.33, 8.18; 10.17 (−54.45, −42.85, −25.35 $^{\circ}C$ ; total phase change enthalpy, Chickos et al. 1999)

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

41.81, 46.2 (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):

75.2 (shake flask-GC, Sutton & Calder 1975)

62.7\* (vapor saturation-UV spec., measured range 15–45 $^{\circ}C$ , Sanemasa et al. 1982)

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

69\* (IUPAC recommended value, temp range 15–45 $^{\circ}C$ , Shaw 1989b)

$\ln x = -39.5173 + 5289.13/(T/K) + 1.149 \times 10^{-4} \cdot (T/K)^2$ ; temp range 5–50 $^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

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

133.3\* (16.8 $^{\circ}C$ , summary of literature data, Stull 1947)

6417\* (90.332 $^{\circ}C$ , ebulliometry, measured range 90.332–177.126 $^{\circ}C$ , Forziati et al. 1949)

$\log (P/mmHg) = 7.04082 - 1593.958/(207.078 + t/^{\circ}C)$ ; temp range 90.3–177.1 $^{\circ}C$  (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

206 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.04082 - 1593.958/(207.078 + t/^{\circ}C)$ ; temp range 75–230 $^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log (P/mmHg) = 7.04082 - 1593.958/(207.078 + t/^{\circ}C)$ ; temp range 56.79–205.36 $^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = [-0.2185 \times 10781.9/(T/K)] + 8.154069$ ; temp range 16.8–176 $^{\circ}C$  (Antoine eq., Weast 1972–73)

217 (calculated-bp, Mackay et al. 1982; Eastcott et al. 1988)

$\log (P/atm) = (1 - 449.175/T) \times 10^{(0.869047 - 6.33423 \times 10^4 \cdot T + 5.14963 \times 10^7 \cdot T^2)}$ ; T in K, temp range 290.0–660.0 K (Cox vapor pressure eq., Chao et al. 1983)

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



$\log (P/\text{kPa}) = 6.16365 - 1592.422/(206.905 + t/^{\circ}\text{C})$ ; temp range 90.33–177.1 $^{\circ}\text{C}$  (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

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

$\log (P/\text{mmHg}) = 7.04082 - 1593.958/(207.08 + t/^{\circ}\text{C})$ ; temp range 57–205 $^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)

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

$\log (P_L/\text{kPa}) = 6.16477 - 1593.776/(-66.032 + T/\text{K})$ ; temp range 363–456 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 2.7492 - 2.6428 \times 10^3/(T/\text{K}) + 3.6120 \cdot \log (T/\text{K}) - 1.0213 \times 10^{-2} \cdot (T/\text{K}) + 5.0553 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 248–665 K (vapor pressure eq., Yaws 1994)

$\log (P/\text{kPa}) = 6.17303 - 1593.958/[(T/\text{K}) - 66.072]$ ; temp range 5–50 $^{\circ}\text{C}$  (regression eq. from literature data, Shiu & Ma 2000)

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):

441\* (vapor-liquid equilibrium-GC, measured range 15–45 $^{\circ}\text{C}$ , Sanemasa et al. 1982)

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

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

3.66 (Hansch & Leo 1979)

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

3.55 (generator column-HPLC/UV, Tewari et al. 1982b, 1982c)

3.70, 3.86 (RP-HPLC- $k'$  correlation, Sherblom & Eganhouse 1988)

3.63 (recommended, Sangster 1989, 1993)

3.55, 3.59, 3.66 (quoted lit. values, Hansch et al. 1995)

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

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

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

2.80 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)

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 and/or the Arrhenius expression see reference:

$k_{\text{OH}} = (14 \pm 3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ ;  $k_{\text{O}(^3\text{P})} = (6.9 \pm 0.7) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$  with O( $^3\text{P}$ ) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{\text{OH}} = (26.4 \pm 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{O}(^3\text{P})} = 11.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction of O( $^3\text{P}$ ) atom at room temp (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{\text{OH}} = 14.9 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  (Darnall et al. 1976)

$k_{\text{OH}}^* = (33.3 \pm 4.5) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence Perry et al. 1977)

$k_{\text{OH}} = (15\text{--}30) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.2\text{--}0.4 \text{ d}$  for trimethylbenzenes (Mill 1982)

$k = (400 \pm 100) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water at pH 1.7 and 20–23 $^{\circ}\text{C}$  (Hoigné & Bader 1983)

$k_{\text{NO}_3} = 5.6 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 3.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{\text{OH}} = 2.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Ohta & Ohyama 1985)

$k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 3.33 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 1.85 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}} = 3.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{OH}} = 3.27 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 1.78 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 3.99 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biotransformation:

Biodegradation:

Bioconcentration:

#### Half-Lives in the Environment:

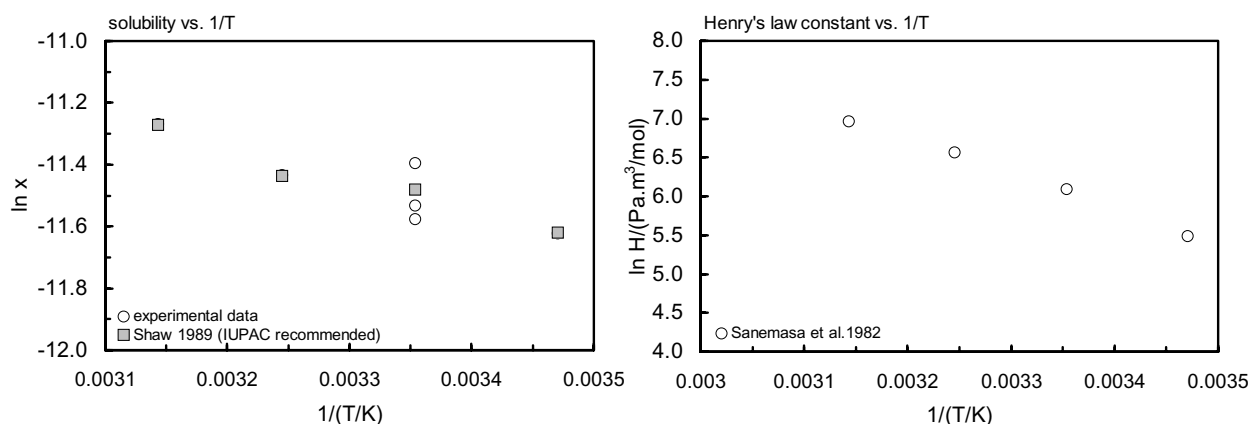
Air:  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

estimated lifetime  $\tau = 1.5 \text{ h}$  under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Perry et al. 1977);

summer daylight lifetime  $\tau = 4.2 \text{ h}$  due to reaction with OH radical (Altshuller 1991)

**TABLE 3.1.1.7.1**  
**Reported aqueous solubilities and Henry's law constants of 1,2,3-trimethylbenzene at various temperatures**

Aqueous solubility				Henry's law constant	
Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Sanemasa et al. 1982	
vapor saturation-UV		recommended values		vapor-liquid equilibrium	
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)
15	75.2	15	60	15	241.2
25	65.5	25	69	25	441
35	72.2	35	72	35	706
45	85.2	45	85	45	1058

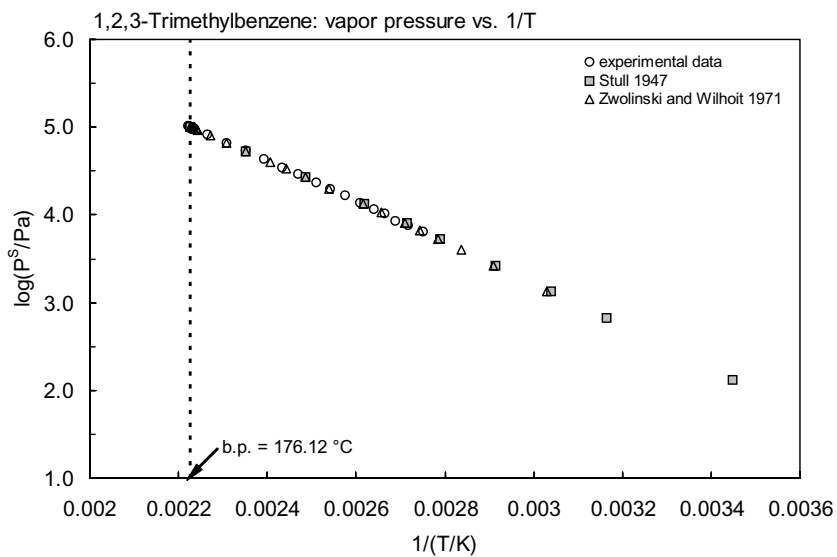


**FIGURE 3.1.1.7.1** Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1,2,3-trimethylbenzene.

TABLE 3.1.1.7.2

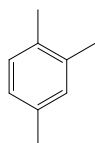
Reported vapor pressures of 1,2,3-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
16.8	133.3	90.332	6417	56.79	1333
42.9	666.6	94.826	7697	70.62	2666
55.9	1333	98.77	8993	79.41	4000
69.9	2666	102.336	10328	86	5333
85.4	5333	105.663	11720	91.313	6666
95.3	7999	110.157	13840	95.802	7999
1088	13332	115.287	16640	103.168	10666
129	26664	120.504	19944	109.132	13332
152	53329	125.333	23474	120.578	19998
176.1	101325	131.8	28978	129.215	26664
		137.737	34918	136.214	33331
mp/ $^{\circ}\text{C}$	-25.5	144.882	43351	142.191	39997
		152.26	53692	152.022	53329
		160.106	66792	160.037	66661
		168.614	83750	166.856	79993
		174.606	97644	172.823	93326
		175.252	99237	173.934	95992
		175.852	100732	175.02	98659
		176.527	102453	176.084	101325
		177.126	103985		
				eq. 2	P/mmHg
				A	7.04082
		eq. 2	P/mmHg	B	1593.958
		A	7.04082	C	207.078
		B	1593.958	bp/ $^{\circ}\text{C}$	176.084
		C	207.078	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				at 25 $^{\circ}\text{C}$	49.06
		bp/ $^{\circ}\text{C}$	176.084	at bp	40.04



**FIGURE 3.1.1.7.2** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3-trimethylbenzene.

## 3.1.1.8 1,2,4-Trimethylbenzene



Common Name: 1,2,4-Trimethylbenzene

Synonym: pseudocumene

Chemical Name: 1,2,4-trimethylbenzene

CAS Registry No: 95-63-6

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_3(CH_3)_3$

Molecular Weight: 120.191

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

−43.77 (Lide 2003)

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

169.38 (Lide 2003)

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

0.8758 (Weast 1982–83)

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

137.2 ( $20^{\circ}C$ , calculated-density)

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

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

13.19 (Chickos et al. 1999)

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

57.53, 46.2 (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  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

57 (shake flask-GC, McAuliffe 1966)

59.0 (shake flask-GC, Sutton & Calder 1975)

51.9 (shake flask-GC, Price 1976)

51.9 (shake flask-GC, Krzyzanowska & Szeliga 1978)

56.5\* (vapor saturation-UV spec., measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)

56\* (IUPAC recommended, temp range  $15$ – $45^{\circ}C$ , Shaw 1989b)

$\ln x = -8.760 - 868.70/(T/K)$ ; temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

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

133.3\* ( $13.6^{\circ}C$ , summary of literature data, Stull 1947)

6417\* ( $84.804^{\circ}C$ , ebulliometry, measured range  $84.804$ – $170.377^{\circ}C$ , Forziati et al. 1949)

$\log (P/mmHg) = 7.04393 - 1573.267/(208.564 + t/^{\circ}C)$ ; temp range  $84.8$ – $170.4^{\circ}C$  (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

280 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.04383 - 1573.267/(208.564 + t/^{\circ}C)$ ; temp range  $70$ – $220^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

2666\* ( $65.405^{\circ}C$ , compiled data, temp range  $65.405$ – $198.215^{\circ}C$ , Bond & Thodos 1960)

$\log (P/mmHg) = 23.2393 - 3301.19/(T/K) - 6.21412 \cdot \log (T/K) + 3.15835[P(mmHg)/(T/K)^2]$ , temp range  $65.4$ – $198^{\circ}C$  (Bond & Thodos 1960)

271\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981; Eastcott et al. 1988)

$\log (P/mmHg) = 7.04383 - 1573.267/(208.564 + t/^{\circ}C)$ ; temp range  $51.75$ – $198.2^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/\text{mmHg}) = [-0.2185 \times 10710.2/(T/K)] + 8.209013$ ; temp range 13.6–169.2°C (Antoine eq., Weast 1972–73)  
 $\log(P/\text{atm}) = (1 - 442.537/T) \times 10^{(0.846724 - 5.41424 \times 10^4/T + 4.22211 \times 10^7/T^2)}$ ; T in K, temp range 253.0–645.0 K (Cox vapor pressure eq., Chao et al. 1983)  
 270 (extrapolated-Antoine eq., Boublik et al. 1984)  
 $\log(P/\text{kPa}) = 6.16282 - 1569.06/(208.089 + t/^\circ\text{C})$ ; temp range 84.8–170.4°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)  
 $\log(P/\text{mmHg}) = 7.04383 - 1573.83/(208.56 + t/^\circ\text{C})$ ; temp range 52–198°C (Antoine eq., Dean 1985, 1992)  
 $\log(P_L/\text{kPa}) = 6.16695 - 1572.687/(-64.593 + T/K)$ ; temp range 357–450 K (liquid, Antoine eq., Stephenson & Malanowski 1987)  
 $\log(P/\text{mmHg}) = 2.1667 - 2.6318 \times 10^3/(T/K) + 4.0350 \cdot \log(T/K) - 1.1776 \times 10^{-2} \cdot (T/K) + 6.0956 \times 10^{-6} \cdot (T/K)^2$ , temp range 229–649 K (vapor pressure eq., Yaws 1994)  
 $\log(P/\text{kPa}) = 6.16866 - 1573.267/[(T/K) - 64.586]$ ; 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):

619\* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)  
 475 (20°C, EPICS-GC, Yurteri et al. 1987)  
 571 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 704, 1135, 1591 (27, 35, 45°C, EPICS-GC, Hansen et al. 1993)  
 $\ln[H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -4298/(T/K) + 14.0$ ; temp range 27–45°C (EPICS-GC, Hansen et al. 1993)  
 529 (20°C, selected from literature experimentally measured data, Staudinger & Roberts, 1996, 2001)  
 $\log K_{AW} = 5.125 - 1697/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

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

3.65 (calculated- $\pi$  substituent constant, Hansch et al. 1968)  
 3.63 (shake flask-HPLC/UV both phases, Wasik et al. 1981)  
 3.78 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 3.82, 4.00 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 3.63 (recommended value, Sangster 1989)  
 3.78 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)  
 3.70 (recommended, Sangster 1993)  
 3.83, 3.78 (quoted lit., Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

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

3.28 (computed- $K_{OW}$ , Kollig 1995)

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

Photolysis: rate constant  $k = 2.686 \times 10^{-2} \text{ h}^{-1}$  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).  
 no photolyzable functional groups (Howard et al. 1991).

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

$k_{OH} = (2.0 \pm 0.3) \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.58 \text{ h}$ ;  $k_{O(3P)} = (6.0 \pm 0.6) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$  with O(<sup>3</sup>P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (33.5 \pm 3.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{NO_3} = 10.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction of O(<sup>3</sup>P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 20 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  (Darnall et al. 1976)

$k_{OH}^* = (40.0 \pm 4.5) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence Perry et al. 1977)

photooxidation  $t_{1/2} = 1056\text{--}43000$  h in water, based on measured rate data with hydroxy radical in aqueous solution (Güsten et al. 1981)

$k_{\text{OH}} = 33.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and residence time of 0.3 d, loss of 96.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = (1.5\text{--}30) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.2\text{--}0.4$  d for trimethylbenzenes (Mill 1982)

$k_{\text{NO}_3} = 5.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 38.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 1.6\text{--}16$  h (Atkinson 1985)

$k_{\text{OH}} = 31.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 25°C (Ohta & Ohyama 1985)

$k_{\text{OH}}(\text{calc}) = 18 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{obs.}) = 40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 1.80 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{\text{OH}} = 3.84 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{OH}} \approx 32.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 1.78 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 39.72 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation: aqueous aerobic biodegradation  $t_{1/2} = 168\text{--}672$  h, based on aqueous screening studies (Marion & Malaney 1964; Kitano 1978; Van der Linden 1978; Tester & Harker 1981; Trzilova & Horska 1988; Howard et al. 1991);

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 0.58$  h estimated from the rate of disappearance for the reaction with OH radical (Doyle et al. 1975)  
 $t_{1/2} = 0.24\text{--}2.4$  h (Darnall et al. 1976);

residence time of 0.3 d, loss of 96.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 1.6\text{--}16$  h, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);

summer daylight lifetime  $\tau = 4.3$  h due to reaction with OH radical (Altshuller 1991);

calculated lifetimes of 4.3 h, 26 d and  $> 4.5$  yr for reactions with OH radical,  $\text{NO}_3$  radical and  $\text{O}_3$ , respectively (Atkinson 2000).

Surface Water:  $t_{1/2} = 168\text{--}672$  h, based on estimated aqueous aerobic biodegradation half-lives (Kitano 1978; Van der Linden 1978; Tester & Harker 1981; Trzilova & Horska 1988; Marion & Malaney 1964; Howard et al. 1991);

photooxidation  $t_{1/2} = 1056\text{--}43000$  h, based on measured rate data with OH radical in aqueous solution (Güsten et al. 1981; Howard et al. 1991).

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

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

Biota:

TABLE 3.1.1.8.1

Reported aqueous solubilities and Henry's law constants of 1,2,4-trimethylbenzene at various temperatures

Aqueous solubility				Henry's law constant			
Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Sanemasa et al. 1982		Hansen et al. 1993	
vapor saturation-UV		recommended values		vapor-liquid equilibrium		EPICS-GC	
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)	t/°C	H/(Pa m <sup>3</sup> /mol)
15	52.3	15	52	15	377	27	704
25	56.5	25	56	25	619	35	1135
35	62.1	35	62	35	1042	45	1591
45	69.3	45	69	45	1663		

$\ln [H/(\text{kPa m}^3/\text{mol})] =$   
 $A - B/(T/K)$   
 $A \quad 14.0$   
 $B \quad 4298$

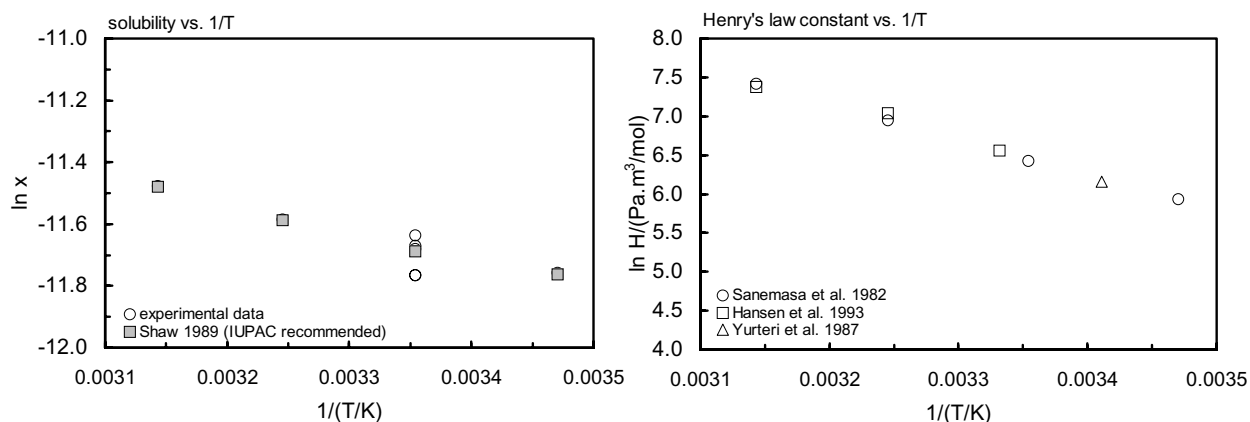


FIGURE 3.1.1.8.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1,2,4-trimethylbenzene.

TABLE 3.1.1.8.2

Reported vapor pressures of 1,2,4-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

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

Stull 1947		Forziati et al. 1949		Bond & Thodos 1960		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
13.6	133.3	84.804	6417	65.405	2666	51.75	1333
38.4	666.6	89.259	7697	97.49	10666	65.39	2666
50.7	1333	93.155	8991	153.55	66661	74.05	4000
64.5	2666	96.65	10328	180.505	133322	80.54	5333



TABLE 3.1.1.8.2 (Continued)

Stull 1947		Forziati et al. 1949		Bond & Thodos 1960		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
79.8	5333	99.94	11720	198.215	199984	85.787	6666
89.5	7999	104.369	13840	bp/°C	169.366	90.214	7999
102.8	13332	109.418	16640			97.475	10666
122.7	26664	114.572	19944			103.355	13332
145.4	53329	119.328	23474	eq. 5	P/mmHg	114.639	19998
169.2	101325	125.694	28978	A	23.2393	123.153	26664
mp/°C	−44.1	131.556	34918	B	3301.19	130.072	33331
		138.599	43351	C	6.21412	135.944	39997
		145.867	53692	D	3.15835	145.634	53329
		153.604	66792			153.534	66661
		161.991	83750			160.256	79993
		167.896	97644			166.137	93326
		168.534	99237			167.231	95992
		169.121	100732			168.302	98659
		169.788	102453			169.351	101325
		170.377	103985				

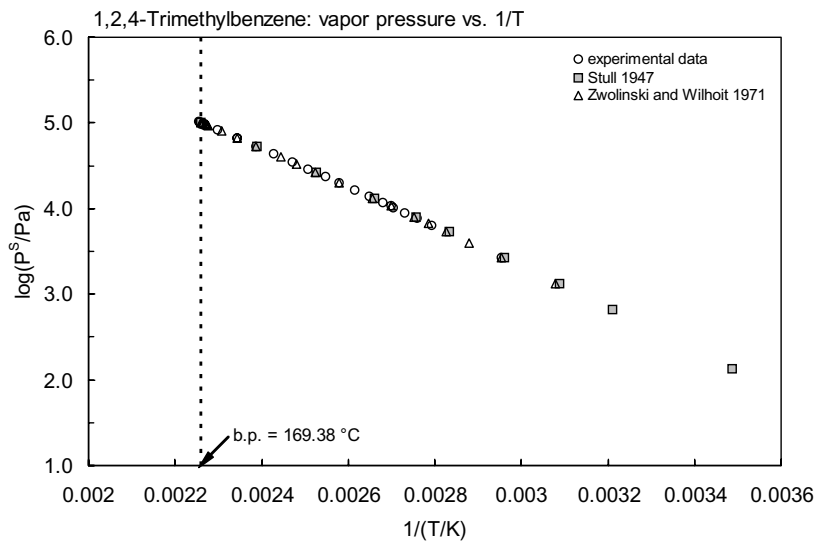
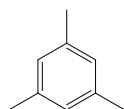


FIGURE 3.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4-trimethylbenzene.

## 3.1.1.9 1,3,5-Trimethylbenzene



Common Name: 1,3,5-Trimethylbenzene

Synonym: mesitylene

Chemical Name: 1,3,5-trimethylbenzene

CAS Registry No: 108-67-8

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_3(CH_3)_3$ 

Molecular Weight: 120.191

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

-44.7 (Weast 1982–83; Lide 2003)

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

164.74 (Lide 2003)

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

0.880 (Weast 1982–83)

Molar Volume ( $cm^3/mol$ ):136.6 ( $20^{\circ}C$ , calculated-density)

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

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):47.48, 39.04 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

51.85 (calculated-bp, Govers &amp; Evers 1992)

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

9.514 (Riddick et al. 1986)

9.51 (Chickos et al. 1999)

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

41.66, 46.2 (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  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

173 (residue-volume method, Booth &amp; Everson 1948)

97 (shake flask-UV, Andrews &amp; Keffer 1950)

39.4 (shake flask-UV, Vesala 1974)

48.2 (shake flask-GC, Sutton &amp; Calder 1975)

49.5\* (vapor saturation-UV, temp range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1981)50\* (vapor saturation-UV, temp range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)49.5 (HPLC- $k'$  correlation, converted from reported  $\gamma_w$ , Hafkenscheid & Tomlinson 1983)48.9\* (recommended, temp range  $15$ – $45^{\circ}C$ , Shaw 1989b)64\* ( $30^{\circ}C$ , equilibrium flow cell-GC, measured range  $30$ – $100^{\circ}C$ , Chen & Wagner 1994c)

$\ln x = 26.26 - 35.26 \cdot (T_r/K)^{-1} + 7.905 \cdot (T_r/K)^{-2}$ ;  $T_r = T/T_c$ , the reduced temp, system temp  $T$  divided by critical temp  $T_c$ , temp range  $303.15$ – $373.15\ K$  (equilibrium flow cell-GC, Chen & Wagner 1994c)

$\ln x = -9.533 - 678.83/(T/K)$ ; temp range  $5$ – $50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

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

121.3\* ( $10.6^{\circ}C$ , mercury manometer, Linder 1931)248\* ( $20^{\circ}C$ , mercury manometer, Kassel 1936)

$\log (P/mmHg) = -3104.5/(T/K) - 5 \cdot \log (T/K) + 23.1929$ ; temp range  $0$ – $80^{\circ}C$  (vapor pressure eq. from Hg manometer measurements, Kassel 1936)

507\* ( $30^{\circ}C$ , mercury manometer, measured range  $10$ – $50^{\circ}C$ , Rintelen et al. 1937)

- log (P/mmHg) =  $-3122.45/(T/K) - 5 \cdot \log (T/K) + 22.23680$ ; temp range 4–75°C (manometer, vapor pressure eq. from exptl. data, Stuckey & Saylor 1940)
- 133.3\* (9.6°C, summary of literature data, Stull 1947)
- 6415\* (81.488°C, ebulliometry, measured range 81.488–165.725°C, Forziati et al. 1949)
- log (P/mmHg) =  $7.07437 - 1569.622/(209.578 + t/^\circ\text{C})$ ; temp range 81.5–165.7°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
- 331 (extrapolated-Antoine eq., Dreisbach 1955)
- log (P/mmHg) =  $7.07436 - 1569.622/(209.578 + t/^\circ\text{C})$ ; temp range 70–210°C (Antoine eq. for liquid state, Dreisbach 1955)
- 328\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981; Eastcott et al. 1988)
- log (P/mmHg) =  $7.07435 - 1569.622/(209.578 + t/^\circ\text{C})$ ; temp range 48.82–193.07°C (Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) =  $[-0.2185 \times 10516.8/(T/K)] + 8.161663$ ; temp range 9.6–164.7°C (Antoine eq., Weast 1972–73)
- 366 (calculated-bp, Mackay et al. 1982)
- log (P/atm) =  $(1 - 437.769/T) \times 10^{(0.872945 - 6.55508 \times 10^4 \cdot T + 5.47586 \times 10^7 \cdot T^2)}$ ; T in K, temp range 253.0–635.0 K (Cox vapor pressure eq., Chao et al. 1983)
- 323 (extrapolated-Antoine eq., Boublik et al. 1984)
- log (P/kPa) =  $6.20212 - 1571.575/(209.79 + t/^\circ\text{C})$ ; temp range 81.488–165.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 322 (extrapolated-Antoine eq., Dean 1985)
- 330 (selected lit., Riddick et al. 1986)
- log (P/kPa) =  $6.21017 - 1577.80/(210.526 + t/^\circ\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)
- log (P/mmHg) =  $7.07436 - 1569.622/(209.58 + t/^\circ\text{C})$ ; temp range 49–193°C (Antoine eq., Dean 1985, 1992)
- 330 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $6.19762 - 1569.749/(-63.565 + T/K)$ ; temp range 354–445 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P<sub>L</sub>/kPa) =  $6.62312 - 1810.653/(-43.307 + T/K)$ ; temp range 249–356 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
- 360 (computed-expert system SPARC, Kollig 1995)
- log (P/kPa) =  $6.18965 - 1569.622/[(T/K) \pm 63.572]$ ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

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

- 929\* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1981)
- 887\* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)
- 682; 849 (EPICS; batch stripping, Ashworth et al. 1988)
- 682\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
- ln [H/(atm m<sup>3</sup>/mol)] =  $7.241 - 3628/(T/K)$ ; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
- 803 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 704 (infinite activity coeff.  $\gamma^\infty$  in water determined by inert gas stripping-GC, Li et al. 1993)
- 597 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
- log K<sub>AW</sub> =  $4.329 - 1448/(T/K)$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

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

- 3.42 (Leo et al. 1971; Hansch & Leo 1979)
- 3.78 (HPLC-k' correlation, Hammers et al. 1982)
- 3.82 (HPLC-k' correlation, Hafkenscheid & Tomlinson 1983)
- 3.42 (HPLC-RV correlation, Garst 1984)
- 3.89 (normal phase HPLC-k' correlation, Govers & Evers 1992)
- 3.42 (recommended value, Sangster 1993)
- 3.42 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

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

- 2.82 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)
- 2.77 (soil, calculated-MCI  $\chi$ , Sabljic 1987a)
- 2.75 (soil, calculated-MCI  $\chi$ , Sabljic 1987b)
- 2.85 (soil, calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 2.82 (soil, calculated-QSAR- $\chi$ , Sabljic et al. 1995)
- 3.37 (computed- $K_{OW}$ , Kollig 1995)

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

Volatilization:

Photolysis: rate constant  $k = 1.606 \times 10^{-2} \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  under photolysis at  $25^\circ\text{C}$  in F-113 solution and with  $\text{HO}\cdot$  in the gas (Dilling et al. 1988).

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

$k_{O_3} < 60 \text{ L mol}^{-1} \text{ s}^{-1}$  for vapor phase reaction with ozone at  $30^\circ\text{C}$  (Bufalini & Altshuller 1965)

$k_{OH} = (31 \pm 4) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ ;  $k_{O(3P)} = (16.8 \pm 2.0) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $\text{O}(^3\text{P})$  atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (47.2 \pm 4.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{O(3P)} = (27.9 \pm 3.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the reaction of  $\text{O}(^3\text{P})$  atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 29.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  (Darnall et al. 1976)

$k_{OH}^* = (62.4 \pm 7.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

photooxidation in water,  $t_{1/2} = 3208\text{--}1.28 \times 10^5 \text{ h}$ , based on measured rate constant for reaction with hydroxyl radical in water (Mill et al. 1980)

$k_{OH} = 49.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and residence time of 0.2 d, loss of 99.3% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{O_3} = 4200 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  for the reaction with ozone at 300 K (Lyman et al. 1982)

$k_{OH} = (15\text{--}30) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.2\text{--}0.4 \text{ d}$  for trimethylbenzenes (Mill 1982)

$k = (700 \pm 200) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water at pH 1.7 and  $20\text{--}23^\circ\text{C}$  (Hoigné & Bader 1983)

$k_{NO_3} = 2.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Atkinson et al. 1984)

$k_{OH} = 60.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{OH} = 38.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Ohta & Ohyama 1985)

$k_{NO_3} = 7.91 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{OH} = 6.05 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson 1985; Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{OH}(\text{calc}) = 38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs.}) = 62.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH}^* = 57.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 3.72 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{OH}(\text{calc}) = 54.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: unacclimated aerobic aqueous biodegradation  $t_{1/2} = 48\text{--}192 \text{ h}$ , based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991);  $t_{1/2}(\text{aq. anaerobic}) = 192\text{--}768 \text{ h}$ , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Bioconcentration:

Half-Lives in the Environment:

Air:  $0.24\text{--}2.4 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

estimated lifetime under photochemical smog conditions in S.E. England is 0.7 h (Brice & Derwent 1978; Perry et al. 1977 and Darnall et al. 1976);

residence time of 0.2 d, loss of 99.3% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 9.72\text{--}97.2$  h, based on estimated photooxidation half-life in air (Atkinson 1987).

Surface Water:  $t_{1/2} = 48\text{--}192$  h, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991);

$t_{1/2} = 1$  d in surface waters in case a first order reduction process may be assumed (estimated, Zoeteman et al. 1980).

Ground water:  $t_{1/2} = 96\text{--}384$  h, based on a soil column study in which aerobic ground water was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991).

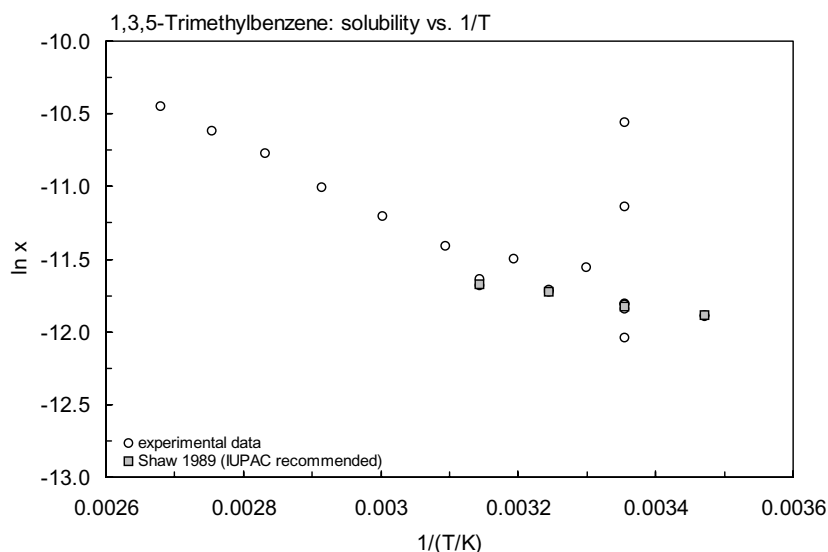
Soil:  $t_{1/2} = 48\text{--}192$  h, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991).

Biota:

**TABLE 3.1.1.9.1**

**Reported aqueous solubilities of 1,3,5-trimethylbenzene at various temperatures**

Sanemasa et al. 1981		Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Chen & Wagner 1994c	
vapor saturation-UV		vapor saturation-UV		recommended values		shake flask-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
15	45.6	15	46	15	46	30	64
25	49.5	25	50	25	48.9	40	67.8
35	54.2	35	54.9	35	54	50	74.12
45	56.5	45	58.9	45	57	60	90.82
						70	111
						80	140
						90	164
						100	194
						$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 4.49$	
						at 25°C	



**FIGURE 3.1.1.9.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,3,5-trimethylbenzene.

TABLE 3.1.1.9.2

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

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

1.

Linder 1931		Kassel 1936		Rintelen et al. 1937		Stull 1947	
Hg manometer		mercury manometer		mercury manometer		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-1.7	45.3	0	58.7	10	80	9.6	133.3
0	50	10	124	30	507	34.7	266.6
2.3	66.7	20	248	50	1523	47.4	1333
3.2	70.7	30	521	<b>Stuckey &amp; Saylor 1940</b>		61	2666
-2.75	38.66	40	844	<b>mercury manometer</b>		76.1	5333
-1.20	44	50	1467	<b>t/°C</b>	<b>P/Pa</b>	85.8	7999
1.5	57.3	60	2440	measured 4–75°C		98.9	13332
10.6	121.3	70	3933	eq. 4	P/mmHg	118.6	26664
-4.20	37.33	80	6133	A	23.2367	141	53323
2.7	66.66	90	9319	B	3122.45	164.7	101325
10.2	121.32	100	13786	C	5	mp/°C	44.8
		eq. 4	P/mmHg				
		A	22.1929	bp/°C	164.54		
		B	3104.5				
		C	5.0				

2.

Forziati et al. 1949				Zwolinski & Wilhoit 1971			
ebulliometry				selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
81.488	6415	163.911	99244	48.82	1333	161.556	93326
85.857	7697	164.489	100733	62.3	2666	162.632	95991
89.662	8991	165.146	102454	70.85	4000	163.686	98659
93.131	10328	165.725	103987	77.25	5333	164.716	101325
96.386	11722			82.424	6666		
100.747	13840	eq. 2	P/mmHg	86.789	7999	eq. 2	P/mmHg
105.716	16641	A	7.07437	93.949	10666	A	7.07436
110.789	19944	B	1573.267	99.746	13332	B	1569.622
115.498	23474	C	208.564	110.866	19998	C	209.578
121.765	28979			119.254	26664		
134.464	43352	bp/°C	164.716	126.068	33331	bp/°C	164.716
141.618	53692			131.849	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
149.238	66792			141.387	53329	at 25°C	47.48
157.477	83752			149.161	66661	at bp	39.04
163.289	97644			155.772	79993		

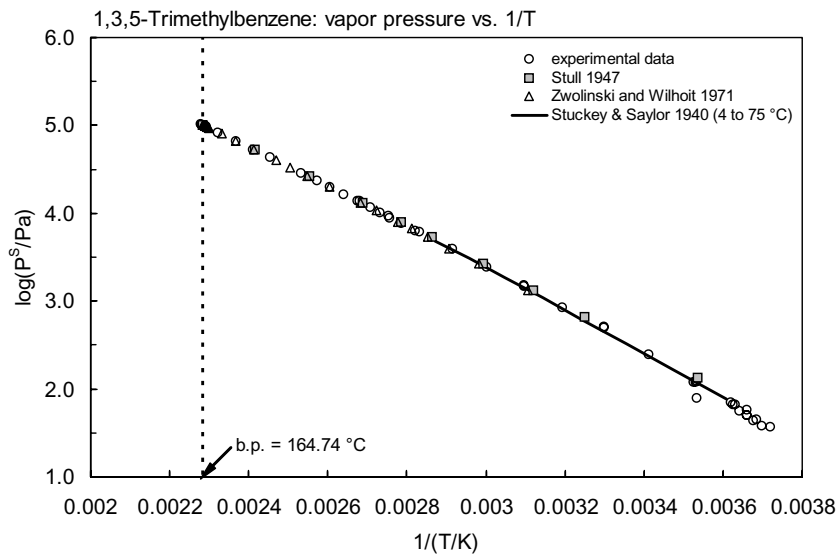
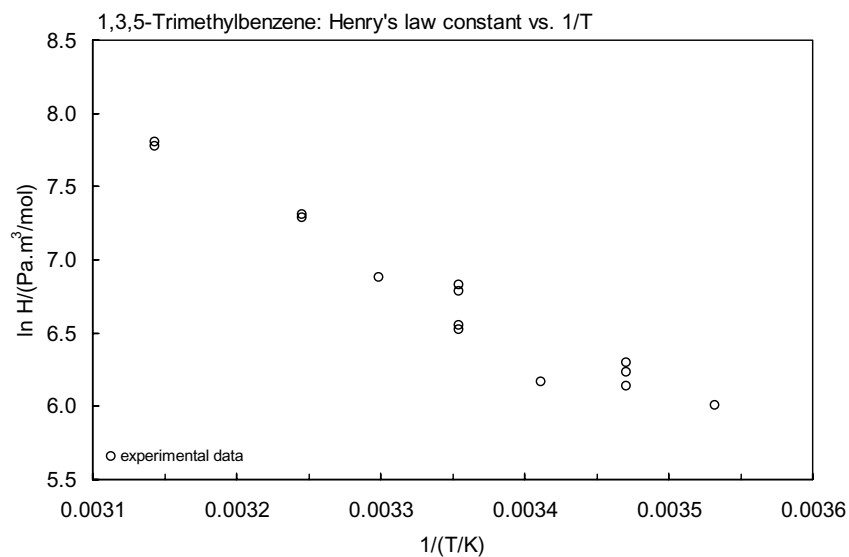


FIGURE 3.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trimethylbenzene.

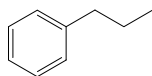
TABLE 3.1.1.9.3  
Reported Henry’s law constants of 1,3,5-trimethylbenzene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(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)			
Sanemasa et al. 1981			Sanemasa et al. 1982		
vapor-liquid equilibrium			vapor-liquid equilibrium		
t/°C	H/(Pa m <sup>3</sup> /mol)		t/°C	H/(Pa m <sup>3</sup> /mol)	
15	547		15	511	
25	929		25	887	
35	1501		35	1365	
45	2466		45	2394	
			Ashworth et al. 1988		
			EPICS-GC		
			t/°C	H/(Pa m <sup>3</sup> /mol)	
			10	408	
			15	466	
			20	477	
			25	682	
			30	976	
			eq. 4a		
			H/(atm m <sup>3</sup> /mol)		
			A	7.241	
			B	3628	



**FIGURE 3.1.1.9.3** Logarithm of Henry's law constant versus reciprocal temperature for 1,3,5-trimethylbenzene.



3.1.1.10 *n*-Propylbenzene

Common Name: *n*-Propylbenzene

Synonym: 1-phenylpropane, propylbenzene

Chemical Name: *n*-propylbenzene

CAS Registry No: 103-65-1

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_5(CH_2)_2CH_3$

Molecular Weight: 120.191

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

−99.6 (Lide 2003)

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

159.24 (Lide 2003)

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

0.862 (Weast 1982–83)

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

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

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

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

9.27 (Chickos et al. 1999)

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

53.39, 59.3 (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  $25^{\circ}C$  or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

60 ( $15^{\circ}C$ , volumetric, Fühner 1924; quoted, Chiou et al. 1982; Chiou 1985)

120 (shake flask-turbidimetric, Stearns et al. 1947)

55 (shake flask-UV, Andrews & Keffer 1950)

120 (shake flask-UV, Klevens 1951)

60 (shake flask-GC, Hermann 1972)

70 (shake flask-GC, Krasnoshchekova & Gubergrits 1975)

66.4 (shake flask-UV spec., Ben-Naim & Wiff 1979)

51.9\* (generator column-HPLC/UV,  $15$ – $30^{\circ}C$ , DeVoe et al. 1981)

51.0\* (vapor saturation-UV spec., measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)

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

52.2 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)

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

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

45.2 (vapor saturation-UV spec., Sanemasa et al. 1984)

51.7\* (generator column-HPLC/UV, measured range  $10$ – $45^{\circ}C$ , Owens et al. 1986)

55.0\* (IUPAC recommended, temp range  $15$ – $45^{\circ}C$ , Shaw 1989b)

48.2\* (vapor absorption technique-HPLC/UV, measured range  $0.5$ – $55^{\circ}C$ , Dohányosová et al. 2001)

55.0\* (shake flask-UV, measured range  $0$ – $50^{\circ}C$ , Sawamura et al. 2001)

$\ln x = -304.679 + 12774.71/(T/K) + 43.8994 \cdot \ln(T/K)$ ; temp range  $290$ – $400\ K$  (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at  $25^{\circ}C$  or as indicated and reported temperature dependence equations; \*data at other temperatures are tabulated at end of section):

260\* ( $13.9^{\circ}C$ , mercury manometer, Linder 1931)

6353\* ( $75.646^{\circ}C$ , ebulliometry, measured range  $75.646$ – $160.202^{\circ}C$ , Willingham et al. 1945)

- $\log (P/\text{mmHg}) = 6.95178 - 1649.548/(207.171 + t/^{\circ}\text{C})$ ; temp range 75.6–160.2°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)  
 667\* (31.3°C, summary of literature data, Stull 1947)  
 6402\* (75.818°C, ebulliometry, measured range 75.818–160.239°C, Forziati et al. 1949)  
 $\log (P/\text{mmHg}) = 6.95094 - 1490.963/(207.100 + t/^{\circ}\text{C})$ ; temp range 75.8–160.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)  
 458 (extrapolated-Antoine eq., Dreisbach 1955)  
 $\log (P/\text{mmHg}) = 6.95142 - 1491.297/(207.140 + t/^{\circ}\text{C})$ ; temp range 65–205°C (Antoine eq. for liquid state, Dreisbach 1955)  
 449\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)  
 $\log (P/\text{mmHg}) = 6.95142 - 1491.297/(207.140 + t/^{\circ}\text{C})$ ; temp range 43.33–187.87°C (Antoine eq., Zwolinski & Wilhoit 1971)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 10424.1/(T/\text{K})] + 8.185880$ ; temp range 6.3–159.2°C (Antoine eq., Weast 1972–73)  
 $\log (P/\text{atm}) = (1 - 432.321/T) \times 10^{(0.891023 - 6.89092 \times 10^4/T + 5.79948 \times 10^7/T^2)}$ ; T in K, temp range 280.0–635.0 K (Cox vapor pressure eq., Chao et al. 1983)  
 450 (extrapolated-Antoine eq., Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.08028 - 1493.914/(207.427 + t/^{\circ}\text{C})$ ; temp range 75.2–160.24°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)  
 $\log (P/\text{mmHg}) = 6.95142 - 1491.297/(207.14 + t/^{\circ}\text{C})$ ; temp range 43–188°C (Antoine eq., Dean 1985, 1992)  
 449 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.07438 - 1490.61/(-66.029 + T/\text{K})$ ; temp range 348–433 K (liquid, Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P/\text{mmHg}) = 39.8219 - 3.6978 \times 10^3/(T/\text{K}) - 10.962 \cdot \log (T/\text{K}) + 8.7429 \times 10^{-11} \cdot (T/\text{K}) + 2.6959 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 174–638 K (Yaws 1994)  
 $\log (P/\text{kPa}) = 6.07625 - 1490.903/[(T/\text{K}) - 66.05]$ ; 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; \*data at other temperatures are tabulated at end of section):

- 1062\* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)  
 1094\* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)  
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 7.835 - 3681/(T/\text{K})$ , temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)  
 1034 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 1102 (infinite activity coeff.  $\gamma^{\infty}$  in water determined by inert gas stripping-GC, Li et al. 1993)  
 1175\* (equilibrium headspace-GC, measured range 10–30°C, Perlinger et al. 1993)  
 902 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)  
 $\log K_{\text{AW}} = 4.587 - 1471/(T/\text{K})$  (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

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

- 3.68 (shake flask-UV, Iwasa et al. 1965; Hansch et al. 1968; 1972)  
 3.57, 3.68 (Leo et al. 1971; Hansch & Leo 1979)  
 3.66 (calculated-fragment const., Rekker 1977)  
 3.44 (shake flask-HPLC, Nahum & Horvath 1980)  
 3.691\* (3.701, 3.72-HPLC/UV, DeVoe et al. 1981)  
 3.71 (generator column-HPLC/UV both phases, Tewari et al. 1982a)  
 3.63 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 3.69 (generator column-HPLC/GC, Tewari et al. 1982b,c; Wasik et al. 1983)  
 3.89 (HPLC- $k'$  correlation, Hafkenscheid & Tomlinson 1983)  
 3.69 (generator column-HPLC/UV, Wasik et al. 1983)  
 3.69 (generator column-RP-HPLC, Schantz & Martire 1987)  
 3.71, 3.88 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 3.69 (recommended, Sangster 1989, 1993)  
 3.69 (HPLC-RT correlation, Jenke et al. 1990)  
 3.72 (recommended, Hansch et al. 1995)

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

4.09 (calculated-measured  $\gamma^\infty$  in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor,  $\log BCF$ :

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

2.87 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)  
 2.83, 2.98 (RP-HPLC- $k'$  correlation, humic acid-silica column, Szabo et al. 1990a,b)  
 2.81, 2.84, 2.87 (RP-HPLC- $k'$  correlation on 3 different stationary phases, Szabo et al. 1995)

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

Volatilization: rate constants:  $k = 0.037 \text{ d}^{-1}$ ,  $t_{1/2} = 19 \text{ d}$  in spring at 8–16°C,  $k = 0.539 \text{ d}^{-1}$ ,  $t_{1/2} = 1.3 \text{ d}$  in summer at 20–22°C,  $k = 0.065 \text{ d}^{-1}$ ,  $t_{1/2} = 11 \text{ d}$  in winter at 3–7°C for the periods when volatilization appears to dominate, and  $k = 0.086 \text{ d}^{-1}$ ,  $t_{1/2} = 8.1 \text{ d}$  with  $\text{HgCl}_2$  in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Photolysis: rate constant  $k = 6.96 \times 10^{-3} \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  under photolysis at 25°C in F-113 solution and with  $\text{HO}$  in the gas (Dilling et al. 1988).

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

$k_{OH} = 3.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 2.4\text{--}24 \text{ h}$  (Darnall et al. 1976)

$k_{OH} = (3.7 \pm 0.8) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  at  $305 \pm 2 \text{ K}$  (relative rate method, Lloyd et al. 1976)

$k_{OH} = (6.40, 5.86) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{OH} = 3.5 \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 1.6 \text{ d}$  (Mill 1982)

$k_{OH} = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{OH} = 6.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Ohta & Ohyama 1985)

$k_{OH}(\text{calc}) = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs.}) = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = 6.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 5.99 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Bioconcentration

Half-Lives in the Environment:

Air:  $t_{1/2} = 2.4\text{--}24 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

estimated lifetime  $\tau = 6 \text{ h}$  under photochemical smog conditions in S.E. England (Brice & Derwent 1978; Darnall et al. 1976).

Surface water:  $t_{1/2} = 19 \text{ d}$  in spring at 6–16°C,  $t_{1/2} = 1.3 \text{ d}$  in summer at 20–22°C,  $t_{1/2} = 11 \text{ d}$  in winter at 3–7°C when volatilization dominates and  $t_{1/2} = 8.1 \text{ d}$  with  $\text{HgCl}_2$  in marine mesocosm experiments (Wakeham et al. 1983)

TABLE 3.1.1.10.1

Reported aqueous solubilities of *n*-propylbenzene at various temperatures

1.

Sanemasa et al. 1982		DeVoe et al. 1981		Owens et al. 1986		Shaw 1989b (IUPAC)	
vapor saturation-UV		generator column-HPLC		generator column-HPLC		recommended values	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
15	46.1	23	51.32	10	53.73	15	47
25	51	15	51.21	15	52.29	25	55
35	55	20	51.09	20	54.33	35	55
45	64.1	25	51.93	25	52.25	45	64
		30	53.49	30	52.53		
				35	56.62		
				40	63.95		
				45	66.59		
				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.70$			
				25°C			

2.

Dohányosová et al. 2001		Sawamura et al. 2001	
vapor absorption-HPLC/UV		shake flask-UV	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
0.5	46.5	0	60.2
5	45.8	5	57.8
15	44.8	10	55.96
25	48.2	15	54.96
35	52.2	20	54.5
45	62.4	25	54.96
55	74.4	30	56.2
		35	58.4
		40	61.3
		45	65.6
		50	90.6
$\Delta_{\text{sol}}H/(\text{kJ mol}^{-1}) = 6.20$			
25°C			

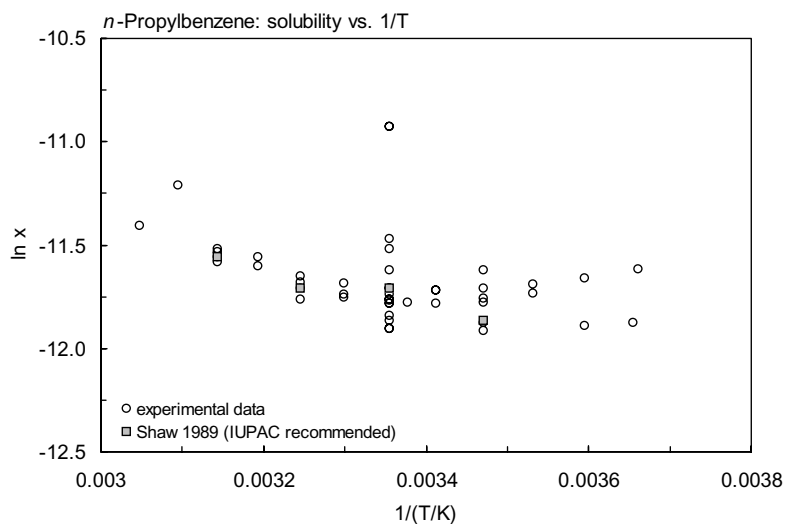
FIGURE 3.1.1.10.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *n*-propylbenzene.

TABLE 3.1.1.10.2

Reported vapor pressures of *n*-propylbenzene 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)							
Linder 1931		Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 71	
mercury manometer		ebulliometry		summary of lit. data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–6.8	46.7	75.646	6353	6.3	133.3	75.818	6402	43.44	1333
–0.7	77.3	80.064	7654	31.3	666.6	80.181	7694	56.79	2666
3.6	113.2	83.909	8965	43.4	1333	83.993	8993	65.28	4000
13.9	260	87.383	10304	56.8	2666	87.457	10332	71.64	5333
		90.622	11696	71.6	5333	90.688	11723	76.784	6666
		94.993	13820	81.1	7999	95.049	13844	81.13	7999
		99.986	16621	94	13332	100.02	16636	88.264	10666
		105.046	19924	113.5	66664	105.085	19946	94.046	13332
		109.744	23450	137.7	53329	109.781	23557	105.142	19998
		116.032	28955	159.2	101325	116.06	23982	113.542	26664
		121.807	34898			128.794	43364	120.367	33331
		128.764	43323	mp/°C	–99.5	135.972	53702	126.163	39997
		135.942	53654			143.625	66799	135.737	53329
		143.598	66757			151.921	83753	143.551	66661
		151.908	83718			157.779	97649	150.205	79993
		157.76	97607			158.408	99239	156.031	93326
		158.389	99203			158.991	100730	157.116	95992
		158.972	100694			159.654	102465	158.178	98659
		159.625	102386			160.239	104003	159.217	101325
		160.202	103910						
						eq. 2	P/mmHg	eq. 2	P/mmHg
		eq. 2	P/mmHg			A	6.95094	A	695142
		A	695178			B	1490.963	B	1491.297
		B	1491548			C	207.1	C	207.14
		C	207.171						
						bp/°C	159.218	bp/°C	159.217
		bp/°C	159.216					ΔH <sub>v</sub> /(kJ mol <sup>–1</sup> ) =	
								at 25°C	46.23
								at bp	38.24

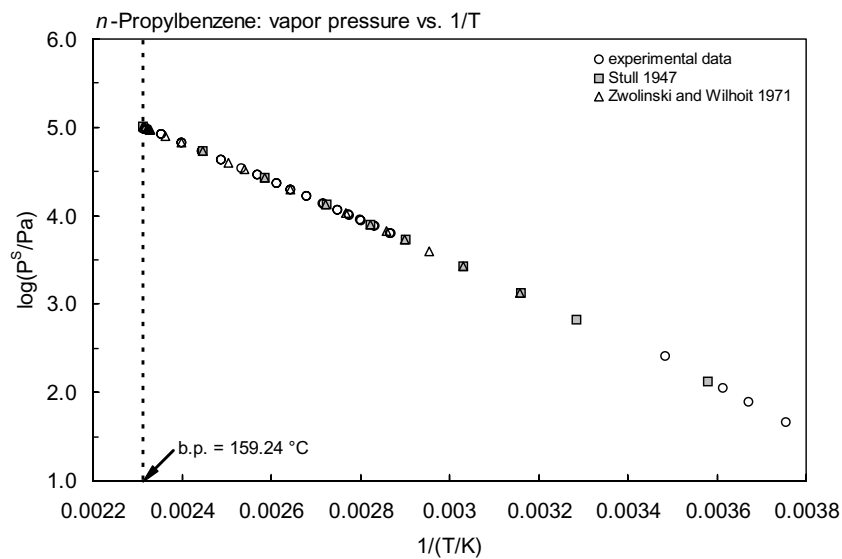


FIGURE 3.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-propylbenzene.

TABLE 3.1.1.10.3  
Reported Henry's law constants and octanol-water partition coefficients of *n*-propylbenzene at various temperatures

Henry's law constant						log $K_{OW}$	
Sanemasa et al. 1982		Ashworth et al. 1988		Perlinger et al. 1993		DeVoe et al. 1981	
vapor-liquid equilibrium		EPICS-GC		equilibrium headspace-GC		generator column-GC	
t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	H/(Pa m <sup>3</sup> /mol)	t/°C	log $K_{OW}$
15	594	10	576	10	441	25	3.691
25	1062	15	741	15	629	25	3.701
35	1818	20	893	20	848	10	3.705
45	2754	25	1094	25	1175	20	3.735
		30	1388	30	1550	25	3.72
						30	3.715
						35	3.682
		ln H = A – B/(T/K)				shake flask-GC	
		H/(atm m <sup>3</sup> /mol)				ambient	3.734
		A	7.835			ambient	3.718
		B	3681			ambient	3.711

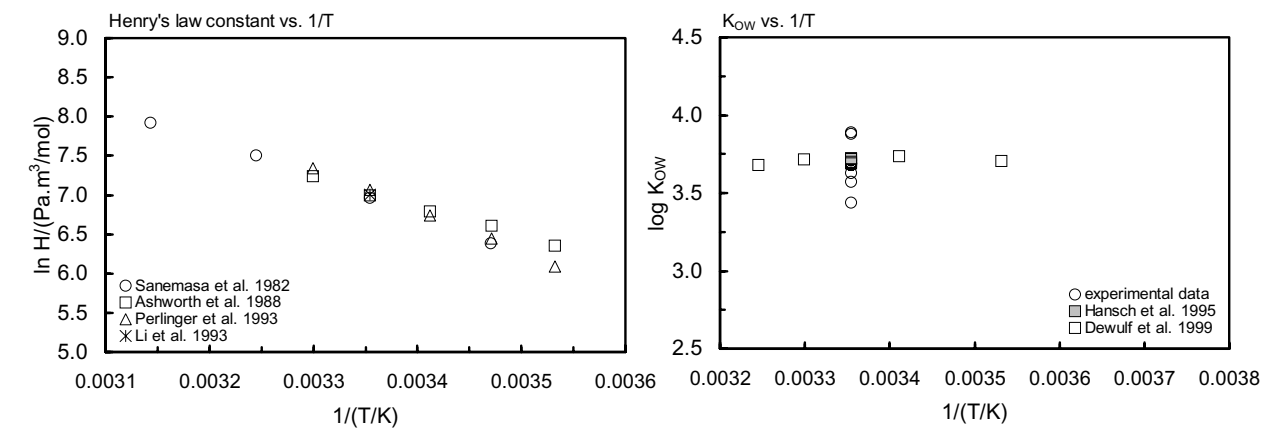
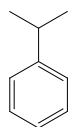


FIGURE 3.1.1.10.3 Logarithm of Henry's law constant and  $K_{OA}$  versus reciprocal temperature for *n*-propylbenzene.

## 3.1.1.11 Isopropylbenzene



Common Name: Isopropylbenzene

Synonym: cumene, 2-phenylpropane, (1-methylethyl)benzene, cumol, *i*-propylbenzene

Chemical Name: isopropylbenzene

CAS Registry No: 98-82-8

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_5CH(CH_3)_2$

Molecular Weight: 120.191

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

−96.02 (Lide 2003)

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

152.41 (Lide 2003)

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

0.8618 (Weast 1982–83)

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

139.5 ( $20^{\circ}C$ , calculated-density)

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

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

45.141, 37.53 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

7.786 (Riddick et al. 1986)

7.32 (Chickos et al. 1999)

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

41.34, 46.3 (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  $25^{\circ}C$ ; or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

170 (shake flask-turbidimetric, Stearns et al. 1947)

73 (shake flask-UV, Andrews & Keffer, 1950)

80.5\* (shake flask-UV, measured range  $25$ – $80^{\circ}C$ , Glew & Robertson 1956)

53 (shake flask-GC, McAuliffe 1963)

50 (shake flask-GC, McAuliffe 1966)

50 (shake flask-GC, Hermann 1972)

65.3 (shake flask-GC, Sutton & Calder 1975)

48.3 (shake flask-GC, Price 1976)

48.3 (shake flask-GC, Krzyzanowska & Szeliga 1978)

61.5\* (vapor saturation-UV, measured range  $15$ – $45^{\circ}C$ , Sanemasa et al. 1982)

56\* (IUPAC recommended, temp range  $15$ – $80^{\circ}C$ , Shaw 1989b)

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):

300\* ( $13.7^{\circ}C$ , mercury manometer, measured range  $-8.2$ – $13.7^{\circ}C$ , Linder 1931)

$\log(P/mmHg) = -2175/(T/K) + 7.991$  (isotenoscope method, temp range not specified, Kobe et al. 1941)

6353\* ( $70.02^{\circ}C$ , ebulliometry, measured range  $70.02$ – $153.367^{\circ}C$ , Willingham et al. 1945)

$\log(P/mmHg) = 6.92929 - 1455.811/(207.202 + t/^{\circ}C)$ ; temp range  $70.0$ – $153.4^{\circ}C$  (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

666.6\* ( $31.3^{\circ}C$ , summary of literature data, temp range  $6.3$ – $159.2^{\circ}C$ , Stull 1947)

6401\* ( $70.16^{\circ}C$ , ebulliometry, measured range  $70.16$ – $153.4^{\circ}C$ , Forziati et al. 1949)

$\log(P/mmHg) = 6.93958 - 1462.717/(207.993 + t/^{\circ}C)$ ; temp range  $70.2$ – $153.4^{\circ}C$  (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)



- 621 (extrapolated-Antoine eq., Dreisbach 1955; quoted, Hine & Mookerjee 1975)  
 $\log (P/\text{mmHg}) = 6.93666 - 1460.793/(207.777 + t/^{\circ}\text{C})$ ; temp range 60–200°C (Antoine eq. for liquid state, Dreisbach 1955)
- 609 (interpolated, Glew & Robertson 1956)
- 611\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)  
 $\log (P/\text{mmHg}) = 6.93666 - 1460.793/(207.777 + t/^{\circ}\text{C})$ ; temp range 38.29–180.67°C (Antoine eq., Zwolinski & Wilhoit 1971)
- $\log (P/\text{mmHg}) = [-0.2185 \times 10335.3/(T/\text{K})] + 8.231760$ ; temp range 2.9–152.4°C (Antoine eq., Weast 1972–73)
- $\log (P/\text{atm}) = (1 - 425.438/T) \times 10^{(0.877964 - 7.34971 \times 10^4/T + 6.06942 \times 10^7/T^2)}$ ; T in K, temp range 264.95–630.0 K (Cox vapor pressure eq., Chao et al. 1983)
- 610 (extrapolated-Antoine eq., Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.0571 - 1457.715/(207.415 + t/^{\circ}\text{C})$ ; temp range 70.02–153.4°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.06528 - 1464.366/(208.235 + t/^{\circ}\text{C})$ ; temp range 56.39–151.69°C (Antoine eq. from reported exptl. data of Dreyer et al. 1955, Boublik et al. 1984)
- 610 (selected lit., Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 6.06588 - 1464.17/(208.207 + t/^{\circ}\text{C})$ ; temp range not specified (Antoine eq., Riddick et al. 1986)
- $\log (P/\text{mmHg}) = 6.93666 - 1460.793/(207.78 + t/^{\circ}\text{C})$ ; temp range 39–181°C (Antoine eq., Dean 1985, 1992)
- 605 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.05949 - 1459.975/(-65.942 + T/\text{K})$ ; temp range 339–433 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
- $\log (P/\text{mmHg}) = -0.9234 - 2.9558 \times 10^3/(T/\text{K}) + 7.1685 \cdot \log (T/\text{K}) - 2.5369 \times 10^{-2} \cdot (T/\text{K}) + 1.4858 \times 10^{-6} \cdot (T/\text{K})^2$ ; temp range 177–631 K (Yaws 1994)
- $\log P/\text{kPa} = 6.06149 - 1460.793/[(T/\text{K}) - 65.373]$ ; 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 and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

- 1469 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 1323\* (28°C, EPICS-GC, measured range 28–46.1°C, Hansen et al. 1993)  
 $\ln [H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -3269/(T/\text{K}) + 11.0$ ; temp range 28–46.1°C (EPICS-GC, Hansen et al. 1993)
- 1126 (infinite activity coeff.  $\gamma^{\infty}$  in water determined by inert gas stripping-GC, Li et al. 1993)
- 960 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
- 902 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
- $\log K_{\text{AW}} = 3.774 - 1256/(T/\text{K})$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 3.43 (calculated- $\pi$  substituent constant, Hansch et al. 1968)
- 3.66 (Leo et al. 1971; Hansch & Leo 1979)
- 3.63 (shake flask-GC, Chiou et al. 1977, 1982)
- 3.51 (headspace GC, Hutchinson et al. 1980)
- 3.52 (HPLC- $k'$  correlation, Hanai et al. 1981)
- 3.52 (HPLC- $k'$  correlation, D'Amboise & Hanai 1982)
- 3.40 (HPLC- $k'$  correlation, Miyake & Terada 1982)
- 3.89, 4.07 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)
- 3.66 (recommended, Sangster 1989, 1993)
- 3.82 (from measured activity coeff., Tse et al. 1994)
- 3.66 (recommended, Hansch et al. 1995)

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

- 3.98 (calculated-measured  $\gamma^{\infty}$  in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

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

- 1.55 (goldfish, Ogata et al. 1984)

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

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

Volatilization:  $t_{1/2} = 5.7$  h from water depth of 1 m (calculated, Mackay & Leinonen 1975).

Photolysis:

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

$k_{OH} = (3.7 \pm 0.8) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  at  $305 \pm 2 \text{ K}$  (relative rate method, Lloyd et al. 1976)

$k_{OH} = 3.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 2.4\text{--}24 \text{ h}$  (Darnall et al. 1976)

$k_{OH} = (7.79 \pm 0.40) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 200 torr He and 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{OH} = 4.6 \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 1.2 \text{ d}$  (Mill 1982)

$k = (11 \pm 3) \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with ozone in water using 100 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{OH} = 6.25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (relative rate method, Ohta & Ohyama 1985)

$k_{OH}(\text{calc}) = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH}(\text{obs.}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 4.69 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Bioconcentration

## Half-Lives in the Environment:

Air:  $t_{1/2} = 2.4\text{--}24 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

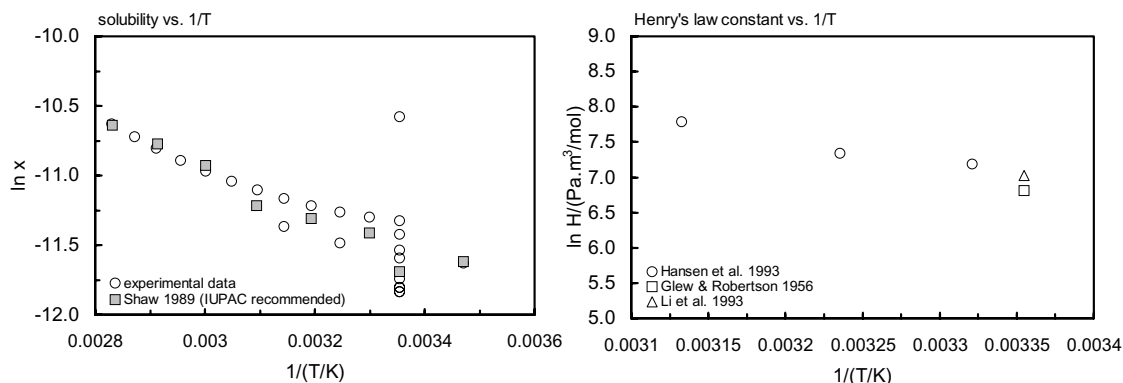
estimated lifetime  $\tau = 6 \text{ h}$  under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Darnall et al. 1976).

Surface Water:  $t_{1/2} = 5.79 \text{ h}$ , calculated half-life based on evaporative loss at 25°C and 1 m depth of water (Mackay & Leinonen 1975).

TABLE 3.1.1.11.1

Reported aqueous solubilities and Henry's law constants of isopropylbenzene at various temperatures

		Aqueous solubility		Henry's law constant			
Glew & Robertson 1956		Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Hansen et al. 1993	
shake flask-UV spec.		vapor equilibrium-UV spec.		recommended values		EPICS-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
24.936	80.47	15	59.5	15	60	28	1323
29.984	82.91	25	61.5	25	56	36	1547
34.918	85.64	35	68.7	30	74	46.1	2422
39.958	89.79	45	77.5	40	82		
44.905	94.57			50	90	$\ln H = A - B/(T/K)$	
49.902	100.4	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 5.10$		60	120	$H/(\text{kPa m}^3/\text{mol})$	
54.916	106.9	at 25°C		70	140	A	11
59.983	115			80	160	B	3299
65.165	124.4						
70.32	135.6						
75.097	147.3						
80.209	161.7						
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.57$							
at 25°C							



**FIGURE 3.1.11.1** Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for isopropylbenzene.

**TABLE 3.1.1.11.2**

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

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

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

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

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

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

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

Linder 1931		Willingham et al.1945		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
Hg manometer		ebulliometry		ebulliometry		selected values	
t/ <sup>°</sup> C	P/Pa	t/ <sup>°</sup> C	P/Pa	t/ <sup>°</sup> C	P/Pa	t/ <sup>°</sup> C	P/Pa
-8.2	57.3	70.02	6353	70.16	6401	36.29	1333
1.3	124	74.365	7654	74.47	7693	51.43	2666
13.7	300	78.155	8965	78.23	8993	59.79	4000
		81.579	10304	81.64	10331	66.06	5333
		84.768	11696	89.11	11722	71.123	6666
		89.077	13820	94.01	13843	75.407	7999
		93.991	16621	99	16636	82.433	10666
		98.975	19924	103.64	19946	88.13	13332
		103.604	23450	109.82	23477	99.076	19998
		109.802	28995	115.52	28980	107.346	26664
		115.495	34898	12.38	34928	114.076	33331
		122.353	43323	129.46	43363	119.789	39997
		129.433	53654	137.01	53701	129.23	53329
		136.983	66757	145.19	66799	136.937	66661
		145.176	83718	150.97	83752	143.501	79993
		150.956	97607	151.59	97649	149.249	93326
		151.576	99203	152.17	100730	150.319	95992
		152.152	100694	152.82	102465	151.367	98659
		152.798	102386	153.4	104003	152.392	101325
		153.367	103910				
		eq. 2	P/mmHg	eq. 2	P/mmHg	eq. 2	P/mmHg
		A	6.92929	A	6.93958	A	6.93666
		B	1455.81	B	1462.717	B	1460.793
		C	207.202	C	207.993	C	207.777
		bp/ <sup>°</sup> C	152.393	bp/ <sup>°</sup> C	152.392	bp/ <sup>°</sup> C	152.392
							$\Delta H_v/(\text{kJ mol}^{-1}) =$
							at 25 <sup>°</sup> C 45.14
							at bp 37.53

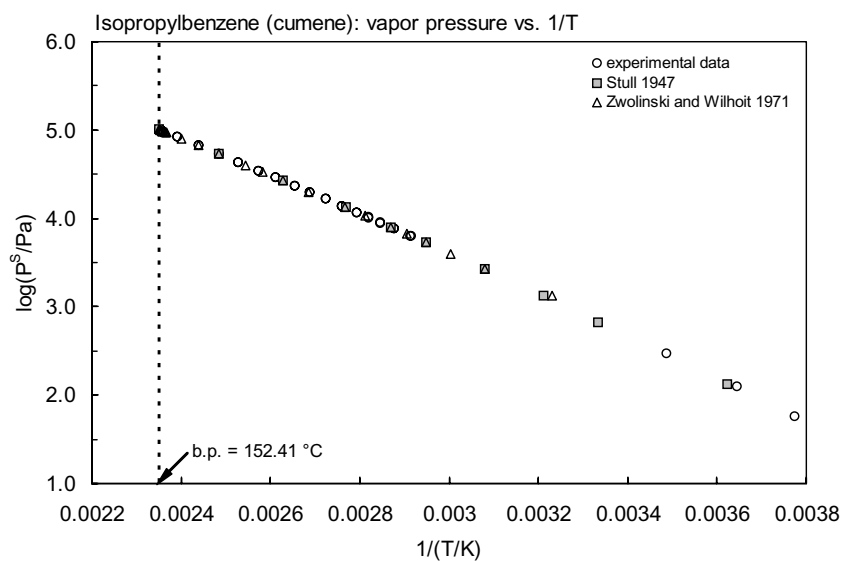
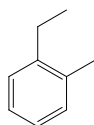


FIGURE 3.1.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for isopropylbenzene.

3.1.1.12 1-Ethyl-2-methylbenzene (*o*-Ethyltoluene)

Common Name: 1-Ethyl-2-methylbenzene

Synonym: 2-ethyltoluene, *o*-ethyltoluene

Chemical Name: 1-ethyl-2-methylbenzene, 1-methyl-2-ethylbenzene

CAS Registry No: 611-14-3

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_4CH_3C_2H_5$

Molecular Weight: 120.191

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

−79.83 (Lide 2003)

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

165.2 (Weast 1982–83; Lide 2003)

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

0.8807 (Weast 1982–83)

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

136.5 ( $20^{\circ}C$ , calculated-density)

162.6 (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  $25^{\circ}C$ ):

40.0 (estimated from nomograph, Kabadi & Danner 1979)

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

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

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\* ( $9.4^{\circ}C$ , summary of literature data, Stull 1947)

6417\* ( $81.146^{\circ}C$ , ebulliometry, measured range  $81.146$ – $157.825^{\circ}C$ , Forziati et al. 1949)

$\log(P/mmHg) = 7.00314 - 1535.374/(207.300 + t/^{\circ}C)$ ; temp range  $81.1$ – $166.2^{\circ}C$  (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

336 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.00314 - 1535.374/(207.3 + t/^{\circ}C)$ ; temp range  $70$ – $215^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P/mmHg) = 7.00314 - 1535.374/(207.300 + t/^{\circ}C)$ ; temp range  $48.46$ – $193.89^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 10448.8/(T/K)] + 8.141032$ ; temp range  $9.4$ – $165.2^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 438.357/T) \times 10^{(0.863837 - 6.34917 \times 10^4/T + 5.19164 \times 10^7/T^2)}$ ; T in K, temp range  $285.0$ – $645.0$  K (Cox vapor pressure eq., Chao et al. 1983)

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

$\log(P/kPa) = 6.11997 - 1529.684/(206.648 + t/^{\circ}C)$ ; temp range  $81.146$ – $166.2^{\circ}C$  (Antoine eq. from reported exptl. data Forziati et al. 1949, Boublik et al. 1984)

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

$\log(P/mmHg) = 7.00314 - 1535.374/(207.30 + t/^{\circ}C)$ ; temp range  $48$ – $194^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.1129 - 1532.449/(-66.123 + T/K)$ ; temp range  $353$ – $443$  K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 15.1142 - 2.9821 \times 10^3/(T/K) - 1.2619 \cdot \log(T/K) - 6.3248 \times 10^{-3} \cdot (T/K) + 3.5155 \times 10^{-6} \cdot (T/K)^2$ , temp range  $192$ – $651$  K (Yaws 1994)

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

565 (EPICS-GC/FID, Ashworth et al. 1988)

$\ln [H/(\text{atm m}^3/\text{mol})] = 5.557 - 3179/(T/\text{K})$ ; temp range  $10\text{--}30^\circ\text{C}$  (EPICS measurements, Ashworth et al. 1988)

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

512 ( $20^\circ\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 1996)

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

3.63 (headspace GC, Hutchinson et al. 1980)

3.53 (generator column-HPLC/UV, DeVoe et al. 1981; Tewari et al. 1982a)

3.78, 3.95 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)

3.53 (recommended, Sangster 1989, 1993)

3.53 (recommended, Hansch et al. 1995)

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

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

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

Volatilization:

Photolysis:

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{\text{OH}}$  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:

$k_{\text{OH}} = (8.2 \pm 1.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  at  $305 \pm 2 \text{ K}$  (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 8.2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with half-life of 0.24–2.4 h (Darnall et al. 1976)

$k_{\text{OH}} = 12.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{\text{OH}} = 12.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (relative rate method, Ohta & Ohyama 1985)

$k_{\text{OH}} = 12.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 17.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

summer daylight lifetime  $\tau = 11 \text{ h}$  due to reaction with OH radical (Altshuller 1991).

Surface water:  $t_{1/2} = 0.5 \text{ d}$  in surface water in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980).

TABLE 3.1.1.12.1

Reported vapor pressures of *o*-ethyltoluene 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		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
9.4	133.3	81.146	6417	48.46	1333
34.8	666.6	85.618	7697	61.96	2666
47.6	1333	89.448	8993	70.54	4000
61.2	2666	92.949	10323	76.97	5333
76.4	5333	96.2	11720	82.165	6666
86	7999	100.584	13840	86.552	7999
99	13332	105.598	16641	93.751	10666
119	26664	110.711	19944	99.582	13332
141.4	53329	115.436	23473	110.777	19998
165.1	101325	121.762	28978	119.29	26664
		127.574	34920	126.1	33331
mp/°C	–104.7	134.57	43351	131.933	39997
		141.792	53693	141.563	53329
		149.582	66792	149.418	66661
		157.825	83749	156.103	79993
				161.954	93326
		eq. 2	P/mmHg	164.044	95992
		A	7.00314	164.11	98659
		B	1535.374	165.534	101325
		C	207.3		
		bp/°C	165.153		

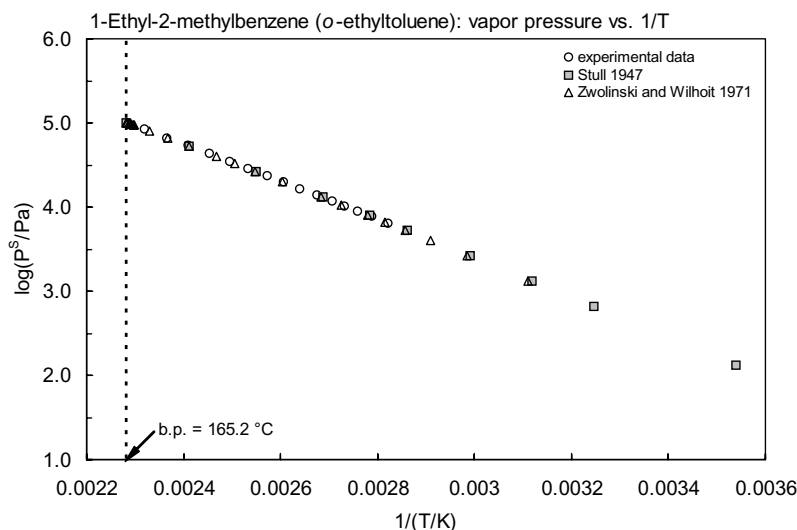
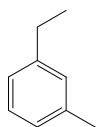


FIGURE 3.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for 1-ethyl-2-methylbenzene (*o*-ethyltoluene).

3.1.1.13 1-Ethyl-3-methylbenzene (*m*-Ethyltoluene)

Common Name: 1-Ethyl-3-methylbenzene

Synonym: 3-ethyltoluene, *m*-ethyl toluene

Chemical Name: 1-ethyl-3-methylbenzene, 1-methyl-3-ethylbenzene

CAS Registry No: 620-14-4

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_4CH_3C_2H_5$

Molecular Weight: 120.191

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

– 95.6 (Lide 2003)

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

161.3 (Forziati et al. 1949, Weast 1982–83; Lide 2003)

Density ( $g/cm^3$ ):

0.8645 ( $20^{\circ}C$ , Weast 1982–83)

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

139.0 ( $20^{\circ}C$ , calculated-density)

162.6 (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  $25^{\circ}C$ ):

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

666.6\* ( $32.3^{\circ}C$ , summary of literature data, temp range  $7.2$ – $161.3^{\circ}C$ , Stull 1947)

3066\* ( $62.1^{\circ}C$ , mercury manometer, measured range  $62.1$ – $160.3^{\circ}C$ , Buck et al. 1949)

6417\* ( $78.105^{\circ}C$ , ebulliometry, measured range  $78.105$ – $154.053^{\circ}C$ , Forziati et al. 1949)

$\log(P/mmHg) = 7.01582 - 1529.784/(208.509 + t/^{\circ}C)$ ; temp range  $78.1$ – $162.3^{\circ}C$  (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

399 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.01582 - 1529.184/(208.509 + t/^{\circ}C)$ ; temp range  $65$ – $210^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P/mmHg) = 7.01582 - 1529.184/(208.509 + t/^{\circ}C)$ ; temp range  $45.68$ – $189.74^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 10416.6/(T/K)] + 8.152199$ ; temp range  $7.2$ – $161.3^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 434.538/T) \times 10^{(0.861399 - 6.30303 \times 10^4 \cdot T + 5.19848 \times 10^7 \cdot T^2)}$ ; T in K, temp range  $280.0$ – $635.0$  K (Cox vapor pressure eq., Chao et al. 1983)

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

$\log(P/kPa) = 6.12947 - 1531.584/(209.417 + t/^{\circ}C)$ ; temp range  $78.3$ – $163^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

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

$\log(P/mmHg) = 7.01582 - 1529.184/(208.51 + t/^{\circ}C)$ ; temp range  $46$ – $190^{\circ}C$  (Antoine eq., Dean 1985, 1992)

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

$\log(P_L/kPa) = 6.13801 - 1527.983/(-64.715 + T/K)$ ; temp range  $348$ – $438$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 39.8909 - 3.6042 \times 10^3/(T/K) - 11.466 \cdot \log(T/K) + 3.5274 \times 10^{-2} \cdot (T/K) + 7.3492 \times 10^{-14} \cdot (T/K)^2$ , temp range  $178$ – $637$  K (Yaws 1994)



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

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

- 3.88, 4.07 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)
- 3.98 (lit. average value, Sangster 1993)
- 3.88 (quoted from Sherblom & Eganhouse 1988; Hansch et al. 1995)

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

Bioconcentration Factor,  $\log \text{BCF}$  or  $\log K_{\text{B}}$ :

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

- 2.42 (aquifer material with  $f_{\text{OC}}$  of 0.006 and measured partition coeff.  $K_{\text{p}} = 1.58 \text{ mL/g.}$ , Abdul et al. 1990)

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

Volatilization:

Photolysis:

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

$k_{\text{OH}} = (11.7 \pm 2.3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  at  $305 \pm \text{K}$  (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 11.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with estimated  $t_{1/2} \sim 0.24\text{--}2.4 \text{ h}$  (Darnall et al. 1976)

$k_{\text{OH}} = (21.3 \pm 1.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (relative rate method, Ohta & Ohshima 1985; Atkinson 1989)

$k_{\text{OH}} = 1.92 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 20.93 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

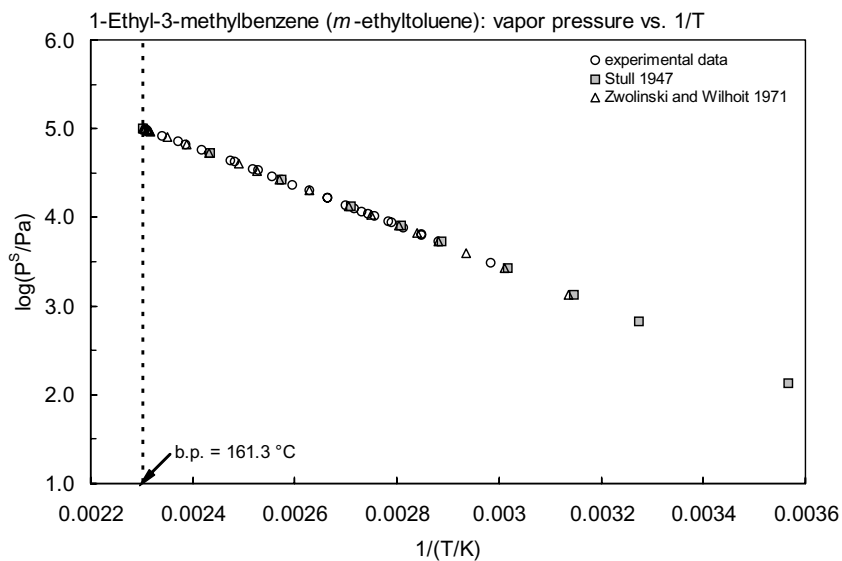
Air:  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al 1976; Howard et al. 1991);

summer daylight lifetime  $\tau = 7.2 \text{ h}$  due to reaction with OH radical (Altshuller 1991).

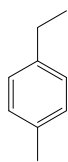
TABLE 3.1.1.13.1

Reported vapor pressures of *m*-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Forziati et al. 1949		Buck et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		mercury manometer		selected values	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
7.2	133.3	78.105	6417	62.1	3066	45.68	1333
32.3	666.6	82.525	7697	74	5386	59.07	2666
44.7	1333	86.293	8993	77.9	6293	67.58	4000
58.2	2666	89.793	10328	85.4	8693	73.95	5333
73.3	5333	93.022	11720	91.3	10879	79.102	6666
82.9	7999	97.368	13840	95.1	12772	83.45	7999
95.9	13332	102.326	16641	102.1	16772	90.584	10666
115.5	26664	107.383	19944	115.3	26398	96.363	13332
137.8	53329	112.074	23473	122.5	34264	107.456	19998
161.3	101325	118.338	28978	129.8	42397	115.829	26664
mp/ $^{\circ}\text{C}$	−104.7	124.082	34920	140.7	58262	122.635	33331
		131.027	43351	148.5	72527	128.412	39997
		138.178	53693	160.3	99592	137.949	53329
		145.795	66792			145.727	66661
		154.053	83749	eq. 4	P/mmHg	152.346	79993
				A	25.08	158.318	93326
		eq. 2	P/mmHg	B	3155	159.217	95992
		A	7.01582	C	5.663	160.272	98659
		B	1529.184			161.305	101325
		C	208.509				
						eq. 2	P/mmHg
						A	7.01582
						B	1529.184
						C	208.509
				bp/ $^{\circ}\text{C}$	161.305		
					$\Delta H_v/(\text{kJ mol}^{-1}) =$		
					at 25 $^{\circ}\text{C}$	46.9	
					at bp	38.53	



**FIGURE 3.1.13.1** Logarithm of vapor pressure versus reciprocal temperature for 1-ethyl-3-methylbenzene (*m*-ethyltoluene).

3.1.1.14 1-Ethyl-4-methylbenzene (*p*-Ethyltoluene)

Common Name: 1-Ethyl-4-methylbenzene

Synonym: 4-ethyltoluene, *p*-ethyl toluene

Chemical Name: 1-ethyl-4-methylbenzene, 1-methyl-4-ethylbenzene

CAS Registry No: 622-96-8

Molecular Formula:  $C_9H_{12}$ ,  $C_6H_4CH_3C_2H_5$

Molecular Weight: 120.191

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

−62.35 (Lide 2003)

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

162 (Weast 1982–83; Lide 2003)

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

0.8614 (Weast 1982–83)

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

139.5 ( $20^{\circ}C$ , calculated -density, Stephenson & Malanowski 1987)

162.6 (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  $25^{\circ}C$ ):

40.0 (estimated from nomograph, Kabadi & Danner 1979)

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

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

666.6\* ( $32.7^{\circ}C$ , summary of literature data, temp range  $7.6$ – $162^{\circ}C$ , Stull 1947)

3840\* ( $66.8^{\circ}C$ , mercury manometer, measured range  $66.8$ – $161.1^{\circ}C$ , Buck et al. 1949)

6417\* ( $78.396^{\circ}C$ , ebulliometry, measured range  $78.396$ – $154.684^{\circ}C$ , Forziati et al. 1949)

$\log(P/mmHg) = 6.99801 - 1527.113/(208.921 + t/^{\circ}C)$ ; temp range  $78.3$ – $163.0^{\circ}C$  (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

402 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 6.99802 - 1527.113/(208.921 + t/^{\circ}C)$ ; temp range  $65$ – $210^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P/mmHg) = 6.99802 - 1527.113/(208.921 + t/^{\circ}C)$ ; temp range  $45.68$ – $190.64^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 10461.1/(T/K)] + 8.175267$ ; temp range  $7.6$ – $162^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 345.228/T) \times 10^{(0.856105 - 6.18307 \times 10^{-4} \cdot T + 5.08568 \times 10^{-7} \cdot T^2)}$ ; T in K, temp range  $280.0$ – $635.0$  K (Cox vapor pressure eq., Chao et al. 1983)

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

$\log(P/mmHg) = 6.99802 - 1527.113/(208.92 + t/^{\circ}C)$ ; temp range  $46$ – $191^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.11098 - 1519.486/(-65.035 + T/K)$ ; temp range  $349$ – $442$  K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 46.9026 - 3.8382 \times 10^3/(T/K) - 14.154 \cdot \log(T/K) + 4.9305 \times 10^{-3} \cdot (T/K) - 1.3901 \times 10^{-13} \cdot (T/K)^2$ ; temp range  $211$ – $640$  K (Yaws 1994)

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

- 498 (calculated-P/C, Mackay & Shiu 1981, Eastcott et al. 1988)
- 498 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

- 3.63 (headspace GC, Hutchinson et al. 1980)
- 3.90, 4.09 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)
- 3.63 (recommended, Sangster 1989, 1993)
- 3.90 (quoted from Sherblom & Eganhouse 1988, Hansch et al. 1995)

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

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

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

Volatilization:

Photolysis:

Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{\text{OH}}$  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:

$k_{\text{OH}} = (7.8 \pm 1.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  at  $305 \pm 2 \text{ K}$  (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 7.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$  (Darnall et al. 1976)

$k_{\text{OH}} = 12.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and residence time of 0.9 d, loss of 67% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = 11.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson 1985)

$k_{\text{OH}} = 12.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (relative rate method, Ohta & Ohyama 1985)

$k_{\text{OH}} = 12.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 21.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (molecular orbital calculations, Klamt 1993)

Half-Lives in the Environment:

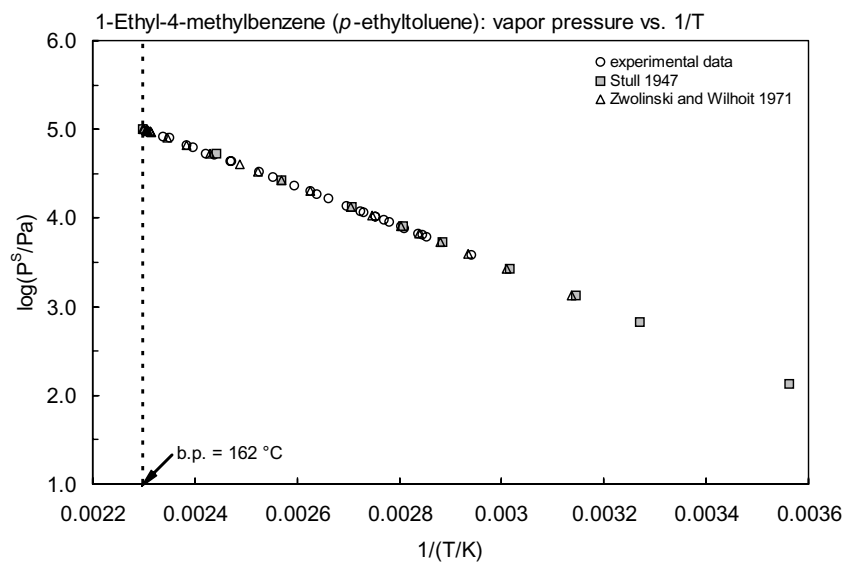
Air:  $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ , based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976)  
residence time of 0.9 d, loss of 67% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

summer daylight lifetime  $\tau = 11 \text{ h}$  due to reaction with OH radical (Altshuller 1991).

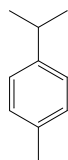
TABLE 3.1.1.14.1

Reported vapor pressures of *p*-ethyltoluene 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		Forziati et al. 1949		Buck et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		mercury manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
7.6	133.3	78.396	6417	66.8	3840	45.68	1333
32.7	666.6	82.701	7657	77.4	6106	59.14	2666
44.9	1333	86.523	8993	79.4	6586	67.68	4000
58.5	2666	89.988	10328	83.5	7999	74.09	5333
73.6	5333	93.252	11720	87.9	9466	79.265	6666
83.2	7999	97.63	13840	90.2	10399	83.637	7999
96.3	13332	102.619	16641	94	11999	90.811	10666
116.1	26664	107.71	19944	105.8	18638	96.623	13332
136.4	53329	112.422	23474	122.7	33197	107.781	19998
162	101325	118.727	28978	131.7	44130	116.205	26664
mp/°C	-	131.499	43351	136.9	51329	123.054	33331
		139.701	53693	144.2	63595	128.869	39997
		146.368	66792	152.5	79727	138.469	53329
		154.684	83750	161.1	100792	146.3	66661
						152.965	79993
		eq. 2	P/mmHg	eq. 4	P/mmHg	158.799	93326
		A	6.99801	A	21.27	159.885	95992
		B	1527.113	B	2939	160.948	98659
		C	208.921	C	4.406	161.989	101325
		bp/°C	161.989			eq. 2	P/mmHg
				A	6.99802		
				B	1527.113		
				C	208.921		
				bp/°C	161.989		
				ΔH <sub>v</sub> /(kJ mol <sup>-1</sup> ) =			
				at 25°C	46.61		
				at bp	38.41		



**FIGURE 3.1.1.14.1** Logarithm of vapor pressure versus reciprocal temperature for 1-ethyl-4-methylbenzene (*p*-ethyltoluene).

3.1.1.15 1-Isopropyl-4-methylbenzene (*p*-Cymene)

Common Name: 1-Isopropyl-4-methylbenzene

Synonym: *p*-cymene, *p*-isopropyltoluene, 1-methyl-4-isopropylbenzene

Chemical Name: 1-isopropyl-4-methylbenzene

CAS Registry No: 99-87-6

Molecular Formula: C<sub>10</sub>H<sub>14</sub>, CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CH(CH<sub>3</sub>)<sub>2</sub>

Molecular Weight: 134.218

Melting Point (°C):

−67.94 (Lide 2003)

Boiling Point (°C):

177.1 (Weast 1982–83; Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.8573 (Weast 1982–83)

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

156.6 (20°C, calculated-density)

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

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

9.66 (Dreisbach 1955)

9.67 (Chickos et al. 1999)

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

47.33, 46.8 (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):

34.15 (residue volume method, Booth & Everson 1948)

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

50.7 ± 2.3 (shake flask-HPLC/UV, Lun et al. 1997)

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

90.7\* (13.3°C, mercury manometer, Linder 1931)

log (P/mmHg) = 8.063 − 10670/(T/K) (isoteniscope method, measured range not specified, Kobe et al. 1941)

133.3\* (19°C, summary of literature data, Stull 1947)

212 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.9260 − 1538.00/(203.10 + t/°C); temp range 80–215°C (Antoine eq. for liquid state, Dreisbach 1955)

12026\* (107.04°C, ebulliometry, measured range 107.04–178.42°C, McDonald et al. 1959)

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

log (P/mmHg) = 6.9237 − 1537.06/(203.05 + t/°C); temp range 56.4–207.1°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/atm) = (1 − 450.311/T) × 10<sup>4</sup>(0.875129 − 6.86627 × 10<sup>4</sup>·T + 5.61507 × 10<sup>7</sup>·T<sup>2</sup>); T in K, temp range 290.0–650.0 K (Cox vapor pressure eq., Chao et al. 1983)

log (P/mmHg) = 7.05074 − 1608.91/(208.72 + t/°C); temp range 107–178°C (Antoine eq., Dean 1985, 1992)

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

log (P<sub>L</sub>/kPa) = 6.16214 − 1599.29/(−65.492 + T/K); temp range 380–452 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = −5.5137 − 3.0256 × 10<sup>3</sup>/(T/K) + 8.9840·log (T/K) − 2.5597 × 10<sup>−2</sup>·(T/K) + 1.3823 × 10<sup>−5</sup>·(T/K)<sup>2</sup>, temp range 205–653 K (Yaws 1994)



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

800	(calculated-P/C, Mackay & Shiu 1981)
942	(computed-expert system SPARC, Kollig 1995)

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

4.10	(shake flask-LSC, Banerjee et al. 1980)
4.14	(calculated-UNIFAC activity coeff., Arbuckle 1983)
3.45	(calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
4.10	(recommended, Sangster 1989)
4.10	(recommended, Hansch et al. 1995)
4.0	(computed-expert system SPARC, Kollig 1995)

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

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

3.70	(computed- $K_{ow}$ , Kollig 1995)
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Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Volatilization:

Photolysis: rate constant of  $1.68 \times 10^{-2} \text{ h}^{-1}$  with  $\text{H}_2\text{O}_2$  under photolysis at  $25^\circ\text{C}$  in F-113 solution and with  $\text{HO}\cdot$  in the gas (Dilling et al. 1988).

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

$k_{OH} = 0.92 \times 10^{11} \text{ M}^{-1} \text{ s}^{-1}$  at room temp. (estimated from structurally similar *p*-ethyltoluene, Winer et al. 1976)

$k_{OH}(\text{calc}) = 1.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (SAR, Atkinson 1987)

$k_{OH} = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Dilling et al. 1988)

$k_{OH} = (1.51 \pm 0.41) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a tropospheric lifetime  $\tau = 1.0\text{--}1.4 \text{ d}$ ;  $k_{NO_3} = (9.9 \pm 1.6) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with a tropospheric lifetime  $\tau = 1.3 \text{ yr}$  and a calculated tropospheric lifetime  $\tau > 330 \text{ d}$  due to reaction with  $\text{O}_3$  at  $295 \pm 2 \text{ K}$  (relative rate method, Corchnoy & Atkinson 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration

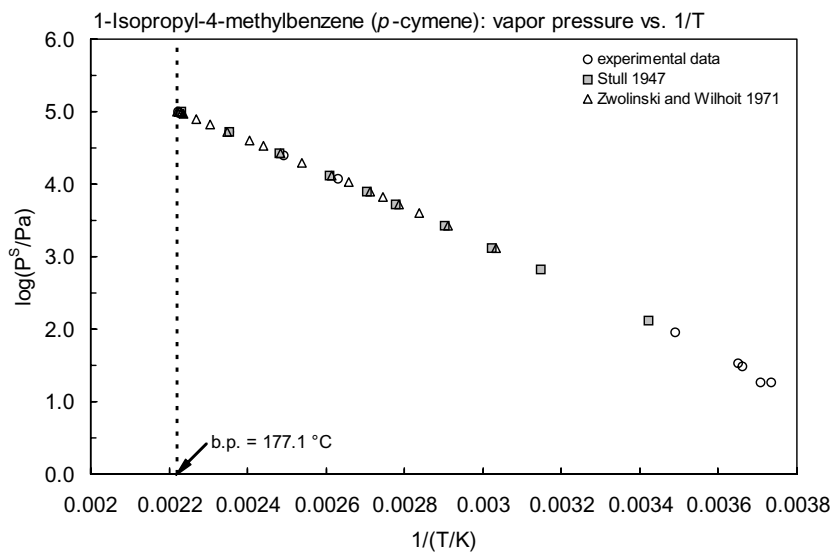
Half-Lives in the Environment:

Air: calculated tropospheric lifetimes of 1.0 d,  $> 330 \text{ d}$  and 1.3 yr due to reactions with OH radical,  $\text{O}_3$  and  $\text{NO}_3$  radical, respectively (Corchnoy & Atkinson 1990)

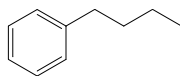
TABLE 3.1.1.15.1

Reported vapor pressures of *p*-cymene 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)					
Linder 1931		Stull 1947		McDonald et al. 1959		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–3.5	18.67	19	133.3	107.04	12026	56.4	1333
–5.3	18.67	44.6	666.6	128.24	25189	70.3	2666
0	30.66	57.6	1333	151.9	51745	79.2	4000
0.8	33.33	71.5	2666	175.35	96965	85.8	5333
13.3	90.66	87	5333	176.46	99792	91.1	6666
		96.8	7999	177.36	101949	95.7	7999
		110.1	13332	178.42	104553	103.1	10666
		130	26664			109.3	13332
		151.8	53329	eq. 2	P/mmHg	120.7	19998
		175	101325	A	7.03724	129.5	26664
				B	1599.29	136.5	33331
		mp/°C		C	207.659	142.6	39997
						152.6	53329
				mp/°C	–67.98	108	66661
						167.7	79993
						173.8	93326
						174.94	95992
						176.05	98659
						177.13	101325
Kobe et al. 1941							
isoteniscope method							
t/°C	P/Pa						
data presented by							
eq. 1	P/mmHg					eq. 2	P/mmHg
A	8.063					A	6.9237
B	2332					B	1537.06
bp/°C	176.8					C	203.05
ΔH <sub>v</sub> /(kJ mol <sup>–1</sup> ) = 44.64						bp/°C	177.13
						ΔH <sub>v</sub> /(kJ mol <sup>–1</sup> ) =	
						at 25°C	50.29
						at bp	38.16



**FIGURE 3.1.15.1** Logarithm of vapor pressure versus reciprocal temperature for 1-isopropyl-4-methylbenzene (*p*-cymene).

3.1.1.16 *n*-ButylbenzeneCommon Name: *n*-Butylbenzene

Synonym: butylbenzene

Chemical Name: *n*-butylbenzene

CAS Registry No: 104-51-8

Molecular Formula: C<sub>10</sub>H<sub>14</sub>, C<sub>6</sub>H<sub>5</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>

Molecular Weight: 134.218

Melting Point (°C):

-87.85 (Lide 2003)

Boiling Point (°C):

183.31 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.8601 (Weast 1982–83)

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

156.1 (20°C, calculated-density)

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

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

10.98 (Dreisbach 1955)

11.22 (Chickos et al. 1999)

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

60.56, 66.5 (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; \*data at other temperatures are tabulated at end of section):

12.6 (shake flask-UV, Andrews &amp; Keefer 1950)

50.5 (shake flask-UV, Klevens 1950)

15.4 (estimated, Deno &amp; Berkheimer 1960)

17.7 (shake flask-GC/ECD, Massaldi &amp; King 1973)

11.8 (shake flask-GC, Sutton &amp; Calder 1975)

12.6 (shake flask-GC, Mackay &amp; Shiu 1981)

13.83 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982)

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

13.76\* (generator column-HPLC/UV, measured range 7–45°C, Owens et al. 1986)

15.0 (IUPAC recommended, Shaw 1989b)

16.7\* (30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen &amp; Wagner 1994c)

ln *x* = -43.2390 - 5720.35/(T/K) - 1.221 × 10<sup>-4</sup>·(T/K)<sup>2</sup>; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

12.25\* (vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)

ln *x* = -346.295 + 14524.83/(T/K) + 49.9130·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations; \*data at other temperatures are tabulated at end of section):

64\* (12.2°C, mercury manometer, Linder 1931)

133.3\* (22.7°C, summary of literature data, Stull 1947)

6415\* (96.233°C, ebulliometry, measured range 96.233–184.329°C, Forziati et al. 1949)

log (P/mmHg) = 6.98318 - 1577.965/(201.378 + t/°C); temp range 96.2–184.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

145 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.98317 - 1577.965/(201.378 + t/°C); temp range 85–220°C (Antoine eq. for liquid state, Dreisbach 1955)

- 137\* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)  
 $\log (P/\text{mmHg}) = 6.98317 - 1577.965/(201.378 + t/^{\circ}\text{C})$ ; temp range 62.36–213.1 $^{\circ}\text{C}$  (Antoine eq., Zwolinski & Wilhoit 1971)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 11052.1/(T/K)] + 8.194170$ ; temp range 22.7–183.1 $^{\circ}\text{C}$  (Antoine eq., Weast 1972–73)  
 $\log (P/\text{atm}) = (1 - 456.368/T) \times 10^{(0.889482 - 7.01171 \times 10^4/T + 5.65027 \times 10^7/T^2)}$ ; T in K, temp range 295.0–660.0 K (Cox vapor pressure eq., Chao et al. 1983)  
 138, 147 (extrapolated-Antoine equations, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.11624 - 1583.708/(202.013 + t/^{\circ}\text{C})$ ; temp range 96.2–184.3 $^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.22353 - 1660.274/(210.314 + t/^{\circ}\text{C})$ ; temp range 101.3–181.8 $^{\circ}\text{C}$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 $\log (P/\text{mmHg}) = 6.98317 - 1577.965/(201.378 + t/^{\circ}\text{C})$ ; temp range 62–213 $^{\circ}\text{C}$  (Antoine eq., Dean 1985, 1992)  
 $\log (P_L/\text{kPa}) = 6.09809 - 1571.648/(-72.413 + T/K)$ ; temp range: 369–463 K (Antoine eq., Stephenson & Malanowski 1987)  
 110 (20.51 $^{\circ}\text{C}$ , static method, measured range 243.8–403.14 K, Kasehgari et al. 1993)  
 $\log (P/\text{kPa}) = 6.41845 - 1779.018/(220.982 + t/^{\circ}\text{C})$ ; temp range 243.8–403.14 K (static method, Kasehgari et al. 1993)  
 $\log (P/\text{mmHg}) = 49.9687 - 4.3981 \times 10^3/(T/K) - 14.352 \cdot \log (T/K) + 4.2054 \times 10^{-11} \cdot (T/K) + 3.4379 \times 10^{-6} \cdot (T/K)^2$ , temp range 185–661 K (Yaws 1994)  
 107 (20.16 $^{\circ}\text{C}$ , static method, measured range 253.76–418.04 K, Mokbel et al. 1998)

Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$  at 25 $^{\circ}\text{C}$ ; \*data at other temperatures are tabulated at end of section):

- 1300 (calculated-P/C, Mackay & Shiu 1981)  
 1332 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 1502 (infinite activity coeff.  $\gamma^{\infty}$  in water determined by inert gas stripping-GC, Li et al. 1993)  
 1692\* (equilibrium headspace-GC, Perlinger et al. 1993)  
 1357.8 (modified EPICS method-GC, Ryu & Park 1999)

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

- 4.26 (Hansch & Leo 1979)  
 4.19 (calculated-fragment const., Rekker 1977)  
 3.86 (headspace GC, Hutchinson et al. 1980)  
 4.26 (HPLC- $k'$  correlation, Hammers et al. 1982)  
 4.28 (generator column-HPLC/UV, Tewari et al. 1982c)  
 4.21 (HPLC methods, Harnisch et al. 1983)  
 4.28 (generator column-HPLC/UV, Wasik et al. 1983)  
 4.29 (generator column-RP-LC, Schantz & Martire 1987)  
 4.26, 4.50 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 4.26 (recommended, Sangster 1989, 1993)  
 4.377 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 4.38 (recommended, Hansch et al. 1995)

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

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

- 3.39 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)  
 3.40 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)  
 3.52 (RP-HPLC- $k'$  correlation, cyanopropyl column, Hodson & Williams 1988)  
 3.15, 3.32 (RP-HPLC- $k'$  correlation, Szabo et al. 1990a,b)  
 3.35, 3.38, 3.39 (RP-HPLC- $k'$  correlation on different stationary phases, Szabo et al. 1995)

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 3.1.1.16.1

Reported aqueous solubilities and Henry's law constants of *n*-butylbenzene at various temperatures

Aqueous solubility						Henry's law constant	
Owens et al. 1986		Chen & Wagner 1994c		Dohányosová et al. 2001		Perlinger et al. 1993	
generator column-HPLC		equilibrium flow cell-GC		vapor abs.-HPLC/UV		equil. headspace-GC	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	H/(Pa m <sup>3</sup> /mol)
7	13.34	30	16.7	0.5	11.5	10	543
10	12.98	40	17.82	5	11.5	15	828
12.5	13.14	50	20.3	15	11.3	20	1115
15	12.97	60	26.9	25	12.25	25	1692
17.5	13.14	70	32.06	35	14.5	30	2168
20	13.66	80	47.72	45	17.6		
25	13.76	90	61.14	55	21.2		
30	14.58	100	83.5				
35	15.4						
40	1763						
45	20.21						
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.60$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.29$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.29$			
at 25°C		at 25°C					

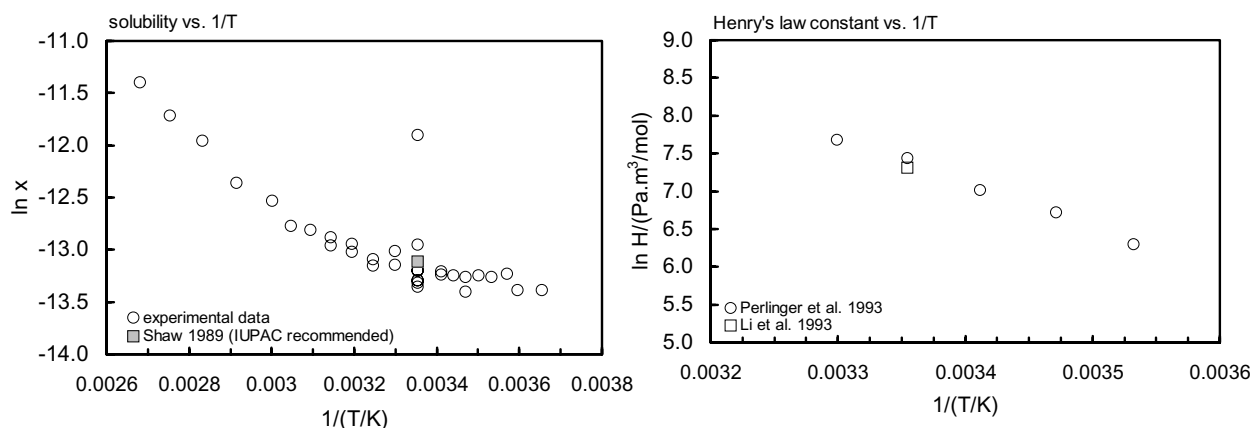
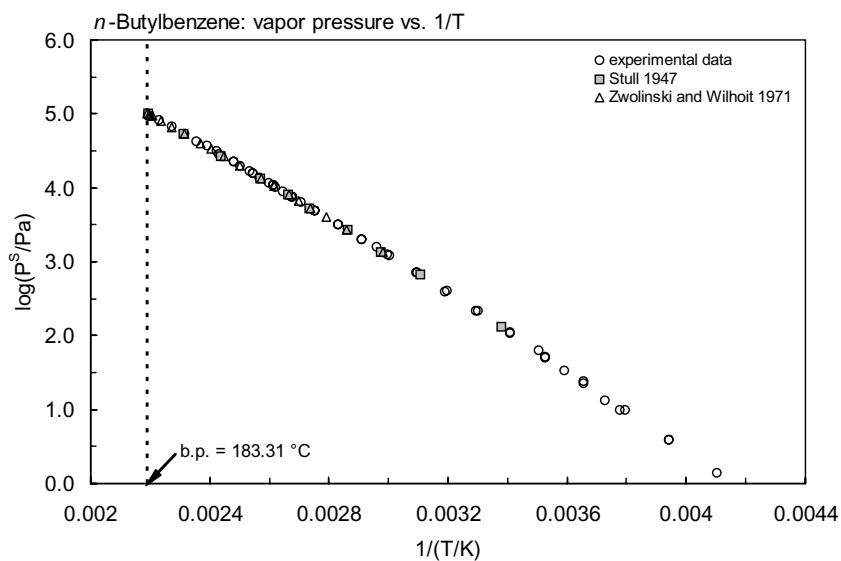
FIGURE 3.1.1.16.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for *n*-butylbenzene.

TABLE 3.1.1.16.2

Reported vapor pressures of *n*-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

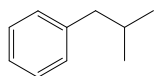
log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–4.7	13.3	22.7	133.3	96.233	6415	62.35	1333
5.5	33.3	48.8	666.6	100.814	7697	76.32	2666
12.2	64	63	1333	104.778	8991	85.21	4000
		76.3	2666	108.403	10328	91.86	5333
		92.4	5333	111.762	11722	97.241	6666
		102.6	7999	116.322	13840	101.785	7999
		116.2	13332	121.506	16640	109.243	10666
		136.9	26664	126.797	19945	115.286	13332
		159.2	53329	138.3	28979	126.89	19998
		183.1	101325	151.541	43352	135.853	26664
				159.032	53693	142.779	33331
		mp/°C	–82.1	167.011	66793	149.829	39997
				175.666	83753	158.82	53329
				181.767	97645	166.971	66661
				182.429	99245	173.91	79993
				183.636	100734	179.985	93326
				183.725	102456	181.116	95992
				184.329	103989	182.223	98659
						183.306	101325
				eq. 2	P/mmHg		
				A	6.98318	eq. 2	P/mmHg
				B	1577.965	A	6.9808
				C	201.378	B	1577.008
						C	201.331
				bp/°C	183.27		
						bp/°C	183.306
						ΔH <sub>v</sub> /(kJ mol <sup>–1</sup> )	
						at 25°C	50.12
						at bp	37.75



**FIGURE 3.1.1.16.2** Logarithm of vapor pressure versus reciprocal temperature for *n*-butylbenzene.



## 3.1.1.17 Isobutylbenzene



Common Name: Isobutylbenzene

Synonym: i-butylbenzene, 2-methylpropylbenzene, methyl-1-phenylpropane

Chemical Name: isobutylbenzene

CAS Registry No: 538-93-2

Molecular Formula:  $C_{10}H_{14}$ ,  $C_6H_5CH_2CH(CH_3)_2$

Molecular Weight: 134.218

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

−51.4 (Lide 2003)

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

170.5 (Stephenson & Malanowski 1987)

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

0.8532 (Weast 1982–83)

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

157.3 ( $20^{\circ}C$ , calculated-density)

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

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

12.51 (Dreisbach 1955)

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

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

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

10.1 (shake flask-GC, Price 1976)

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):

667\* ( $21.1^{\circ}C$ , summary of literature data, Stull 1947)

6415\* ( $86.637^{\circ}C$ , ebulliometry, measured range  $86.637$ – $173.814^{\circ}C$ , Forziati et al. 1949)

$\log(P/mmHg) = 6.93033 - 1526.384/(204.171 + t/^{\circ}C)$ ; temp range  $86.6$ – $173.8^{\circ}C$  (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

257 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 6.93033 - 1526.384/(204.171 + t/^{\circ}C)$ ; temp range  $75$ – $210^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P/mmHg) = 6.92804 - 1525.446/(204.122 + t/^{\circ}C)$ ; temp range  $53.21$ – $202.45^{\circ}C$  (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 8567.8/(T/K)] + 7.048112$ ; temp range:  $-9.8$  to  $170.5^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 445.940/T) \times 10^{(0.870338 - 6.75481 \times 10^{-4} \cdot T + 5.59009 \times 10^{-7} \cdot T^2)}$ ; T in K, temp range  $285.0$ – $645.0$  K (Cox vapor pressure eq., Chao et al. 1983)

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

$\log(P/kPa) = 6.06156 - 1530.811/(204.675 + t/^{\circ}C)$ ; temp range  $86.64$ – $173.8^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.06898 - 1536.514/(-67.788 + T/K)$ ; temp range  $373$ – $447$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -7.0438 - 2.6892 \times 10^3/(T/K) + 8.7843 \cdot \log(T/K) - 2.1426 \times 10^{-2} \cdot (T/K) + 1.1248 \times 10^{-5} \cdot (T/K)^2$ ; temp range  $222$ – $650$  K (Yaws 1994)

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

1160, 1714 (calculated- $C_w/C_A$ , calculated-bond contribution, Hine & Mookerjee 1975)

3300 (calculated-P/C, Mackay & Shiu 1981)

1393 (calculated-QSAR, Nirmalakhandan & Speece 1988b)

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

- 4.01 (headspace GC, Hutchinson et al. 1980)  
 4.54, 4.82 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 4.68 (average lit. value, Sangster 1993)  
 4.54 (Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

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

Environmental Fate Rate Constants or Half-Lives:

Volatilization: estimated  $t_{1/2} \sim 3.2$  h, evaporation from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s at 20°C (Lyman et al. 1982).

Half-Lives in the Environment:

**TABLE 3.1.1.17.1**

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

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(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		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−9.8	133.3	86.637	6415	53.21	1333
21.1	666.6	91.118	7697	66.97	2666
37.3	1333	95.026	8991	75.73	4000
54.7	2666	98.62	10328	82.29	5333
73.2	5333	101.946	11722	87.602	6666
84.1	7999	106.45	13840	92.087	7999
99	13332	111.582	16640	99.452	10666
120.7	26664	116.808	19945	105.422	13332
145.2	53329	121.659	23474	116.893	19998
170.2	101325	128.149	28979	125.561	26664
		134.112	34918	132.614	33331
mp/°C		141.301	43352	138.694	39997
		148.724	53693	149.502	53329
		156.632	66793	156.583	66661
		165.217	83754	163.465	79993
		171.27	97647	169.492	93326
		171.92	99247	170.615	95992
		172.526	100737	171.714	98659
		173.209	102457	172.789	101325
		173.814	103990		
				eq. 2	P/mmHg
		eq. 2	P/mmHg	A	6.92804
		A	6.93033	B	1525.446
		B	1526.384	C	204.122
		C	204.171	bp/°C	172.789
				$\Delta H_v/(kJ\ mol^{-1}) =$	
		bp/°C	172.759	at 25°C	49.45
				at bp	37.82

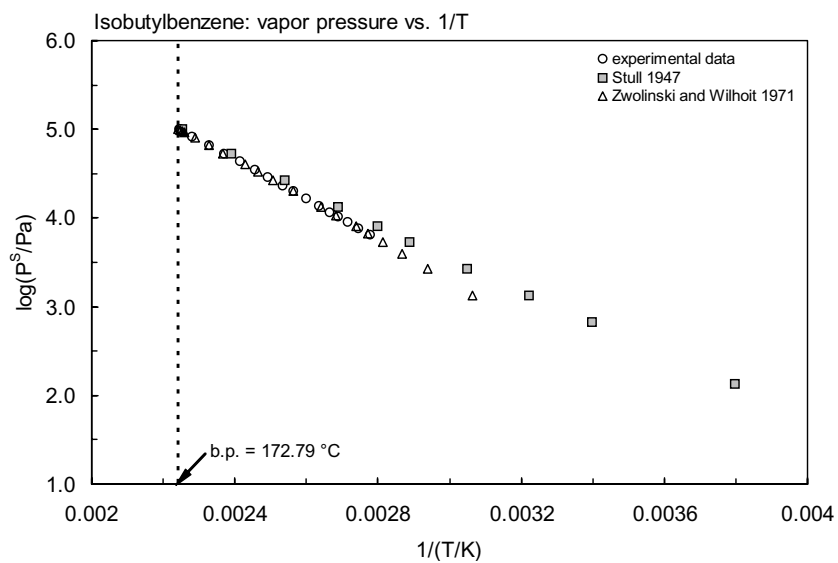
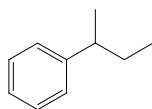


FIGURE 3.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for isobutylbenzene.

3.1.1.18 *sec*-Butylbenzene

Common Name: *sec*-Butylbenzene

Synonym: 2-phenylbutane, (1-methylpropyl)benzene, *s*-butylbenzene

Chemical Name: *sec*-butylbenzene

CAS Registry No: 135-98-8

Molecular Formula:  $C_{10}H_{14}$ ,  $C_6H_5CH(CH_3)C_2H_5$

Molecular Weight: 134.218

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

−82.7 (Lide 2003)

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

173.3 (Lide 2003)

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

0.8621 (Weast 1982–83)

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

155.7 ( $20^{\circ}C$ , calculated from density)

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

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

9.83 (Dreisbach 1955)

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

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

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

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

17.6 (shake flask-GC, Sutton & Calder 1975)

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):

70.7\* ( $9.8^{\circ}C$ , mercury manometer, measured range  $-8.6$  to  $9.8^{\circ}C$ , Linder 1931)

133.3\* ( $18.6^{\circ}C$ , summary of literature data, temp range  $18.6$ – $173.5^{\circ}C$ , Stull 1947)

6415\* ( $87.118^{\circ}C$ , ebulliometry, measured range  $87.118$ – $174.358^{\circ}C$ , Forziati et al. 1949)

$\log(P/mmHg) = 6.95097 - 1540.174/(205.101 + t/^{\circ}C)$ ; temp range  $87.1$ – $174.4^{\circ}C$ , (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

250 (extrapolated, Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 6.95097 - 1540.174/(205.101 + t/^{\circ}C)$ ; temp range  $75$ – $210^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P/mmHg) = 6.94866 - 1539.233/(205.052 + t/^{\circ}C)$ ; temp range  $53.7$ – $202.95^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 11609.3/(T/K)] + 8.318014$ ; temp range  $18.6$ – $173.5^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 446.499/T) \times 10^{(0.870844 - 6.72060 \times 10^{-4} \cdot T + 5.52698 \times 10^{-7} \cdot T^2)}$ ; T in K, temp range  $285.0$ – $645.0\ K$  (Cox vapor pressure eq., Chao et al. 1983)

240 (extrapolated, Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.05072 - 1533.897/(204.382 + t/^{\circ}C)$ ; temp range  $87.12$ – $174.4^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.94219 - 1533.95/(204.39 + t/^{\circ}C)$ ; temp range  $87$ – $174^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.10298 - 1559.452/(C + T/K)$ ; temp range  $384$ – $448\ K$  (Antoine eq., Stephenson & Malanowski 1987)

188\* ( $20.33^{\circ}C$ , static method, measured range  $243.92$ – $373.39\ K$ , Kasehgari et al. 1993)

$\log(P/kPa) = 6.47915 - 1781.723/(208.35 + t/^{\circ}C)$ ; temp range  $243.92$ – $373.39\ K$  (static method, Kasehgari et al. 1993)

$$\log (P/\text{mmHg}) = 61.5904 - 4.5093 \times 10^3/(T/K) - 19.522 \cdot \log (T/K) + 6.9865 \times 10^{-3} \cdot (T/K) + 7.8205 \times 10^{-14} \cdot (T/K)^2,$$

temp range 198–665 K (Yaws 1994)

$$186^* \quad (20.23^\circ\text{C}, \text{ static method, measured range } 263.52\text{--}393.39 \text{ K, Mokbel et al. 1998})$$

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

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

- 4.44, 4.70 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 4.57 (average lit. value, Sangster 1993)  
 4.44 (Hansch et al. 1995)  
 3.90 (computed-expert system SPARC, Kollig 1995)

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

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

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

- 2.71 (aquifer material with  $f_{\text{OC}}$  of 0.006 and measured partition coeff.  $K_p = 3.06 \text{ mL/g.}$ , Abdul et al. 1990)  
 3.60 (computed- $K_{\text{OW}}$ , Kollig 1995)

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

**TABLE 3.1.1.18.1**

**Reported vapor pressures of sec-butylbenzene 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.

Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−8.6	13.33	18.6	133.3	87.118	6415	53.7	1333
−3.0	24	44.2	666.6	91.684	7695	67.49	2666
2.6	42.66	57	1333	95.62	8990	76.26	4000
9.8	70.66	70.6	2666	99.179	10328	82.84	5333
		86.2	5333	102.523	11722	88.15	6666
		96	7999	107.009	13840	92.614	7999
		109.5	13332	112.151	16641	100.012	10666
		128.8	26664	117.387	19945	105.986	13332
		150.3	53329	122.232	23475	117.462	19998
		173.5	101325	128.715	28979	126.132	26664
				134.683	43352	133.185	33331
		mp/°C	−82.87	141.867	53693	139.175	39997
				149.288	66793	149.069	53329
				157.194	83754	157.133	66661
				165.768	97647	164.021	79993

(Continued)

TABLE 3.1.1.18.1 (Continued)

1.

Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				171.82	99245	170.042	93326
				173.068	100737	171.164	95992
				173.754	102457	172.261	98659
				174.358	103990	173.864	101325
				eq. 2	P/mmHg	eq. 2	P/mmHg
				A	6.95097	A	6.94866
				B	1540.174	B	1539.223
				C	205.101	C	205.052
				bp/°C	173.035	bp/°C	173.335
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	49.5
						at bp	37.95

2.

Kasehgari et al. 1993		Mokbel et al. 1998	
static method		static method	
T/K	P/Pa	T/K	P/Pa
243.92	2.92	263.52	16.31
253.79	7.99	273.42	43.34
263.69	19.3	283.40	92.39
273.55	44.9	293.38	186.0
283.50	93.3	303.42	357.0
293.48	188	313.44	652.0
303.49	358	323.55	1145
313.61	654	333.55	1943
313.61	655	343.57	3088
323.60	1136	353.62	4862
323.60	1139	363.43	7329
328.60	1478	373.39	10789
333.57	1904		
343.57	3088	data fitted to Wagner eq.	
363.43	4862		
373.39	7329		
Antoine eq.			
eq. 2	P/kPa		
A	6.47915		
B	1781.723		
C	226.989		

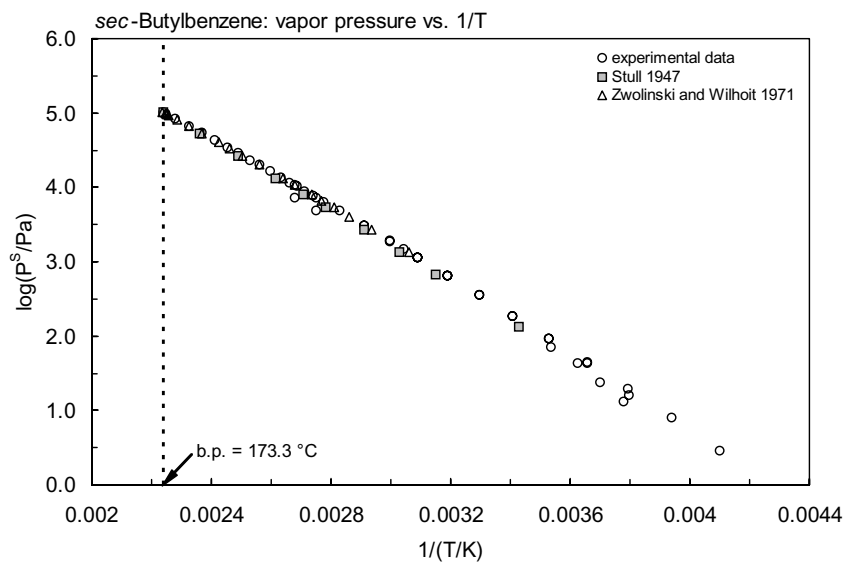
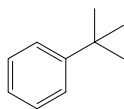


FIGURE 3.1.1.18.1 Logarithm of vapor pressure versus reciprocal temperature for sec-butylbenzene.

3.1.1.19 *tert*-Butylbenzene

Common Name: *tert*-Butylbenzene

Synonym: (1,1-dimethylethyl)benzene, 2-methyl-2-phenylpropane, trimethylphenylmethane, pseudobutylbenzene, *t*-butylbenzene

Chemical Name: *tert*-butylbenzene

CAS Registry No: 98-06-6

Molecular Formula: C<sub>10</sub>H<sub>14</sub>, C<sub>6</sub>H<sub>5</sub>C(CH<sub>3</sub>)<sub>3</sub>

Molecular Weight: 134.218

Melting Point (°C):

−58 (Stephenson & Malanowski 1987)

Boiling Point (°C):

169.1 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.8665 (Weast 1982–83)

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

154.9 (20°C, calculated from density)

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

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

8.38 (Dreisbach 1955)

8.40 (Chickos et al. 1999)

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

39.1, 45.4 (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):

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

29.5 (shake flask-GC, Sutton & Calder 1975)

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):

144\* (13.7°C, mercury manometer, measured range −2 to 13.7°C, Linder 1931)

133.3\* (13°C, summary of literature data, temp range 13–168.5°C, Stull 1947)

6426\* (83.887°C, ebulliometry, measured range 83.887–170.165°C, Forziati et al. 1949)

log (P/mmHg) = 9.2050 − 1504.572/(203.328 + t/°C); temp range 83.9–170.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

295 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.92050 − 1504.572/(203.328 + t/°C); temp range 70–205°C (Antoine eq. for liquid state, Dreisbach 1955)

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

log (P/mmHg) = 6.91829 − 1503.651/(203.280 + t/°C); temp range 50.79–198.54°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [−0.2185 × 10705.5/(T/K)] + 8.195269; temp range 13–168°C (Antoine eq., Weast 1972–73)

log (P/atm) = (1 − 442.319/T) × 10<sup>4</sup>(0.881530 − 7.21114 × 10<sup>4</sup>·T + 6.01764 × 10<sup>7</sup>·T<sup>2</sup>); T in K, temp range 285.0–635.0 K (Cox vapor pressure eq., Chao et al. 1983)

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

log (P/kPa) = 6.03861 − 1499.886/(202.792 + t/°C); temp range 83.88–170.2°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

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

log (P/mmHg) = 6.92255 − 1505.987/(203.49 + t/°C); temp range 84–170°C (Antoine eq., Dean 1985, 1992)



$\log (P_L/\text{kPa}) = 6.06067 - 1515.51/(-68.551 + T/\text{K})$ ; temp range 368–444 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 41.4522 - 3.9027 \times 10^3/(T/\text{K}) - 11.410 \cdot \log (T/\text{K}) + 2.4320 \times 10^{-10} \cdot (T/\text{K}) + 2.2517 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 215–660 K (Yaws 1994)

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

1200 (calculated-P/C, Mackay & Shiu 1981)

1300 (calculated- $C_A/C_w$ , Eastcott et al. 1988)

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

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

4.07 (shake flask-HPLC, Nahum & Horvath 1980)

4.25, 4.49 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)

4.11 (recommended, Sangster 1989, 1993)

4.11 (recommended, Hansch et al. 1995)

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

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

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

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

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

Volatilization/Evaporation:

Photolysis:

Oxidation: rate constant  $k = 4.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the gas phase reaction with OH radical at room temp. (Ohta & Ohyama 1985; Atkinson 1989);

rate constant  $k = 4.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for the gas-phase reaction with OH radical at 298 K (Atkinson 1990).

Oxidation:

Hydrolysis:

Biodegradation:

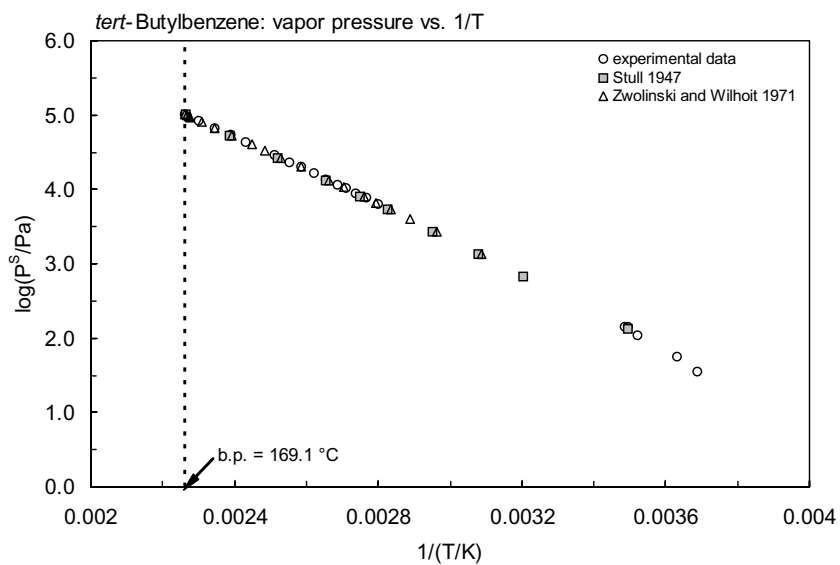
Bioconcentration

Half-Lives in the Environment:

TABLE 3.1.1.19.1

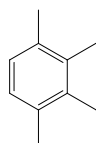
Reported vapor pressures of *tert*-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(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)					
Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−2.0	36	13	133.3	83.887	6426	50.79	1333
2.3	57.3	39	666.6	88.312	7695	64.41	2666
10.8	140	51.7	1333	92.194	8990	73.07	4000
13.7	144	65.6	2666	95.715	10332	79.56	5333
		80.8	5333	99.017	11722	84.816	6666
		90.6	7999	103.471	13840	89.254	7999
		103.8	13332	108.546	16641	96.542	10666
		123.7	26664	113.72	19945	102.449	13332
		145.8	53329	118.524	23475	113.802	19998
		168.5	101325	124.936	28979	122.449	26664
				137.968	43354	129.364	33331
		mp/°C	−58.0	145.315	53692	135.295	39997
				153.149	66781	145.095	53329
				161.649	83754	153.097	66661
				167.646	97647	159.913	79993
				168.287	99247	165.882	93326
				168.886	100737	166.994	95992
				169.565	102458	168.083	98659
				170.165	103991	169.018	101325
				eq. 2	P/mmHg	eq. 2	P/mmHg
				A	6.9205	A	6.91829
				B	1504.572	B	1503.651
				C	203.328	C	203.28
				bp/°C	169.119	bp/°C	169.148
						$\Delta H_v/(kJ\ mol^{-1}) =$	
						at 25°C	49.8
						at bp	37.61



**FIGURE 3.1.1.19.1** Logarithm of vapor pressure versus reciprocal temperature for *tert*-butylbenzene.

## 3.1.1.20 1,2,3,4-Tetramethylbenzene



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

Synonym: perhintene, prebnitene

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

CAS Registry No: 488-23-3

Molecular Formula:  $C_{10}H_{14}$ ,  $C_6H_2(CH_3)_4$

Molecular Weight: 134.218

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

−6.2 (Weast 1982–83; Lide 2003)

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

205 (Weast 1982–83; Lide 2003)

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

0.9052 (Weast 1982–83)

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

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

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

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

11.21 (Dreisbach 1955)

11.23 (Chickos et al. 1999)

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

42.31, 45.7 (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  $25^{\circ}C$ ):

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\* ( $42.6^{\circ}C$ , summary of literature data, temp range  $42.6$ – $204.4^{\circ}C$ , Stull 1947)

49.20 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.0584 - 1689.10/(199.28 + t/^{\circ}C)$ ; temp range  $100$ – $250^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1333\* ( $79.515^{\circ}C$ , compiled data, temp range  $79.515$ – $235.815^{\circ}C$ , Bond & Thodos 1960)

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

$\log(P/mmHg) = 7.0594 - 1690.54/(199.48 + t/^{\circ}C)$ ; temp range  $79.5$ – $235.9^{\circ}C$  (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 12258.0/(T/K)] + 8.534237$ ; temp range  $42.6$ – $204.4^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 478.255/T) \times 10^{(0.889494 - 6.47585 \times 10^4/T + 4.96841 \times 10^7/T^2)}$ ; T in K, temp range  $310.0$ – $690.0\ K$  (Cox vapor pressure eq., Chao et al. 1983)

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

$\log(P/mmHg) = 7.0594 - 1690.54/(199.48 + t/^{\circ}C)$ ; temp range  $80$ – $217^{\circ}C$  (Antoine eq., Dean 1985, 1992)

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

$\log(P_L/kPa) = 6.1843 - 1690.54/(-73.67 + T/K)$ ; temp range  $352$ – $509\ K$  (liquid, Antoine eq., Stephenson & Malanowski 1987)

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

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

3.84 (generator column-HPLC, Wasik et al. 1982)

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

- 4.30, 4.53 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 4.00 (recommended, Sangster 1989, 1993)  
 4.09 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)  
 3.98 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

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

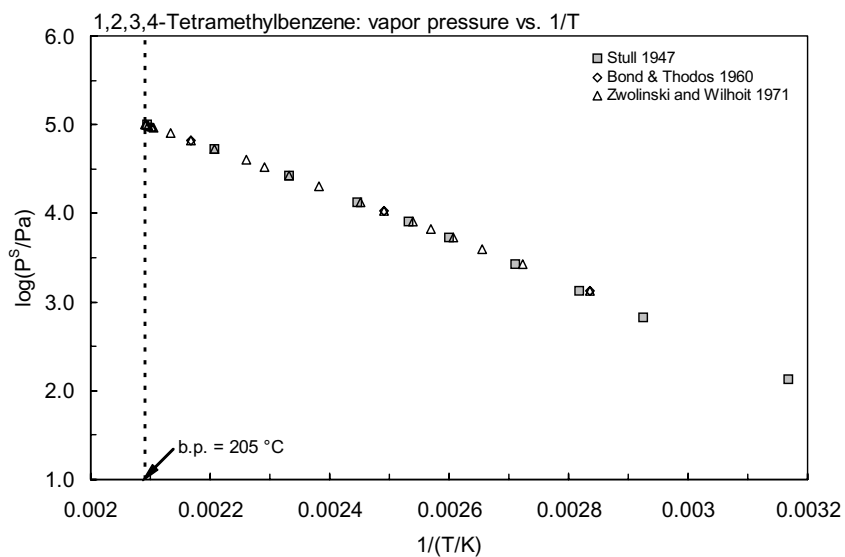
Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 3.1.1.20.1**

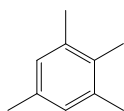
**Reported vapor pressures of 1,2,3,4-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations**

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)					
log P = A – B/(T/K) – C·log (T/K) + D·P/(T/K) <sup>2</sup>		(5)					
Stull 1947		Bond & Thodos 1960		Zwolinski & Wilhoit 1971			
summary of literature data		compiled data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
42.6	133.3	79.515	1333	79.5	1333	201.6	93326
68.7	666.6	128.415	10666	94.1	2666	202.83	95992
81.8	1333	188.185	66661	103.4	4000	204.54	98659
95.8	2666	216.925	133322	110.3	5333	205.09	101325
111.5	5333	235.815	199984	115.9	6666		
121.8	7999			120.6	7999	eq. 2	P/mmHg
135.7	13332	bp/°C	205.055	128.4	10666	A	7.0594
1155.7	26664			134.7	13332	B	1690.54
180	53329	eq. 5	P/mmHg	146.7	19998	C	199.48
204.4	101325	A	27.4323	155.8	26664	bp/°C	205.9
		B	3713.52	163.2	33331	ΔH <sub>v</sub> /(kJ mol <sup>-1</sup> ) =	
mp/°C	–4.0	C	6.77416	169.2	39997	at 25°C	57.15
		D	3.81118	179.8	53329	at bp	45.02
				188.22	66661		
				195.99	79993		



**FIGURE 3.1.1.20.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,4-tetramethylbenzene.

## 3.1.1.21 1,2,3,5-Tetramethylbenzene



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

Synonym: isodurene

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

CAS Registry No: 527-53-7

Molecular Formula:  $C_{10}H_{14}$ ,  $C_6H_2(CH_3)_4$

Molecular Weight: 134.218

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

−24.1 (Stephenson & Malanowski 1987)

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

198 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

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

0.8903 (Weast 1982–83)

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

150.8 ( $20^{\circ}C$ , calculated-density)

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

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

12.93 (Chickos et al. 1999)

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

52.01, 46.7 (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  $25^{\circ}C$ ):

16.2, 16.4, 19.4 (15, 25,  $35^{\circ}C$ , estimated- RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

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

133.3\* ( $40.6^{\circ}C$ , summary of literature data, temp range  $40.6$ – $197.9^{\circ}C$ , Stull 1947)

67.10 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.0769 - 1674.00/(200.94 + t/^{\circ}C)$ ; temp range  $95$ – $240^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P/mmHg) = 7.70779 - 1675.43/(201.14 + t/^{\circ}C)$ ; temp range  $74.5$ – $228.3^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 12358.4/(T/K)] + 8.680246$ ; temp range  $40.6$ – $197.9^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 471.208/T) \times 10^{(0.891876 - 6.64575 \times 10^4/T + 5.21861 \times 10^7/T^2)}$ ; T in K, temp range  $305.0$ – $675.0$  K (Cox vapor pressure eq., Chao et al. 1983)

62.22 (extrapolated, Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.0779 - 1675.43/(201.14 + t/^{\circ}C)$ ; temp range  $75$ – $228^{\circ}C$  (Antoine eq., Dean 1985, 1992)

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

$\log(P_L/kPa) = 6.2028 - 1675.43/(-72.01 + T/K)$ ; temp range  $348$ – $502$  K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -3.9778 - 2.960 \times 10^3/(T/K) + 7.3226 \cdot \log(T/K) - 1.7725 \times 10^{-2} \cdot (T/K) + 8.6365 \times 10^{-6} \cdot (T/K)^2$ , temp range  $249$ – $679$  K (Yaws 1994)

Henry's Law Constant ( $Pa m^3/mol$ ):

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

4.04 (generator column-HPLC/UV, Wasik et al. 1982)

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

- 4.30 (average value, RP-HPLC- $k'$  correlation, Sherblom & Eganhouse 1988)  
 4.10 (recommended, Sangster 1989, 1993)  
 4.23 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)  
 4.04 (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 3.1.1.21.1**

**Reported vapor pressures of 1,2,3,5-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations**

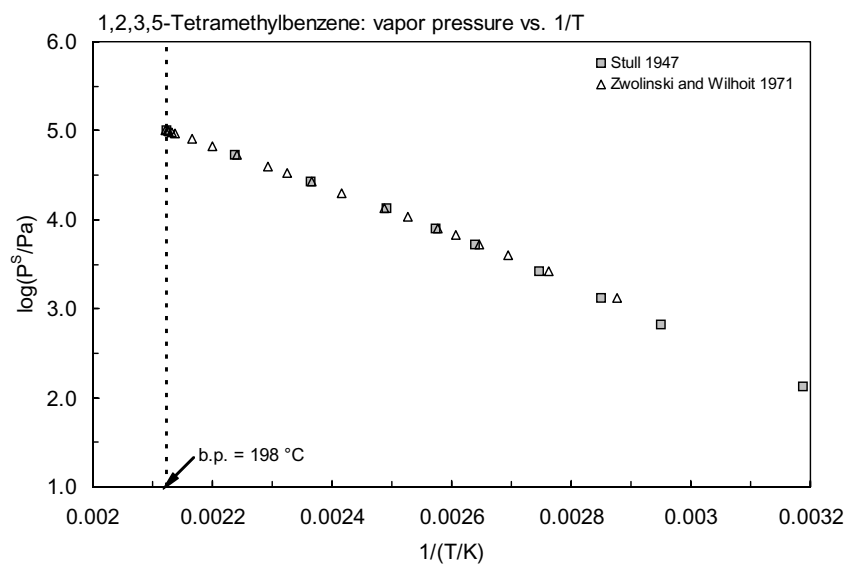
$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}C) & (2) & \ln P = A - B/(C + t/^{\circ}C) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

**Stull 1947**

**Zwolinski & Wilhoit 1971**

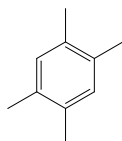
summary of literature data		selected values			
$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa
40.6	133.3	74.5	1333	194.68	93326
65.8	666.6	88.9	2666	195.83	95992
77.8	1333	98	4000	196.95	98659
91	2666	104.8	5333	198.05	101325
105.8	5333	110.3	6666		
115.4	7999	115	7999	eq. 2	P/mmHg
128.3	13332	122.6	10666	A	7.0779
149.9	26664	128.8	13332	B	1675.43
173.7	53329	140.7	19998	C	201.14
197.9	101325	149.6	26664		
		156.9	33331	bp/ $^{\circ}C$	198.05
mp/ $^{\circ}C$	-24.0	163	39997	$\Delta H_v/(kJ\ mol^{-1}) =$	
		173.2	53329	at 25 $^{\circ}C$	55.82
		181.5	66661	at bp	43.81
		188.5	79993		





**FIGURE 3.1.1.21.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetramethylbenzene.

## 3.1.1.22 1,2,4,5-Tetramethylbenzene



Common Name: 1,2,4,5-Tetramethylbenzene

Synonym: durene

Chemical Name: 1,2,4,5-tetramethylbenzene

CAS Registry No: 95-93-2

Molecular Formula:  $C_{10}H_{14}$ ,  $C_6H_2(CH_3)_4$

Molecular Weight: 134.218

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

79.3 (Lide 2003)

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

196.8 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density ( $g/cm^3$  at  $20^{\circ}C$ ): 0.838

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

160.1 ( $20^{\circ}C$ , calculated-density)

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

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

21.0 (Dreisbach 1955; Tsonopoulos & Prausnitz 1971)

20.88 (Chickos et al. 1999)

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

59.83 (Tsonopoulos & Prausnitz 1971)

59.25, 46.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ , F: 0.293 (mp at  $79.3^{\circ}C$ ))

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

19.5 (Deno & Berkheimer 1960)

3.48 (shake flask-GC, Price 1976)

3.48 (shake flask-GC, Krzyzanowska & Szeliga 1978)

13.9 (HPLC- $k'$  correlation, converted from reported activity coeff  $\gamma_w$ , Hafkenscheid & Tomlinson 1983)

17.2, 18.6, 28.2 (15, 25,  $35^{\circ}C$ , RP-HPLC- $k'$  correlation, Finizio & Di Guardo 2001)

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

4.4\* ( $1.75^{\circ}C$ , mercury manometer, measured range  $-1.7$ – $1.75^{\circ}C$ , Linder 1931)

133.3\* ( $45^{\circ}C$ , summary of literature data, temp range  $45$ – $195.9^{\circ}C$ , Stull 1947)

70.9 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.0790 - 1671.0/(201.23 + t/^{\circ}C)$ ; temp range  $95$ – $240^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P/mmHg) = 7.0800 - 1672.43/(201.43 + t/^{\circ}C)$ ; temp range  $73.6$ – $227^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 12582.6/(T/K)] + 8.822113$ ; temp range  $45$ – $195.9^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 470.032/T) \times 10^{(0.884259 - 6.36677 \times 10^{-4} \cdot T + 4.97646 \times 10^{-7} \cdot T^2)}$ ; T in K, temp range  $346.75$ – $675.0\ K$  (Cox vapor pressure eq., Chao et al. 1983)

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

$\log(P/mmHg) = 7.0800 - 1672.43/(201.43 + t/^{\circ}C)$ ; temp range  $74$ – $277^{\circ}C$  (Antoine eq., Dean 1985, 1992)

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

$\log(P_L/kPa) = 6.2049 - 1672.43/(-71.72 + T/K)$ ; temp range  $353$ – $500\ K$  (Antoine eq., Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = -51.3593 - 1.6523 \times 10^3/(T/K) + 26.656 \cdot \log (T/K) - 3.5721 \times 10^{-2} \cdot (T/K) + 1.5018 \times 10^{-5} \cdot (T/K)^2,$$

temp range 352–Y675K (Yaws 1994)

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

2541 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

4.00 (Hansch & Leo 1979)  
 4.24 (HPLC-RV correlation, Garst 1984)  
 4.13, 4.34 (RP-HPLC-k' correlations, Sherblom & Eganhouse 1988)  
 4.10 (recommended, Sangster 1989, 1993)  
 4.27 (normal phase HPLC-k' correlation, Govers & Evers 1992)  
 4.00 (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>:

3.12 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)  
 2.99 (soil, calculated-MCI  $\chi$ , Sabljic 1987a,b)  
 2.76 (aquifer material with f<sub>OC</sub> of 0.006 and measured K<sub>p</sub> = 3.42 mL/g., Abdul et al. 1990)

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

Volatilization:

Photolysis:

Oxidation: rate constant k = 1.1 × 10<sup>4</sup> cm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup> for reaction with ozone at 300 K (estimated, Lyman 1982).

Hydrolysis:

Biodegradation:

Bioconcentration:

Half-Lives in the Environment:

TABLE 3.1.1.22.1

Reported vapor pressures of 1,2,4,5-tetramethylbenzene 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)					
Linder 1931		Stull 1947		Zwolinski & Wilhoit 1971			
Hg manometer		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−1.7	1.733	45	133.3	73.6	1333	193.49	93326
−1.3	21.33	63	666.6	88	2666	194.63	95992
1.3	4.4	74.6	1333	97.1	4000	195.75	98659
1.75	4.4	88	2666	103.9	5333	196.84	101325
		104.2	5333	109.4	6666		
		114.8	7999	114	7999	eq. 2	P/mmHg
		128.1	13332	121.6	10666	A	7.08
		149.5	26664	127.8	13332	B	1672.43
		172.1	53329	139.6	19998	C	201.43
		195.9	101325	148.5	26664		
				155.8	33331	bp/°C	196.84
		mp/°C	79.5	161.9	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				172.1	53329	at 25°C	75
				180.3	66661	at bp	44.52
				187.3	79993		

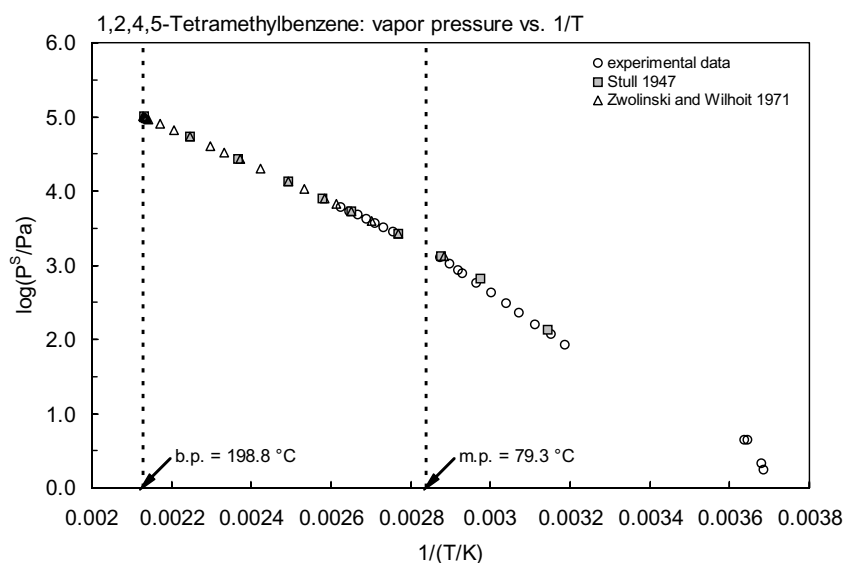
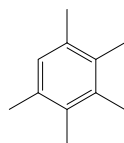


FIGURE 3.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4,5-tetramethylbenzene.

## 3.1.1.23 Pentamethylbenzene



Common Name: Pentamethylbenzene

Synonym:

Chemical Name: pentamethylbenzene

CAS Registry No: 700-12-9

Molecular Formula:  $C_{11}H_{16}$ ,  $C_6H(CH_3)_5$

Molecular Weight: 148.245

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

54.5 (Weast 1982–83; Lide 2003)

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

232 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

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

0.917, 0.913 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

0.917 (Weast 1982–83)

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

161.7 ( $20^{\circ}C$ , calculated from density)

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

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

12.34 (Tsonopoulos & Prausnitz 1971)

1.98, 10.67; 12.65 ( $23.65$ ,  $55.05^{\circ}C$ ; total phase change enthalpy, Chickos et al. 1999)

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

37.70 (Tsonopoulos & Prausnitz 1971)

39.33, 47.3 (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: 0.514 (mp at  $54.5^{\circ}C$ )

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

15.6 (Deno & Berkheimer 1960)

15.52 (calculated- $K_{OW}$ , Yalkowsky et al. 1983)

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

13.84 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.13756 - 1833.8/(199.0 + t/^{\circ}C)$ ; temp range  $125$ – $280^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log(P_L/kPa) = 6.3509 - 1867/(-75.15 + T/K)$ ; temp range  $338$ – $503\ K$  (Antoine eq., Stephenson & Malanowski 1987)

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

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

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

4.57 (HPLC-RV correlation, Garst 1984)

4.56 (recommended, Sangster 1989, 1993)

4.59 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)

4.56 (recommended, Hansch et al. 1995)

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

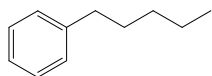
Bioconcentration Factor,  $\log BCF$ :

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

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

Half-Lives in the Environment:

## 3.1.1.24 Pentylbenzene



Common Name: *n*-Pentylbenzene

Synonym: phenylpentane

Chemical Name: pentylbenzene

CAS Registry No: 538-68-1

Molecular Formula:  $C_{11}H_{16}$ ,  $C_6H_5(CH_2)_4CH_3$

Molecular Weight: 148.245

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

−75 (Dreisbach 1955; Weast 1982–83; Lide 2003)

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

205.4 (Weast 1982–83; Lide 2003)

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

0.8585 (Weast 1982–83)

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

172.7 ( $20^{\circ}C$ , calculated from density)

207.0 (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  $25^{\circ}C$ , 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):

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

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

3.37\* (generator column-HPLC/UV, measured range  $7$ – $45^{\circ}C$ , Owens et al. 1986)

$\ln x = -387.920 + 16274.64/(T/K) + 55.9266 \cdot \ln (T/K)$ ; temp range  $290$ – $400\ K$  (eq. derived from literature calorimetric and solubility data, Tsionopoulos 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):

43.7 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.04709 - 1670.68/(195.6 + t/^{\circ}C)$ ; temp range  $105$ – $270^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log (P/mmHg) = 6.97833 - 1639.91/(194.76 + t/^{\circ}C)$ ; temp range  $80$ – $237^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 34.2755 - 3.6829 \times 10^3/(T/K) - 9.3387 \cdot \log (T/K) + 2.7727 \times 10^{-3} \cdot (T/K) - 8.8315 \times 10^{-15} \cdot (T/K)^2$ , temp range  $198$ – $680\ K$  (Yaws 1994)

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

600 (calculated-P/C, Mackay & Shiu 1981)

617 (calculated- $C_A/C_w$ , Eastcott et al. 1988)

1689 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

1628.2 (modified EPICS method-GC, Ryu & Park 1999)

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

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

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

4.90 (recommended, Sangster 1989, 1993)

4.90 (recommended, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

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

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

Volatilization:

Photolysis:

Oxidation: rate constant  $k = 5.0 \times 10^4 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  for the reaction with ozone at 300 K (Lyman 1982).

Hydrolysis:

Biodegradation:

Bioconcentration:

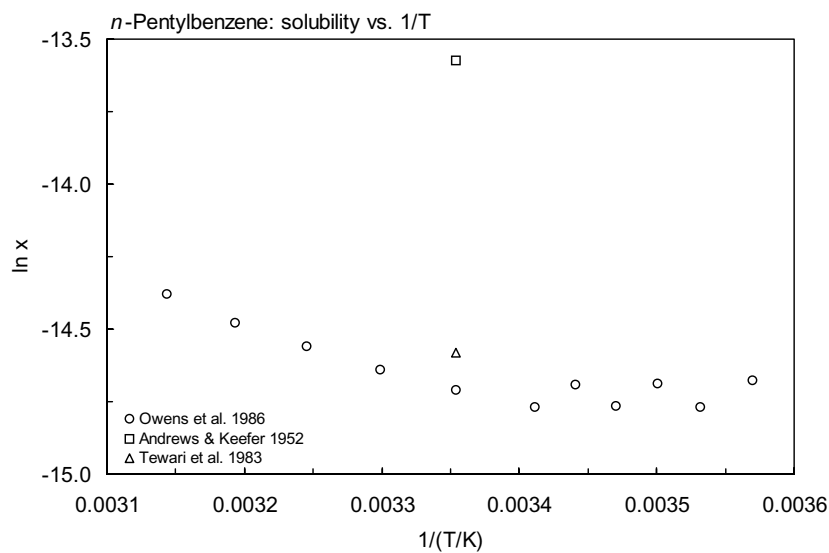
Half-Lives in the Environment:

**TABLE 3.1.1.24.1**

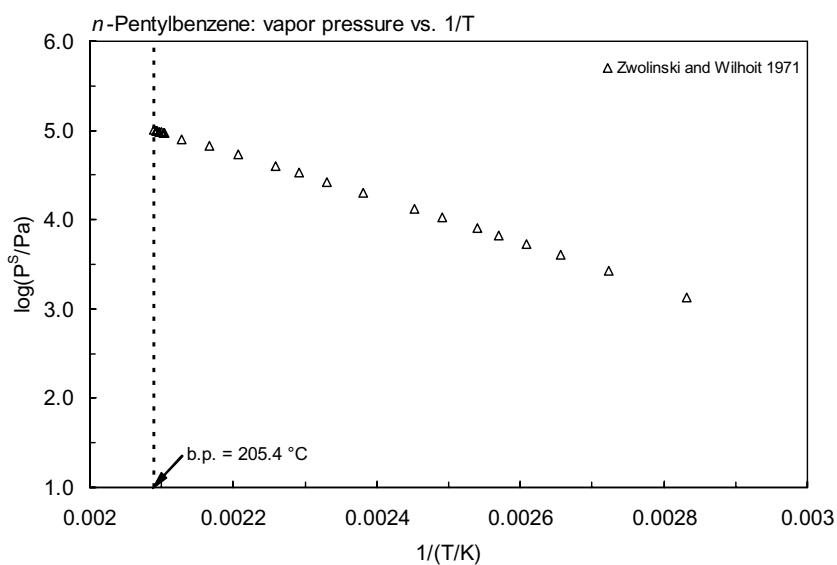
**Reported aqueous solubilities and vapor pressures of *n*-pentylbenzene at various temperatures**

Aqueous solubility		Vapor pressure			
Owens et al. 1986		Zwolinski & Wilhoit 1971			
generator column-HPLC		selected values			
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{P/Pa}$	$t/^{\circ}\text{C}$	$\text{P/Pa}$
7	3.48	80	1333	283.18	95992
10	3.18	94	2666	203.16	97325
12.5	3.44	103.3	4000	204.33	98659
15	3.19	110.3	5333	204.9	99992
17.5	3.43	115.87	6666	205.46	101325
20	3.18	120.6	7999		
25	3.37	128.36	10666	$\log P = A - B/(C + t/^{\circ}\text{C})$	
30	3.61	134.65	13332	Antoine eq.	P/mmHg
35	3.92	146.73	19998	A	6.97833
40	4.25	155.85	26664	B	1639.91
45	4.69	163.27	33331	C	194.76
		169.57	39997		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.50$		179.97	53329	bp/ $^{\circ}\text{C}$	205.46
at $25^{\circ}\text{C}$		188.45	66661	$\Delta H_v/(\text{kJ mol}^{-1})$	
		196.68	79993	at $25^{\circ}\text{C}$	55.06
		202	93326	at $25^{\circ}\text{C}$	41.21
		202.59	94659		



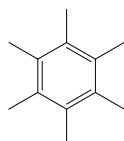


**FIGURE 3.1.1.24.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *n*-pentylbenzene.



**FIGURE 3.1.1.24.2** Logarithm of vapor pressure versus reciprocal temperature for *n*-pentylbenzene.

## 3.1.1.25 Hexamethylbenzene



Common Name: *n*-Hexamethylbenzene

Synonym: mellitene

Chemical Name: *n*-hexamethylbenzene

CAS Registry No: 87-95-4

Molecular Formula:  $C_{12}H_{18}$ ,  $C_6(CH_3)_6$

Molecular Weight: 162.271

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

165.5 (Lide 2003)

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

263.4 (Weast 1982–83)

Density ( $g/cm^3$  at  $25^{\circ}C$ ):

1.063 (Weast 1982–83)

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

152.6 ( $25^{\circ}C$ , calculated-density)

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

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

20.46 (Tsonopoulos & Prausnitz 1971)

1.76, 20.63; 22.38 ( $110.5$ ,  $165.55^{\circ}C$ ; total phase change enthalpy, Chickos et al. 1999)

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

46.44 (Tsonopoulos & Prausnitz 1971)

51.6, 47.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ,  $F: 0.042$  ( $mp = 166.5^{\circ}C$ ))

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

0.235 (generator column-GC, Doucette & Andren 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):

1.004\* ( $41.07^{\circ}C$ , transpiration method, measured range  $41$ – $90.5^{\circ}C$ , Overberger et al. 1969)

0.28\* ( $30^{\circ}C$ , diaphragm pressure gauge, measured range  $30$ – $70^{\circ}C$ , Ambrose et al. 1976)

0.160 (calculated-vapor pressure eq., Ambrose et al. 1976)

$\log(P/Pa) = 13.134 - 3855/[(T/K) - 21]$ ; temp range  $202$ – $343\ K$  (diaphragm pressure gauge measurements, Antoine eq., Ambrose et al. 1976)

$\log(P/atm) = (1 - 571.163/T) \times 10^{(1.00973 - 5.04725 \times 10^{-4} \cdot T - 6.310130 \times 10^{-7} \cdot T^2)}$ ;  $T$  in  $K$ , temp range  $303.1$ – $343.02\ K$  (Cox vapor pressure eq., Chao et al. 1983)

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

$\log(P_s/kPa) = 8.6223 - 2965.633/(-59.583 + T/K)$ ; temp range  $303$ – $343\ K$  (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.89588 - 1629.9/(-118.46 + T/K)$ ; temp range  $443$ – $537\ K$  (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

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

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

4.61 (generator column-HPLC, Wasik et al. 1982)

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

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

4.60 (shake flask/slow stirring-GC, Brooke et al. 1986)

- 4.60, 4.88 (reversed phase HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 4.75 (recommended, Sangster 1989)  
 4.95 (normal phase HPLC- $k'$  correlation, Govers & Evers 1992)  
 5.11 (recommended, Sangster 1993)  
 4.61 (recommended, Hansch et al. 1995)

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

- 6.31 (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,  $t_{1/2}$ :

Volatilization:

Photolysis:

Oxidation: rate constant  $k = 2.4 \times 10^5 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$  for the reaction with ozone at 300K (Lyman et al. 1982)

Hydrolysis:

Biodegradation:

Bioconcentration

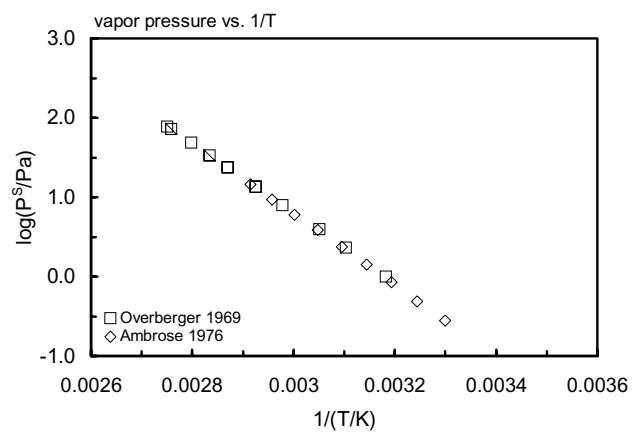
Half-Lives in the Environment:

**TABLE 3.1.1.25.1**

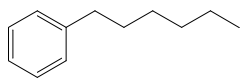
**Reported vapor pressures of hexamethylbenzene at various temperatures and the coefficients for the vapor pressure equations**

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

Overberger et al. 1969		Ambrose et al. 1976	
transpiration method		diaphragm gauge	
$t/^{\circ}\text{C}$	$P/\text{Pa}$	$t/^{\circ}\text{C}$	$P/\text{Pa}$
41.07	1.004	29.95	0.28
49.11	2.306	35.07	0.49
54.68	3.912	40.02	0.85
62.62	8.015	44.96	1.41
68.71	13.62	49.95	2.34
68.72	13.58	55.04	3.81
75.21	23.71	59.95	6.05
75.33	23.79	64.91	9.39
79.75	33.69	69.87	14.4
79.75	33.5		
84.2	48.3	mp/ $^{\circ}\text{C}$	165.55
89.46	72		
89.48	72.16	eq. 3	$P/\text{Pa}$
90.54	77.91	A	13.134
		B	3855
		C	-21.0



**FIGURE 3.1.1.25.1** Logarithm of vapor pressure versus reciprocal temperature for *n*-hexamethylbenzene.

3.1.1.26 *n*-Hexylbenzene

Common Name: *n*-Hexylbenzene

Synonym: 1-phenylhexane, hexylbenzene

Chemical Name: *n*-hexylbenzene

CAS Registry No: 1077-16-3

Molecular Formula:  $C_{12}H_{18}$ ,  $C_6H_5(CH_2)_5CH_3$

Molecular Weight: 162.271

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

−61.0 (Dreisbach 1955; Lide 2003)

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

226.1 (Lide 2003)

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

0.8613 (Weast 1982–83)

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

188.4 ( $20^{\circ}C$ , calculated from density)

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

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

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

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

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

0.995\* (generator column-HPLC, measured range  $5$ – $29^{\circ}C$ , May et al. 1983)

0.902\* (generator column-HPLC/UV, measured range  $7$ – $45^{\circ}C$ , Owens et al. 1986)

$\ln x = -429.463 + 18024.83/(T/K) + 61.9402 \cdot \ln (T/K)$ ; temp range  $290$ – $400\ K$  (eq. derived from literature calorimetric and solubility data, Tsionopoulos 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):

14.01 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.18284 - 1813.74/(195.5 + t/^{\circ}C)$ ; temp range  $120$ – $290^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log (P/mmHg) = 6.9853 - 1700.5/(188.2 + t/^{\circ}C)$ ; temp range  $96$ – $258^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

10.52\* ( $20.51^{\circ}C$ , static method, measured range  $273.73$ – $462.97\ K$ , Kasehgari et al. 1993)

$\log (P/kPa) = 6.50020 - 1946.435/(208.935 + t/^{\circ}C)$ ; temp range  $273.73$ – $462.97\ K$  (static method, Kasehgari et al. 1993)

$\log (P/mmHg) = 6.7694 - 3.6050 \times 10^3/(T/K) + 3.3416 \cdot \log (T/K) - 1.5306 \times 10^{-2} \cdot (T/K) + 7.8479 \times 10^{-6} \cdot (T/K)^2$ , temp range  $212$ – $698\ K$  (Yaws 1994)

10.52\* ( $20.51^{\circ}C$ , measured range  $263.88$ – $462.97\ K$ , Mokbel et al. 1998)

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

1977 (calculated- $C_A/C_W$ , Eastcott et al. 1988)

2172 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

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

5.25 (calculated-fragment const., Rekker 1977)

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

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

- 5.45, 5.25 (quoted of HPLC methods, Harnisch et al. 1983)  
 5.26, 5.62 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)  
 5.52 (recommended, Sangster 1989, 1993)  
 5.52 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

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

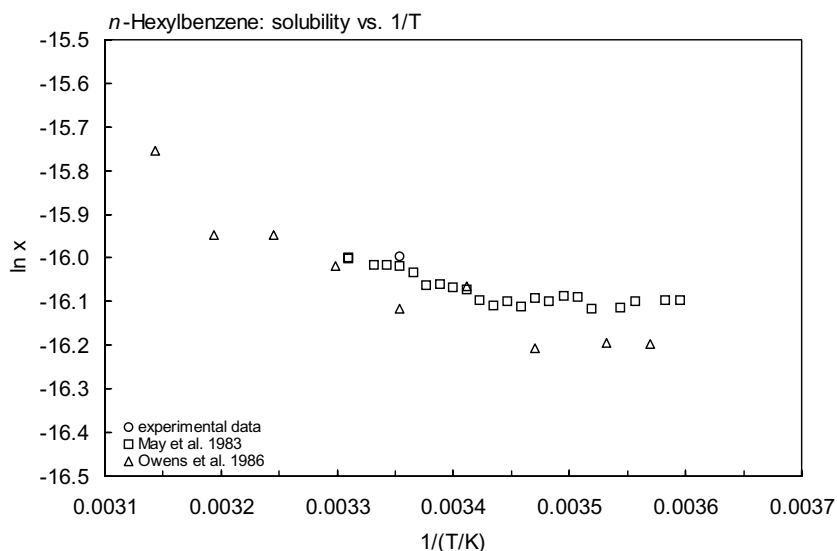
Environmental Fate Rate Constants,  $k$ , or Half-Lives,  $t_{1/2}$ :

Half-Lives in the Environment:

**TABLE 3.1.1.26.1**

**Reported aqueous solubilities of *n*-hexylbenzene at various temperatures**

May et al. 1983				Owens et al. 1986	
generator column-HPLC				generator column-HPLC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
5	0.921	20	0.043	7	0.834
6	0.921	21	0.949	10	0.836
8	0.92	22	0.956	15	0.826
9	0.996	23	0.953	20	0.951
11	0.904	24	0.983	25	0.902
12	0.928	25	0.995	30	0.996
13	0.93	26	0.999	35	1.069
14	0.92	27	0.999	40	1.069
15	0.925	29	1.012	45	1.298
16.01	0.908	29	1.016		
17	0.919				
18	0.91	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 7.60$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 8.0$	
19	0.921	at $25^{\circ}\text{C}$		at $25^{\circ}\text{C}$	



**FIGURE 3.1.1.26.1** Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for *n*-hexylbenzene.

TABLE 3.1.1.26.2

Reported vapor pressures of *n*-hexylbenzene at various temperatures and the coefficients for the vapor pressure equations

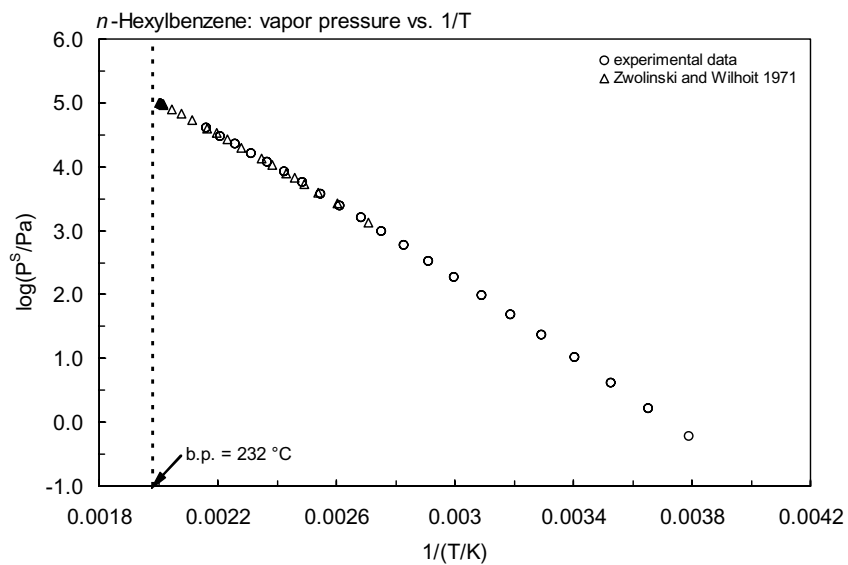
$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

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

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

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

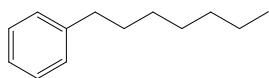
Zwolinski & Wilhoit 1971		Kasehgari et al. 1993		Mokbel et al. 1998	
selected values		static method		static method	
t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
96	1333	273.73	1.653	263.88	0.609
111	2666	283.63	4.239	273.73	1.648
121	4000	293.66	10.52	283.63	4.236
128	5333	303.64	23.20	293.66	10.52
133.5	6666	313.62	48.66	303.64	23.20
138.4	7999	323.59	97.32	313.62	48.72
146.4	10666	333.58	184.9	323.59	97.36
152.9	13332	343.57	336.63	333.58	185.0
165.4	19998	353.58	589.1	343.57	336.0
174.8	26664	363.58	997.8	353.58	589.0
182.5	33331	372.84	1606	363.58	998.0
189.0	39997	382.77	2519	372.84	1606
199.8	53329	392.70	3841	382.77	2520
208.5	66661	402.74	5722	392.70	3841
216.0	79993	412.76	8320	402.74	5722
222.5	93326	422.76	11828	412.76	8321
223.1	94659	432.75	16516	422.76	11829
223.7	95992	442.89	22640	432.75	16517
224.3	97325	452.83	30575	442.80	22641
224.9	98659	462.97	40693	452.83	30576
225.5	99992			462.79	40694
226.1	101325	eq. 2	P/kPa		
		A	6.50020	data fitted to Wagner eq.	
Antoine eq.	P/mmHg	B	1946.435		
A	6.9853	C	208.935		
B	1700.5				
C	1882.2				
bp/°C	226.1				
$\Delta H_v/(\text{kJ mol}^{-1}) =$					
at 25°C	60				
at bp	43.1				



**FIGURE 3.1.1.26.2** Logarithm of vapor pressure versus reciprocal temperature for *n*-hexylbenzene.



## 3.1.1.27 Heptylbenzene



Common Name: Heptylbenzene

Synonym: 1-phenylheptane

Chemical Name: *n*-heptylbenzene

CAS Registry No: 1078-71-3

Molecular Formula:  $C_{13}H_{20}$ ,  $C_6H_5(CH_2)_6CH_3$

Molecular Weight: 176.298

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

−48 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

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

240 (Lide 2003)

Density ( $g/cm^3$ ):

0.8567 ( $20^{\circ}C$ , Weast 1982–83)

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

205.8 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

0.686; 0.925 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

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

133.3\* ( $66.2^{\circ}C$ , summary of literature data, temp range  $66.2$ – $233^{\circ}C$ , Stull 1947)

1333\* ( $112^{\circ}C$ , derived from compiled data, temp range  $112$ – $246^{\circ}C$ , Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0006 - 1761.2/(181.5 + t/^{\circ}C)$ ; temp range  $112$ – $279^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.1255 - [1761.2/(T - 91.65)]$ ; temp range  $423$ – $527$  K (liquid, Antoine equation, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 89.2811 - 6.4093 \times 10^3/(T/K) - 29.248 \cdot \log(T/K) + 1.0328 \times 10^{-2} \cdot (T/K) + 6.2451 \times 10^{-14} \cdot (T/K)^2$ , temp range  $225$ – $714$  K (Yaws 1994)

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

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

5.768 (HPLC- $k'$  correlation, Hanai & Hubert 1981)

5.37 (HPLC- $k'$  correlation, Ritter et al. 1995)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

TABLE 3.1.1.27.1

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

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

Stull 1947		Zwolinski & Wilhoit 1971			
summary of literature data		selected values			
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
66.2	133.3	112	1333	243	94659
94.8	666.6	128	2666	243.6	95992
109	1333	137	4000	244.2	97325
124.2	2666	145	5333	244.8	98659
141.6	5333	150.7	6666	245.4	99992
151.5	7999	155.7	7999	246	101325
165.7	13332	164	10666		
186.6	26664	170.7	13332	eq. 2	P/mmHg
210	53329	183.6	19998	A	6.97833
233	101325	193.3	26664	B	1639.91
		201.1	33331	C	194.76
mp/ $^{\circ}\text{C}$	-	207.8	39997		
		218.9	53329	bp/ $^{\circ}\text{C}$	205.46
		227.9	66661	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
		235.6	79993	at 25 $^{\circ}\text{C}$	55.06
		242.3	93326	at bp	41.21

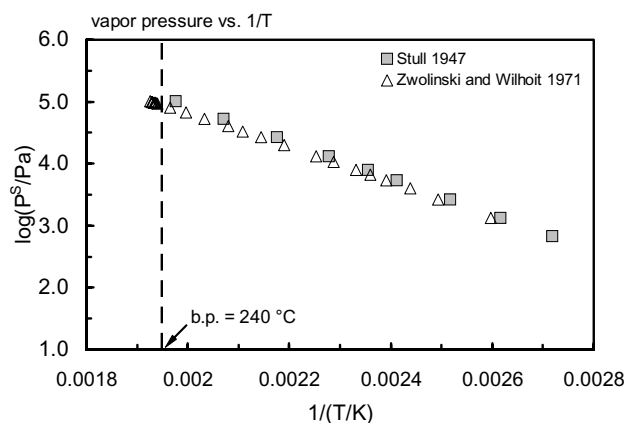
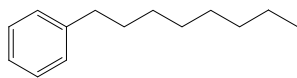


FIGURE 3.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for heptylbenzene.

3.1.1.28 *n*-Octylbenzene

Common Name: *n*-Octylbenzene

Synonym: 1-phenyloctane, octylbenzene

Chemical Name: *n*-octylbenzene

CAS Registry No: 2189-60-8

Molecular Formula:  $C_{14}H_{22}$ ,  $C_6H_5(CH_2)_7CH_3$

Molecular Weight: 190.325

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

−36 (Lide 2003)

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

264 (Lide 2003)

Density ( $g/cm^3$ ):

0.8582 (20 $^{\circ}C$ , Weast 1982–83)

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

222.2 (20 $^{\circ}C$ , calculated-density)

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

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

29.96 (Chickos et al. 1999)

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

127.91, 110.4 (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 $^{\circ}C$ ):

0.219; 0.204 (calculated-regression eq.; calculated-molar volume correlation, Wang et al. 1992)

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

1333\* (127 $^{\circ}C$ , derived from compiled data, temp range 127–264.4 $^{\circ}C$ , Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0086 - 1812.2/(174.6 + t/^{\circ}C)$ ; temp range 127–298 $^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

7.666\* (43 $^{\circ}C$ , gas saturation, measured range 43–125.6 $^{\circ}C$ , Allemand et al. 1986)

$\log(P/kPa) = 8.35571 - 3293.744/(T/K)$ ; temp range 368–400 K (liquid, Antoine equation, Stephenson & Malanowski 1987)

1.15\* (20.01 $^{\circ}C$ , static method, measured range 293.16–462.87 K, Kasehgari et al. 1993)

$\log(P/kPa) = 6.50210 - 2183.874/(207.887 + t/^{\circ}C)$ ; temp range 293.16–462.87 K (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = 1.8919 - 4.1324 \times 10^3/(T/K) + 6.1473 \cdot \log(T/K) - 2.0294 \times 10^{-2} \cdot (T/K) + 9.6879 \times 10^{-6} \cdot (T/K)^2$ , temp range 237–729 K (Yaws 1994)

1.105\* (20.34 $^{\circ}C$ , static method, measured range 293.49–462.87 K, Mokbel et al. 1998)

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

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

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

6.52, 6.29 (RP-HPLC- $k'$  correlation, Harnisch et al. 1982)

6.297 (HPLC- $k'$  correlation, Hanai & Hubert 1984)

6.35, 6.85 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)

6.30 (recommended, Sangster 1993)

5.89 (HPLC- $k'$  correlation, Ritter et al. 1995)

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

Bioconcentration Factor, log BCF or log  $K_B$ :

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

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

Half-Lives in the Environment:

**TABLE 3.1.1.28.1**

**Reported vapor pressures of octylbenzene 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)					
Zwolinski & Wilhoit 1971		Allemand et al. 1986		Kasehgari et al. 1993		Mokbel et al. 1998	
selected values		gas saturation		static method		static method	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
127	1333	43.0	7.666	293.16	1.15	293.49	1.105
143	2666	52.43	14.8	303.13	3.01	313.49	2.690
153	4000	72.75	66.8	313.01	6.87	303.48	6.316
161	5333	84.2	134.7	323.01	15.3	23.47	13.92
166.7	6666	95.39	262.7	333.15	31.5	333.48	28.76
171.9	7999	106.0	437.3	343.15	60.8	343.45	57.64
180.4	10666	125.64	1205	353.13	114	353.45	109.0
187.2	13332			363.14	207	363.42	198.0
200.3	19998			373.22	362	373.45	350.0
210.4	26664			383.25	609	403.00	1513
218.4	33331			393.32	994	412.96	2329
225.3	39997			403.33	1574	422.92	3504
236.7	53329			412.96	2329	432.94	5143
235.9	66661			422.92	3504	442.96	7395
253.8	79993			432.94	5143	452.90	10366
260.7	93326			442.96	7395	462.87	14266
261.9	95992			452.90	10370		
263.2	98659			462.87	14270		data fitted to Wagner eq.
264.4	101325						
				Antoine eq.			
eq. 2	P/mmHg			eq. 2	P/kPa		
A	7.0086			A	6.50210		
B	1812.2			B	2183.874		
C	174.6			C	207.887		
bp/°C	264.4						
ΔH <sub>v</sub> /(kJ mol <sup>-1</sup> ) =							
at 25°C	69.96						
at bp	46.9						

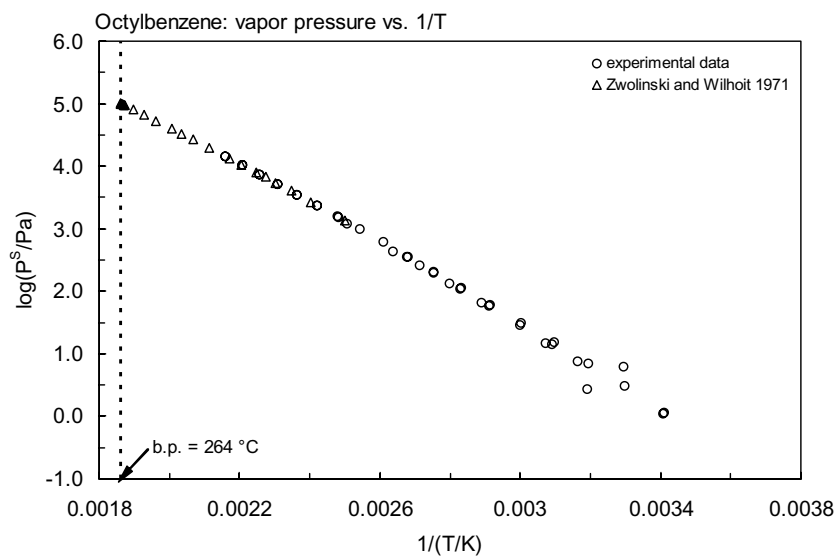
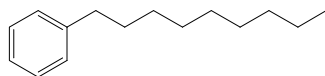


FIGURE 3.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for octylbenzene.

## 3.1.1.29 Nonylbenzene



Common Name: Nonylbenzene

Synonym: 1-phenylnonane

Chemical Name: *n*-nonylbenzene

CAS Registry No: 1081-77-2

Molecular Formula:  $C_{15}H_{24}$ ,  $C_6H_5(CH_2)_8CH_3$

Molecular Weight: 204.352

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

-24 (Dreisbach 1955; Lide 2003)

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

280.5 (Lide 2003)

Density ( $g/cm^3$ ):

0.8558, 0.8522 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

0.8584 ( $20^{\circ}C$ , Weast 1982-83)

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

238.1 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

0.0725; 0.112 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

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

0.573 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.19041 - 1991.0/(180.0 + t/^{\circ}C)$ ; temp range  $165-330^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1333\* ( $142^{\circ}C$ , derived from compiled data, temp range  $142-282^{\circ}C$ , Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0245 - 1862.6/(167.5 + t/^{\circ}C)$ ; temp range  $142-316^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

2.906\* ( $43^{\circ}C$ , gas saturation, measured range  $43-142^{\circ}C$ , Allemand et al. 1986)

0.338 (GC-RT correlation, Sherblom et al. 1992)

$\log(P/mmHg) = -0.9235 - 4.2232 \times 10^3/(T/K) + 7.3073 \cdot \log(T/K) - 2.0964 \times 10^{-2} \cdot (T/K) + 9.7152 \times 10^{-6} \cdot (T/K)^2$ , temp range 249-741 K (Yaws 1994)

0.8747\* ( $30.52^{\circ}C$ , static method, measured range  $313.67-466.46 K$ , Mokbel et al. 1998)

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

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

6.828 (HPLC- $k'$  correlation, Hanai & Hubert 1981)

6.83, 7.40 (RP-HPLC- $k'$  correlations, Sherblom & Eganhouse 1988)

7.11 (recommended, Sangster 1993)

6.41 (HPLC- $k'$  correlation, Ritter et al. 1995)

6.83 (quoted from Sherblom & Eganhouse 1988, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

TABLE 3.1.1.29.1  
Reported vapor pressures of nonylbenzene 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)							
Zwolinski & Wilhoit 1971				Allemand et al. 1986		Mokbel et al. 1998	
selected values				gas saturation		static method	
t/°C	P/Pa			t/°C	P/Pa	T/K	P/Pa
142	1333	eq. 2	P/mmHg	43	2.906	303.67	0.8474
158	2666	A	7.0245	50	5.186	313.65	2.271
168	4000	B	1862.6	59	10.36	323.67	5.369
176	5333	C	167.5	64	15.07	333.61	12.07
182.3	6666			74.32	31.73	343.53	25.20
187.5	7999	bp/°C	282.0	85.0	64.26	351.83	44.97
196.2	10666	$\Delta H_v/(kJ\ mol^{-1})$		91.3	95.33	361.84	85.44
203.2	13332	at 25°C	74.81	98.28	146.7	371.75	155
216.7	19998	at bp	49.0	108.57	260.0	381.65	270
226.8	26664			120.0	480.0	391.62	459
235.1	33331			130.73	780.0	401.56	752
247.1	39997			142.0	1352	411.48	1207
253.7	53329					411.60	1203
263.1	66661					421.45	1881
271.1	79993					431.44	2835
278.2	93326					441.49	4201
279.5	95992					451.48	6053
280.7	98659					461.48	8591
282	101325					466.46	10099

data fitted to Wagner eq.

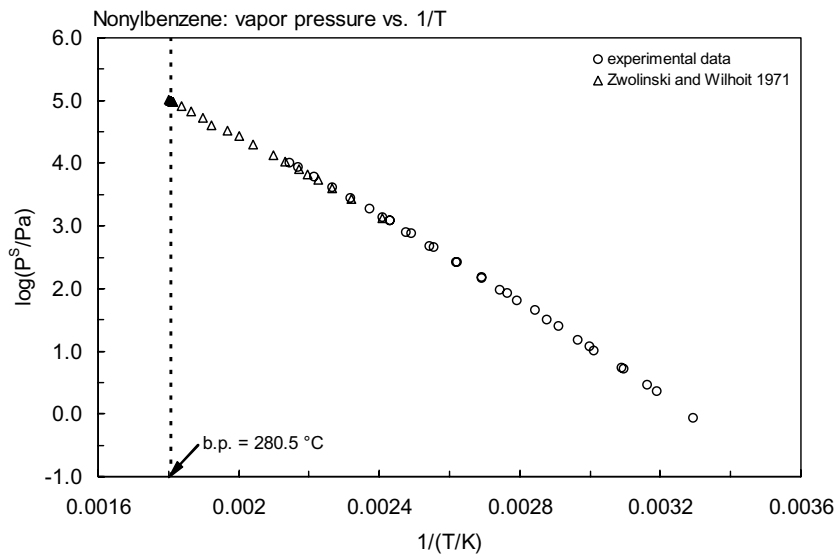
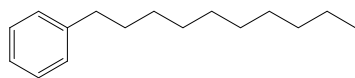


FIGURE 3.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for nonylbenzene.

## 3.1.1.30 Decylbenzene



Common Name: Decylbenzene

Synonym: 1-phenyldecane

Chemical Name: *n*-decylbenzene

CAS Registry No: 104-72-3

Molecular Formula:  $C_{16}H_{26}$ ,  $C_6H_5(CH_2)_9CH_3$

Molecular Weight: 218.337

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

-14.4 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)

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

293 (Lide 2003)

Density ( $g/cm^3$ ):

0.85553, 0.85189 (20 $^{\circ}C$ , 25 $^{\circ}C$ , Camin et al. 1954; Dreisbach 1955)

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

255.3 (20 $^{\circ}C$ , calculated-density)

318.0 (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 $^{\circ}C$ , F: 1.0

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

2.50 (vapor-phase saturation, shake flask-GC, Sherblom et al. 1992)

5.59, 8.47, 10.55 (calculated- $V_M$ ,  $K_{ow}$ , TSA, Sherblom et al. 1992)

0.023; 0.0188 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

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

8329\* (202.987 $^{\circ}C$ , ebulliometry, measured range 202.987–297.799 $^{\circ}C$ , Camin et al. 1954)

$\log(P/mmHg) = 7.03642 - 1904.132/(160.318 + t/^{\circ}C)$ ; temp range 202.9–297.9 $^{\circ}C$  (Antoine eq., manometer measurements, Camin et al. 1954)

0.20 (extrapolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.27177 - 2107.7/(180.0 + t/^{\circ}C)$ ; temp range 185–345 $^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1333\* (155.1 $^{\circ}C$ , derived from compiled data, temp range 155.1–297.89 $^{\circ}C$ , Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.03642 - 1904.132/(160.318 + t/^{\circ}C)$ ; temp range 155.1–322.9 $^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.16274 - 1905.56/(160.503 + t/^{\circ}C)$ ; temp range 203–297.8 $^{\circ}C$  (Antoine eq. from reported exptl. data of Camin et al. 1954, Boublik et al. 1984)

$\log(P/kPa) = 4.03653 - 876.208/(T/K - 203.15)$ ; temp range 317–427 K (liquid, Antoine equation, Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.15658 - [1900.916/(T/K - 113.16)]$ ; temp range 475–571 K (liquid, Antoine equation, Stephenson & Malanowski 1987)

0.133, 0.127 ( $P_L$ , GC-RT correlation, Sherblom et al. 1992)

0.707\* (39.85 $^{\circ}C$ , static method, measured range 313.0–433.23 K, Kasehgari et al. 1993)

$\log(P/kPa) = 6.37655 - 2098.329/(180.620 + t/^{\circ}C)$ ; temp range 313.0–433.23 K (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = -4.4754 - 4.4669 \times 10^3/(T/K) + 9.1965 \cdot \log(T/K) - 2.4010 \times 10^{-2} \cdot (T/K) + 1.0848 \times 10^{-5} \cdot (T/K)^2$ , temp range 259–753 K (Yaws 1994)



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

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

- 7.35 (RP-TLC retention time correlation, Bruggeman et al. 1982)
- 7.60, 7.33 (RP-HPLC-k' correlations, Harnisch et al. 1982)
- 7.358 (HPLC-k' correlation, Hanai & Hubert 1984)
- 7.37, 8.01 (RP-HPLC-k' correlation, Sherblom & Eganhouse 1988)
- 7.38 (HPLC-k' correlation, Sherblom et al. 1992)
- 7.35 (recommended, Sangster 1993)
- 6.94 (HPLC-k' correlation, Ritter et al. 1995)
- 7.37 (quoted from Sherblom & Eganhouse 1988, Hansch et al. 1995)

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>:

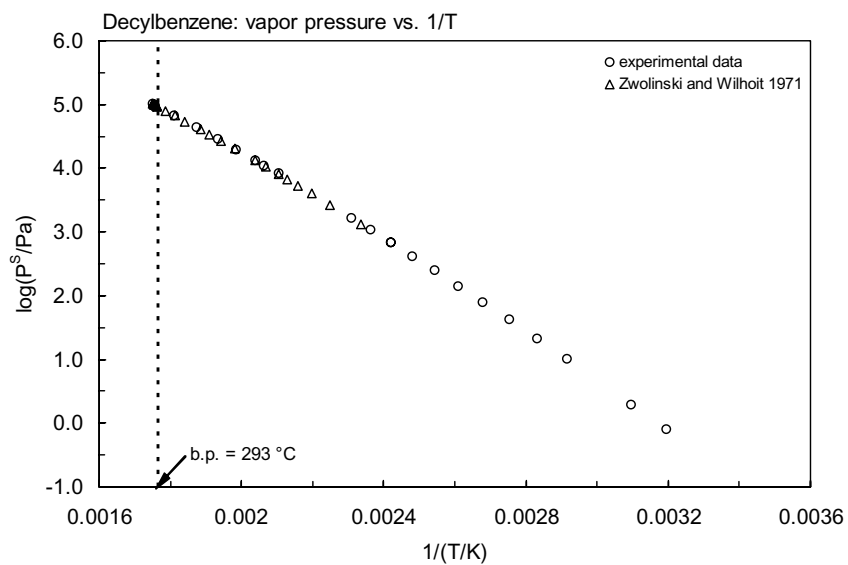
Environmental Fate Rate Constants, k, and Half-Lives, t<sub>1/2</sub>:

Half-Lives in the Environment:

**TABLE 3.1.1.30.1**

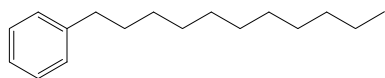
**Reported vapor pressures of decylbenzene at various temperatures and the coefficients for the vapor pressure equations**

$\log P = A - B/(T/K)$		(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)					
Camin et al. 1954		Zwolinski & Wilhoit 1971				Kasehgari et al. 1993	
ebulliometry		selected values				static method	
t/°C	P/Pa	t/°C	P/Pa			T/K	P/Pa
202.987	8329	155.1	1333	eq. 2	P/mmHg	313.0	0.797
211.392	10938	171.7	2666	A	7.03642	323.13	1.92
217.156	13088	182.19	4000	B	1904.132	343.15	10.3
230.476	19442	190.07	5333	C	160.318	353.11	21.6
244.331	28555	196.431	6666			363.12	41.9
260.372	43172	201.803	7999	bp/°C	297.89	373.25	78.5
278.950	67077	210.617	10666	$\Delta H_v/(kJ\ mol^{-1}) =$		383.28	142
296.370	98146	217.755	13332	at 25°C	79.75	393.34	248
297.799	101113	231.452	19998	at bp	50.6	403.37	417
		241.789	26664			413.33	683
bp/°C	297.083	250.19	33331			413.33	684
		257.18	39997			423.21	1081
		269.86	53329			433.23	1687
		278.68	66661				
		286.843	79993				
		293.986	93326			Antoine eq	
		295.969	95992			eq. 2	P/kPa
		296.616	98659			A	6.37655
		297.89	101325			B	2098.329
						C	180.620



**FIGURE 3.1.1.30.1** Logarithm of vapor pressure versus reciprocal temperature for decylbenzene.

### 3.1.1.31 Undecylbenzene



Common Name: Undecylbenzene

Synonym: 1-phenylundecane

Chemical Name: *n*-undecylbenzene

CAS Registry No: 6742-54-7

Molecular formula:  $C_{17}H_{28}$ ,  $C_6H_5(CH_2)_{10}CH_3$

Molecular Weight: 232.404

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

-5.0 (Dreisbach 1955; Lide 2003)

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

316 (Dreisbach 1955; Lide 2003)

Density ( $g/cm^3$ ):

0.8553, 0.8517 (20 $^{\circ}C$ , 25 $^{\circ}C$ , Dreisbach 1961)

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

271.7 (20 $^{\circ}C$ , calculated-density)

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

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

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

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

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

0.00702; 0.00377 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

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

0.080 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.34672 - 2215.1/(180.0 + t/^{\circ}C)$ ; temp range 195–375 $^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1333\* (168 $^{\circ}C$ , derived from compiled data, temp range 168–313.2 $^{\circ}C$ , Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0509 - 1944.1/(153.0 + t/^{\circ}C)$ ; temp range 168–349 $^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

0.050, 0.047 ( $P_L$ , GC-RT correlation, Sherblom et al. 1992)

$\log(P/mmHg) = 124.1549 - 8.8970 \times 10^3/(T/K) - 41.223 \cdot \log(T/K) + 1.3662 \times 10^{-2} \cdot (T/K) - 8.1321 \times 10^{-14} \cdot (T/K)^2$ , temp range 268–764 K (Yaws 1994)

0.7156\* (50.42 $^{\circ}C$ , static method, measured range 323.57–467.33 $^{\circ}C$ , data fitted to Wagner eq., Mokbel et al. 1998)

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

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

8.14 (RP-HPLC-RT correlation, Sherblom et al. 1992, quoted, Sangster 1993)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

TABLE 3.1.1.31.1

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

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

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

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

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

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

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

Zwolinski & Wilhoit 1971				Mokbel et al. 1998			
selected values				static method			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
168	1333	309.2	93326	323.57	0.7156	462.28	3088
185	2666	310.6	95992	333.59	1.820	467.33	37726
196	4000	311.9	98659	343.71	4.304		
204	5333	313.2	101325	352.69	9.405	data fitted to Wagner eq.	
210.3	6666			363.78	19.39		
215.7	7999	eq. 2	P/mmHg	372.07	34.36		
224.7	10666	A	7.0590	382.06	64.41		
231.9	13332	B	1944.1	392.06	117		
245.8	19998	C	153.0	402.11	204		
256.3	26664			412.11	344		
264.8	33331	bp/°C	313.2	422.09	564		
272.1	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$		422.19	568		
284	53329	at 25°C	84.68	432.25	908		
293.7	66661	at bp	52.3	442.27	1369		
302	79993			452.29	2080		

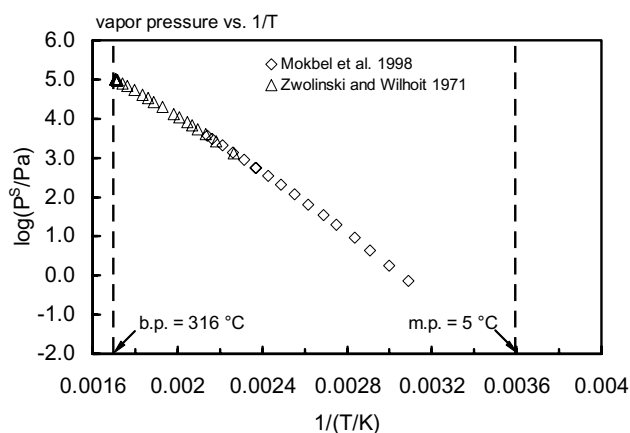
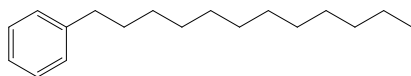


FIGURE 3.1.1.31.1 Logarithm of vapor pressure versus reciprocal temperature for undecylbenzene.

## 3.1.1.32 Dodecylbenzene



Common Name: Dodecylbenzene

Synonym: 1-phenyldodecane

Chemical Name: *n*-dodecylbenzene

CAS Registry No: 123-01-3

Molecular Formula:  $C_{18}H_{30}$ ,  $C_6H_5(CH_2)_{11}CH_3$

Molecular Weight: 246.431

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

3.0 (Dreisbach 1955; Lide 2003)

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

328 (Lide 2003)

Density ( $g/cm^3$ ):

0.8551, 0.8516 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

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

288.2 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

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):

26.66\* ( $78.4^{\circ}C$ , ebulliometry-McLeod gauge, measured range  $78.4$ – $288.6^{\circ}C$ , Myers & Fenske 1955)

0.032 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.41934 - 2319.2/(180.0 + t/^{\circ}C)$ ; temp range  $210$ – $385^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1333\* ( $181^{\circ}C$ , derived from compiled data, temp range  $181$ – $327.6^{\circ}C$ , Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0693 - 1981.6/(145.5 + t/^{\circ}C)$ ; temp range  $181$ – $363^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

1.08\* ( $53.7^{\circ}C$ , gas saturation, measured range  $53.7$ – $192.7^{\circ}C$ , Allemand et al. 1986)

0.019, 0.017 ( $P_L$ , GC-RT correlation, Sherblom et al. 1992)

0.727\* ( $69.771^{\circ}C$ , static method, measured range  $332.92$ – $453.26\ K$ , Kasehgari et al. 1993)

$\log(P/kPa) = 6.66087 - 2371.902/(182.311 + t/^{\circ}C)$ ; temp range  $332.92$ – $453.26\ K$  (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = 145.6916 - 1.0165 \times 10^3/(T/K) - 48.761 \cdot \log(T/K) + 1.5985 \times 10^{-2} \cdot (T/K) + 4.881 \times 10^{-13} \cdot (T/K)^2$ , temp range  $276$ – $774\ K$  (Yaws 1994)

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

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

8.65 (RP-HPLC- $k'$  correlation, Sherblom et al. 1992)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

TABLE 3.1.1.32.1

Reported vapor pressures of dodecylbenzene 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)					
Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Allemand et al. 1986		Kasehgari et al. 1993	
ebulliometry-McLeod gauge		selected values		gas saturation		static method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
78.4	26.66	181	1333	53.7	1.080	343.21	0.640
91.2	66.66	198	2666	86.19	6.733	353.26	1.61
102.3	133.3	209	4000	93.0	11.15	363.23	3.72
114.2	266.6	217	5333	103.0	21.60	363.23	3.73
122.4	400.0	223.5	6666	111.0	36.40	373.21	8.11
128.2	533.3	229.0	7999	124.02	79.86	383.22	16.9
133.4	666.6	238.1	10666	136.47	158.7	393.22	32.8
137.0	800	245.4	13332	160.44	540	403.27	59.5
143.5	1067	259.5	19998	192.71	1464	413.28	106
148.8	1333	270.1	26664			423.29	182
158.5	2000	278.7	33331			433.37	306
165.6	2666	286	39997			443.39	493
176.4	4000	298.1	53329			453.33	760
184.2	5333	307.9	66661			463.38	1167
191.0	6666	316.3	79993				
196.0	7999	323.6	93326				
205.5	10666	325	95992			Antoine eq	
212.0	13332	326.3	98659			eq. 2	P/kPa
225.4	19998	327.6	101325			A	6.66087
235.8	26664					B	2371.902
250.3	39997					C	182.311
262.0	53329	eq. 2	P/mmHg				
270.4	66661	A	7.0693				
278.2	79992	B	1981.6				
285.5	93326	C	145.5				
288.6	101325						
		bp/°C	327.6				
		$\Delta H_v/(\text{kJ mol}^{-1})$					
		at 25°C	89.62				
		at bp	54.4				

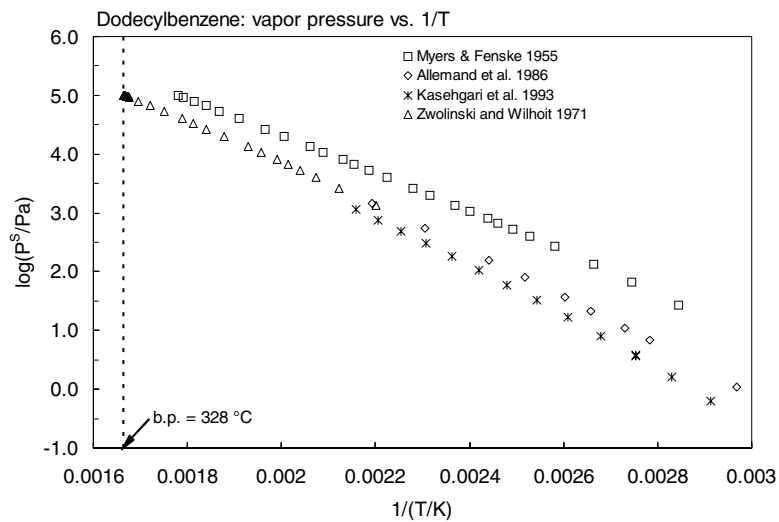
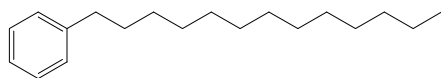


FIGURE 3.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for dodecylbenzene.

## 3.1.1.33 Tridecylbenzene



Common Name: Tridecylbenzene

Synonym: 1-phenyltridecane

Chemical Name: *n*-tridecylbenzene

CAS Registry No: 123-02-4

Molecular Formula:  $C_{19}H_{32}$ ,  $C_6H_5(CH_2)_{12}CH_3$

Molecular Weight: 260.457

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

10 (Dreisbach 1955; Lide 2003)

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

346 (Dreisbach 1955; Lide 2003)

Density ( $g/cm^3$ ):

0.8550, 0.8515 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

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

304.6 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

0.233 (vapor saturation-shake flask-GC, Sherblom et al. 1992)

0.233, 0.0885, 0.181 (calculated- $V_m$ ,  $K_{OW}$ , TSA, Sherblom et al. 1992)

0.00067; 0.00137 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

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

0.0125 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.49437 - 2626.7/(180.0 + t/^{\circ}C)$ ; temp range  $226-405^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1333\* ( $193^{\circ}C$ , derived from compiled data, temp range  $193-341.2^{\circ}C$ , Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0843 - 2013.9/(137.9 + t/^{\circ}C)$ ; temp range  $193-376^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

0.008, 0.07 ( $P_L$ , GC-RT correlation, Sherblom et al. 1992)

0.64\* ( $70.06^{\circ}C$ , static method, measured range  $343.21-463.38$  K, Kasehgari et al. 1993)

$\log(P/kPa) = 6.13410 - 2087.968/(153.790 + t/^{\circ}C)$ ; temp range  $343.21-463.38$  K (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = 160.3924 - 1.1093 \times 10^4/(T/K) - 53.875 \cdot \log(T/K) + 1.7532 \times 10^{-2} \cdot (T/K) + 3.727 \times 10^{-13} \cdot (T/K)^2$ , temp range  $283-783$  K (Yaws 1994)

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

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

9.36 (RP-HPLC- $k'$  correlation, Sherblom et al. 1992)

8.97; 8.54 (calculated-fragment const., calculated-molar volume correlation, Wang et al. 1992)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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



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

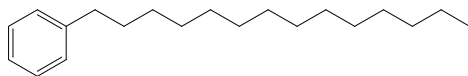
Half-Lives in the Environment:

**TABLE 3.1.1.33.1**

**Reported vapor pressures of tridecylbenzene at various temperatures**

Zwolinski & Wilhoit 1971				Kasehgari et al. 1993	
selected values				static method	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	T/K	P/Pa
193	1333	338.5	95992	343.20	$6.40 \times 10^{-4}$
210	2666	339.9	98659	353.26	$1.61 \times 10^{-3}$
221	4000	341.2	101325	363.23	$3.73 \times 10^{-3}$
229	5333			373.21	$8.11 \times 10^{-3}$
236	6666	$\log P = A - B/(C + t/^{\circ}\text{C})$		383.22	0.0169
242	7999		P/mmHg	393.22	0.0328
251	10666	A	7.0843	403.27	0.0595
258.2	13332	B	2013.9	413.28	0.106
271.6	19998	C	137.9	423.29	0.182
283.1	26664			433.37	0.306
291.8	33331	bp/ $^{\circ}\text{C}$	341.2	443.39	0.493
299.2	39997	$\Delta H_v/(\text{kJ mol}^{-1})$		453.33	0.760
311.4	53329	at $25^{\circ}\text{C}$	94.6	463.38	1.167
321.3	66661	at bp	56.1		
329.8	79993				
337.2	93326				

## 3.1.1.34 Tetradecylbenzene



Common Name: Tetradecylbenzene

Synonym: 1-phenyltetradecane

Chemical Name: *n*-tetradecylbenzene

CAS Registry No: 1459-10-5

Molecular Formula:  $C_{20}H_{34}$ ,  $C_6H_5(CH_2)_{13}CH_3$

Molecular Weight: 274.484

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

16 (Dreisbach 1955; Lide 2003)

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

359 (Dreisbach 1955; Lide 2003)

Density ( $g/cm^3$ ):

0.8549, 0.8514 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

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

321.7 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

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):

1333\* ( $205^{\circ}C$ , derived from compiled data, temp range  $205$ – $354^{\circ}C$ , Zwolinski & Wilhoit 1971)

0.0055 (extrapolated-Antoine eq., Dreisbach 1955; quoted, Sherblom et al. 1992)

$\log(P/mmHg) = 7.56143 - 2522.8/(180.0 + t/^{\circ}C)$ ; temp range  $235$ – $410^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = 7.101 - 2042/(130 + t/^{\circ}C)$ ; temp range  $205$ – $300^{\circ}C$  (Antoine eq., Zwolinski & Wilhoit 1971)

0.002 ( $P_L$ , GC-RT correlation, Sherblom et al. 1992)

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

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

9.95 (RP-HPLC- $k'$  correlation, Sherblom et al. 1992)

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

Bioconcentration Factor,  $\log BCF$  or  $\log K_B$ :

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

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

Half-Lives in the Environment:

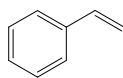
TABLE 3.1.1.34.1

Reported vapor pressures of tetradecylbenzene at various temperatures

Zwolinski &amp; Wilhoit 1971

selected values			
t/°C	P/Pa	t/°C	P/Pa
205	1333	351	95992
222	2666	353	98659
233	4000	354	101325
241	5333		
248	6666		
254	7999	log P = A - B/(C + t/°C)	
263	10666	eq. 2	P/mmHg
270	13332	A	7.010
285	19998	B	2042.0
295	26664	C	130.0
304	33331	bp/°C	354.0
312	39997	$\Delta H_v$ /(kJ mol <sup>-1</sup> )	
324	53329	at 25°C	99.6
334	66661	at bp	57.7
342	79993		
350	93326		

## 3.1.1.35 Styrene



Common Name: Styrene

Synonym: phenylethene, styrol, styrolene cinnamene, cinnamol, phenylethylene, vinylbenzene, ethenylbenzene

Chemical Name: styrene

CAS Registry No: 100-42-5

Molecular Formula:  $C_8H_8$ ,  $C_6H_5CH=CH_2$

Molecular Weight: 104.150

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

-30.65 (Lide 2003)

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

145 (Lide 2003)

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

0.9060, 0.9012 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach & Martin 1949; Dreisbach 1955; Riddick et al. 1986)

0.906 (Weast 1982-83)

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

115.0 ( $20^{\circ}C$ , calculated-density)

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

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

43.932, 38.7 ( $25^{\circ}C$ , bp, Riddick et al. 1986)

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

10.95 (Riddick et al. 1986; Chickos et al. 1999)

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

45.15, 52.2 (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  $25^{\circ}C$  or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \* are compiled at the end of this section):

330\* ( $24^{\circ}C$ , shake flask-Karl Fischer titration, measured range  $7-51^{\circ}C$ , Lane 1946)

310\* (cloud point method, measured range  $10-60^{\circ}C$ , Lane 1946)

220 (shake flask-method not specified, Friette & Hohenstein 1948)

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

160 (shake flask-HPLC/UV, Banerjee et al. 1980)

250\* (recommended best value, temp range  $10-60^{\circ}C$ , Shaw 1989b)

$\ln x = -19.471 - 1655.9/(T/K) - 4.6244 \times 10^{-5} \cdot (T/K)^2$ ; temp range  $5-50^{\circ}C$  (regression eq. of literature data, Shiu & Ma 2000)

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

288\* ( $8.2^{\circ}C$ , mercury manometer, measured range  $-7.7$  to  $8.2^{\circ}C$ , Linder 1931)

$\log (P/mmHg) = 7.929 - 2103/(T/K)$ ; temp range  $33.5-116.3^{\circ}C$  (isoteniscope method, Burchfield 1942)

841.3\* (static-Hg manometer, measured range  $12.5-60^{\circ}C$ , Pitzer et al. 1946)

969.4\* (calculated-Antoine eq. regression, Stull 1947)

$\log (P/mmHg) = 7.22302 - 1629.2/(230 + t/^{\circ}C)$  (Antoine eq., Dreisbach & Martin 1949)

6799\* ( $66.7^{\circ}C$ , mercury manometer, Buck et al. 1949)

$\log (P/mmHg) = -3151/(T/K) - 6.294 \cdot \log (T/K) + 26.92$ ; temp range  $80-120^{\circ}C$  (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)

807 (extrapolated by formula, Dreisbach 1955)

$\log (P/mmHg) = 6.92409 - 1430.0/(206.0 + t/^{\circ}C)$ ; temp range  $55-205^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

1093\* ( $29.92^{\circ}C$ , measured range  $29.92-110.06^{\circ}C$ , Dreyer et al. 1955)

1333\* ( $32.24^{\circ}C$ , measured range  $32.4-82.9^{\circ}C$ , Chaiyavech & van Winkle 1959)

- $\log (P/\text{mmHg}) = 8.2696 - 2221.21/(T/K)$ ; temp range 32.4–82.9°C (Chaiyavech & van Winkle 1959)  
 $\log (P/\text{mmHg}) = [-0.2185 \times 9634.7/(T/K)] + 7.922049$ ; temp range –7.0 to 145.2°C (Antoine eq., Weast 1972–73)  
 879, 812 (extrapolated-Antoine eq., Boublik et al. 1973)  
 $\log (P/\text{mmHg}) = 7.14016 - 1574.511/(224.087 + t/^\circ\text{C})$ ; temp range 32.4–62.19°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 $\log (P/\text{mmHg}) = 7.06623 - 1507.434/(214.985 + t/^\circ\text{C})$ ; temp range 29.92–144.77°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)  
 $\log (P/\text{atm}) = (1 - 418.675/T) \times 10^{(0.886470 - 8.14267 \times 10^4 \cdot T + 7.57896 \times 10^7 \cdot T^2)}$ ; T in K, temp range 281.35–417.92 K (Cox vapor pressure eq., Chao et al. 1983)  
 878, 811 (extrapolated-Antoine eq., Boublik et al. 1984)  
 $\log (P_L/\text{kPa}) = 6.235 - 1557.406/(222.538 + T/K)$ ; temp range 32.4–62.19°C (Antoine eq., Boublik et al. 1984)  
 $\log (P/\text{kPa}) = 6.18301 - 1501.162/(214.42 + t/^\circ\text{C})$ ; temp range 29.92–144.77°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)  
 879 (extrapolated, Antoine eq., Dean 1985, 1992)  
 $\log (P/\text{mmHg}) = 7.14016 - 1774.51/(224.09 + t/^\circ\text{C})$ ; temp range 32–82°C (Antoine eq., Dean, 1985, 1992)  
 841 (lit. average, Riddick et al. 1986)  
 $\log (P/\text{kPa}) = 6.34792 - 1629.20/(230.0 + t/^\circ\text{C})$ , temp range not specified (Antoine eq., Riddick et al. 1986)  
 880 (interpolated-Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 7.3945 - 2221.3/(T/K)$ ; temp range 245–334 K (Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P_L/\text{kPa}) = 6.08201 - 1445.58/(-63.72 + T/K)$ ; temp range 334–419 K (Antoine eq., Stephenson & Malanowski 1987)  
 $\log (P/\text{mmHg}) = 55.8621 - 4.024 \times 10^3/(T/K) - 17.609 \cdot \log (T/K) + 6.6842 \times 10^{-3} \cdot (T/K) + 1.9438 \times 10^{-13} \cdot (T/K)^2$ , temp range 243–648 K (Yaws 1994)  
 $\log (P/\text{kPa}) = 7.3945 - 2221.3/(T/K)$ ; 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):

- 233 (calculated-P/C, Mackay & Shiu 1990)  
 285, 527 (quoted, Howard et al. 1989)  
 267 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
 297 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)  
 261 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)  
 $\log K_{AW} = 5.628 - 1935/(T/K)$  (summary of literature data, Staudinger & Roberts 2001)

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

- 3.14 (calculated-fragment const., Rekker 1977)  
 2.95 (shake flask, Hansch & Leo 1979)  
 3.16 (shake flask-HPLC, Banerjee et al. 1980)  
 2.76 (HPLC-RT correlation Fujisawa & Masuhara 1981)  
 2.90 (HPLC-RT correlation, Wang et al. 1986)  
 3.05 (recommended, Sangster 1989, 1993)  
 2.95 (recommended, Hansch et al. 1995)

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

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

- 1.13 (goldfish, Ogata et al. 1984)

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

- 3.42–2.74 (Swann et al. 1983)  
 2.96, 2.71 (quoted exptl., calculated-MCI  $\chi$ , Meylan et al. 1992)

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

Volatilization: Volatilization and biodegradation may be dominant transport and transformation processes for styrene in water; calculated volatilization  $t_{1/2} = 3$  h from a river 1-m deep with a current speed of 1.0 m/s and wind velocity of 3 m/s (Howard 1989);

volatilized rapidly from shallow layers of lake water with  $t_{1/2} = 1$  to 3 h, but much slower from soil (Fu & Alexander 1992).

**Photolysis:**

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

$k_{O_3} = 1.8 \times 10^4 \text{ L mol}^{-1} \text{ s}^{-1}$  for the reaction with ozone at 30°C (Bufalini & Altshuller 1965)

$k_{O_3} = (22.6 \pm 4.6) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $296 \pm 2 \text{ K}$  (relative rate method, Atkinson et al. 1982)

$k_{OH} = 5.25 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson 1985)

$k_{O_3} = 22 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{OH} = (5.87 \pm 0.15) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{NO_3} = (1.51 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (Atkinson & Aschmann 1988)

$k_{OH} = 5.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1989)

$k_{O_3} = 1.71 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 296 K (Tuazon et al. 1993)

**Hydrolysis:** no hydrolyzable groups (Howard et al. 1991).

**Biodegradation:**  $t_{1/2}(\text{aerobic}) = 336\text{--}672 \text{ h}$ , based on unacclimated grab samples of aerobic soil and a subsurface sample;  $t_{1/2}(\text{anaerobic}) = 1344\text{--}2688 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

styrene will be rapidly destroyed by biodegradation in most aerobic environments, and the rate may be slow at low concentrations in aquifers and lake waters and in environments at low pH (Fu & Alexander 1992)

$t_{1/2}(\text{aerobic}) = 14 \text{ d}$ ,  $t_{1/2} = 56 \text{ d}$  in natural waters (Capel & Larson 1995)

**Biotransformation:**

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

**Half-Lives in the Environment:**

**Air:** atmospheric  $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ , based on the EPA Reactivity Classification of Organics (Darnall et al. 1976); will react rapidly with both hydroxyl radical and ozone in air with a combined  $t_{1/2}(\text{calc}) = 2.5 \text{ h}$ , the reaction  $t_{1/2} = 3.5 \text{ h}$  with OH radicals and  $t_{1/2} = 9 \text{ h}$  with ozone (Howard 1989);

photooxidation  $t_{1/2} = 0.9$  to  $7.3 \text{ h}$ , based on measured rate data for the reaction with OH radical and  $O_3$  in air (Howard et al. 1991);

calculated lifetimes of styrene due to reaction with OH radicals,  $NO_3$  radicals and  $O_3$  are  $\sim 3 \text{ h}$ ,  $\sim 4 \text{ h}$  and  $1 \text{ d}$ , respectively, for ambient atmospheric conditions (Tuazon et al. 1993);

calculated lifetimes of  $1.4 \text{ h}$ ,  $3.7 \text{ h}$  and  $1.0 \text{ d}$  for reactions with OH radical,  $NO_3$  radical and  $O_3$  respectively (Atkinson 2000).

**Surface water:**  $t_{1/2} = 0.6 \text{ d}$  in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 336\text{--}672 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}(\text{calc}) = 0.75\text{--}51 \text{ d}$  for styrene loss from surface waters (Fu & Alexander 1992).

**Ground water:**  $t_{1/2} = 672\text{--}5040 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life and acclimated aqueous screening test data (Howard et al. 1991).

**Sediment:**

**Soil:**  $t_{1/2} = 336\text{--}672 \text{ h}$ , based on unacclimated grab samples of aerobic soil and acclimated aqueous screening test data (Howard et al. 1991).

**Biota:**

TABLE 3.1.1.35.1

Reported aqueous solubilities of styrene at various temperatures

Lane 1946				Shaw 1989b (IUPAC)	
shake flask-titration		shake flask-cloud pt.		recommended values	
t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>	t/°C	S/g·m <sup>-3</sup>
7	290	15	250	10	290
24	330	25	310	20	300
32	360	44	400	25	340
40	400	49	450	30	340
51	450	65	500	40	400
				50	460
				60	530

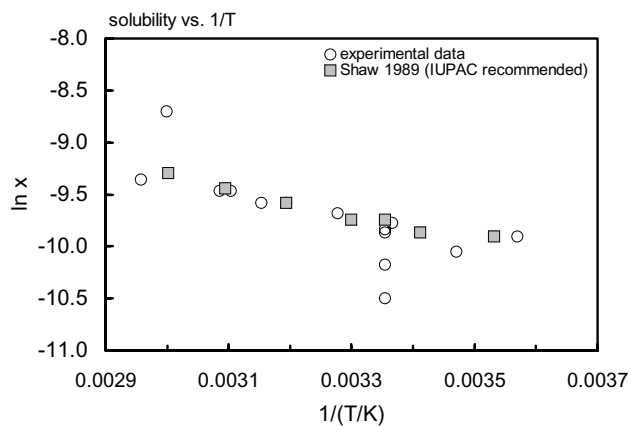
FIGURE 3.1.1.35.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for styrene.

TABLE 3.1.1.35.2

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

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

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

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

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

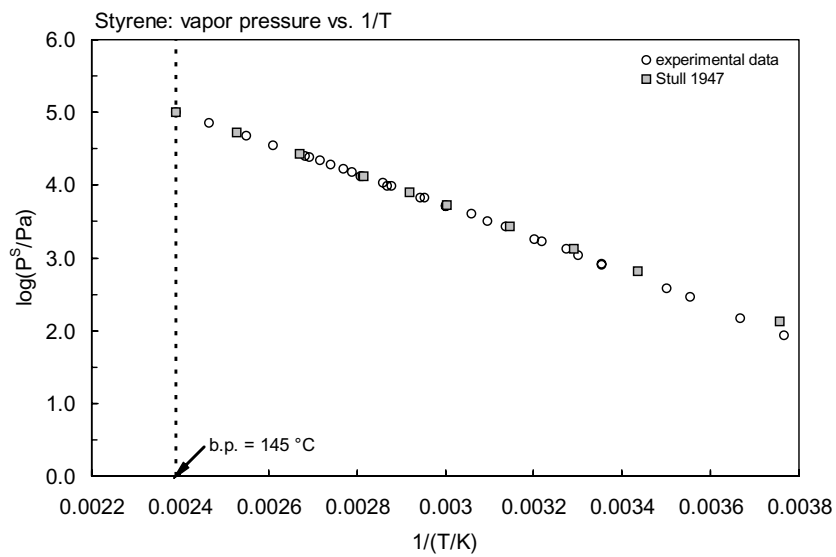
## 1.

Linder 1931		Pitzer et al. 1946		Stull 1947		Buck et al. 1949	
Hg manometer		static-Hg manometer		summary of literature data		Hg manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-7.7	86.66	12.5	384	-7.0	133.3	66.7	6799
-0.5	105.7	25	841.3	18	666.6	75.4	9866
8.2	288	37.5	1692	30.8	1333	82.4	13332
		50	3230	44.6	2666	88	16665
		60	5177	59.8	5333	91.7	18932
				69.5	7999	95.1	21732
<b>Burchfield 1942</b>				82	13332	98.2	24665
<b>isoteniscope method</b>		mp/°C	-30.68	101.3	26664	119.1	48129
t/°C	P/Pa			122.5	53329	132.6	71461
data presented by		eq. 4	P/mmHg	145.2	101325	145	100658
Clausius-Clapeyron eq.		A	28.8631				
		B	3203				
		C	7	mp/°C	-30.6		
eq. 1	P/mmHg					eq. 4	P/mmHg
A	7.929	$\Delta H_{\text{fus}}(\text{kJ mol}^{-1}) = 10.95$				A	26.92
B	2103					B	3151
measured temp range:		$\Delta H_{\text{v}}(\text{kJ mol}^{-1}) = 43.93$				C	6.294
33.5–116.3°C		at 25°C					

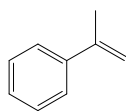
## 2.

Dreyer et al. 1955		Chaiyavech & Van Winkle 1959	
t/°C	P/Pa	t/°C	P/Pa
29.92	1093	32.4	1333
39.21	1827	35.6	2666
60.04	5106	53.86	4000
74.42	9639	60.05	5333
85.53	14999	65.45	6666
99.51	25105	76.6	10666
110.06	56877	82.9	13332
		eq. 1	P/mmHg
		A	8.2696
		B	2221.3





**FIGURE 3.1.135.2** Logarithm of vapor pressure versus reciprocal temperature for styrene.

3.1.1.36  $\alpha$ -Methylstyrene

Common Name:  $\alpha$ -Methylstyrene

Synonym: isopropenylbenzene

Chemical Name:  $\alpha$ -Methylstyrene

CAS Registry No: 98-83-9

Molecular Formula:  $C_9H_{10}$ ,  $C_6H_5C(CH_3)=CH_2$

Molecular Weight: 118.175

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

-23.2 (Lide 2003)

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

165.4 (Lide 2003)

Density ( $g/cm^3$ ):

0.9106, 0.9062 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

0.9082 ( $20^{\circ}C$ , Weast 1982-83)

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

129.8 ( $20^{\circ}C$ , calculated-density)

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

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

11.92 (Chickos et al. 1999)

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

47.55, 53.8 (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  $25^{\circ}C$ ):

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\* ( $7.4^{\circ}C$ , summary of literature data, temp range  $7.4$ – $165.4^{\circ}C$ , Stull 1947)

$\log(P/mmHg) = 7.28240 - 1740.3/(230 + t/^{\circ}C)$  (Antoine eq., Dreisbach & Martin 1949)

333 (extrapolated by formula., Dreisbach 1855)

$\log(P/mmHg) = 6.92366 - 1486.88/(202.4 + t/^{\circ}C)$ ; temp range  $70$ – $220^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 10214.6/(T/K)] + 7.959753$ ; temp range  $7.4$ – $165.4^{\circ}C$  (Antoine eq., Weast 1972-73)

$\log(P/mmHg) = 6.92366 - 1486.88/(202.4 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.04856 - 1486.88/(-70.75 + T/K)$ ; temp range  $343$ – $493 K$  (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.294 - 1599.88/(-63.72 + T/K)$ ; temp range  $353$ – $413 K$  (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -0.8626 - 2.5638 \times 10^3/(T/K) + 5.3807 \cdot \log(T/K) - 1.3516 \times 10^{-2} \cdot (T/K) + 6.7181 \times 10^{-6} \cdot (T/K)^2$ , temp range  $250$ – $654 K$  (Yaws 1994)

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

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

3.48 (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<sub>OC</sub>:

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

Volatilization:

Photolysis:

Photooxidation: k = (52 ± 6) × 10<sup>-12</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for the gas-phase reactions with OH radical at 298 ± 2 K (Atkinson 1989).

Hydrolysis:

Biodegradation:

Biotransformation:

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

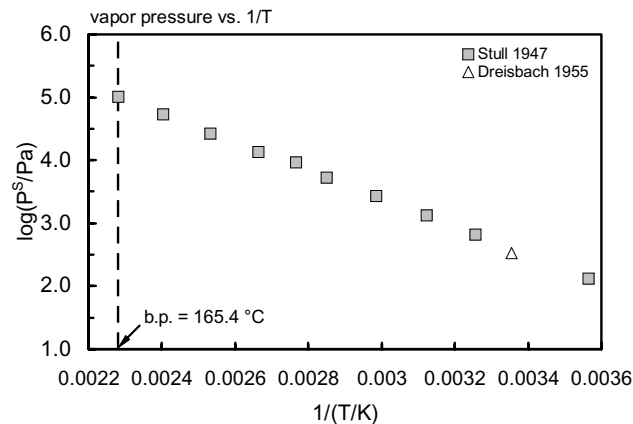
Half-Lives in the Environment:

**TABLE 3.1.1.36.1**  
**Reported vapor pressures of α-methylstyrene at various temperatures and the coefficients for the vapor pressure equations**

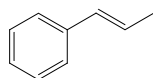
log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		

**Stull 1947**

summary of literature data	
t/°C	P/Pa
7.4	133.3
34.0	666.6
47.1	1333
61.8	2666
77.8	5333
88.3	7999
102.2	13332
121.8	26664
143	53329
165.4	101325
mp/°C	–23.2



**FIGURE 3.1.1.36.1** Logarithm of vapor pressure versus reciprocal temperature for α-methylstyrene.

3.1.1.37  $\beta$ -Methylstyrene

Common Name:  $\beta$ -Methylstyrene

Synonym: propenylbenzene

Chemical Name:  $\beta$ -Methylstyrene

CAS Registry No: 766-90-5 (*cis*-); 873-66-5 (*trans*-)

Molecular Formula:  $C_9H_{10}$ ,  $C_6H_5CH=CHCH_3$

Molecular Weight: 118.175

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

-61.6 (*cis*-, Stephenson & Malanowski 1987; Lide 2003)

-29.3 (*trans*-, Stephenson & Malanowski 1987; Lide 2003)

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

174 (*cis*-, Stephenson & Malanowski 1987)

175–176 (*trans*-, Stephenson & Malanowski 1987)

167.5 (*cis*-, Lide 2003)

178.3 (*trans*-, Lide 2003)

Density ( $g/cm^3$ ):

0.9088 ( $20^{\circ}C$ , *cis*-, Lide 2003)

0.9023 ( $25^{\circ}C$ , *trans*-, Lide 2003)

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

129.7 (*cis*-, Stephenson & Malanowski 1987)

131.0 (*trans*-, Stephenson & Malanowski 1987)

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

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

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

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

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

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

133.3\* ( $17.5^{\circ}C$ , summary of literature data, measured range  $32.1$ – $112^{\circ}C$ , temp range  $17.5$ – $179^{\circ}C$ , Stull 1947)

267 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.92339 - 1499.80/(201.0 + t/^{\circ}C)$ ; temp range  $75$ – $200^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 10701.3/(T/K)] + 8.071487$ ; temp range  $17.5$ – $179^{\circ}C$  (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = 6.92339 - 1499.80/(201.0 + t/^{\circ}C)$ ; temp range not specified (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.04829 - 1499.8/(-72.15 + T/K)$ ; temp range  $348$ – $498$  K (*cis*-, liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.58873 - 1915.94/(-33.996 + T/K)$ ; temp range  $291$ – $452$  K (*trans*-, liquid, Antoine eq., Stephenson & Malanowski 1987)

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 Constant and Half-Lives:

Volatilization:

Photolysis:

Photooxidation: rate constant  $k = (59 \pm 6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  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  $k_2$ ):

## Half-Lives in the Environment:

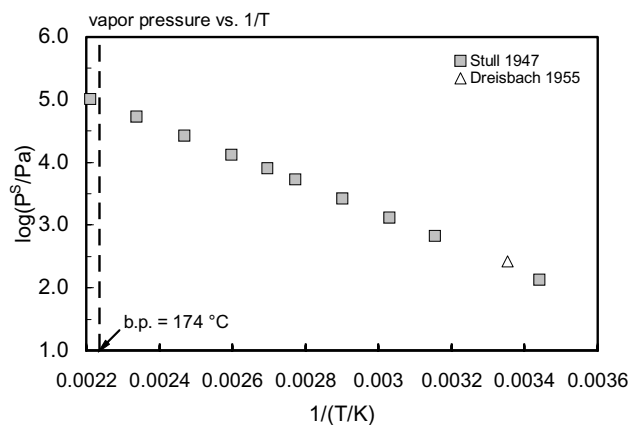
**TABLE 3.1.1.37.1**

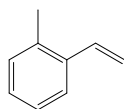
**Reported vapor pressures of  $\beta$ -methylstyrene at various temperatures and the coefficients for the vapor pressure equations**

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

**Stull 1947****summary of literature data**

$t/^{\circ}\text{C}$	$P/\text{Pa}$
17.5	133.3
43.8	666.6
57	1333
71.5	2666
87.7	5333
97.8	7999
111.7	13332
132	26664
154.7	53329
179.0	101325
mp/ $^{\circ}\text{C}$	-30.1

**FIGURE 3.1.1.37.1** Logarithm of vapor pressure versus reciprocal temperature for  $\beta$ -methylstyrene.

3.1.1.38 *o*-Methylstyrene

Common Name: *o*-Methylstyrene

Synonym: 2-methylstyrene, 2-vinyl toluene, *o*-methylvinylbenzene

Chemical Name: 2-methylstyrene

CAS Registry No: 611-15-4

Molecular Formula:  $C_9H_{10}$ ,  $2-CH_3C_6H_4CH=CH_2$

Molecular Weight: 118.175

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

-68.5 (Lide 2003)

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

169.8 (Lide 2003)

Density ( $g/cm^3$ ):

0.9106 ( $20^{\circ}C$ , Weast 1982-83)

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

129.8 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

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

387\* ( $32.1^{\circ}C$ , differential manometer, measured range  $32.1$ – $112^{\circ}C$ , Clements et al. 1953)

$\log (P/mmHg) = 7.15212 - 1628.405/(211.386 + t/^{\circ}C)$ ; temp range  $32.1$ – $112^{\circ}C$  (Antoine eq. from differential manometer measurements, Clements et al. 1953)

240.8 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.09235 - 1582.7/(206.0 + t/^{\circ}C)$ ; temp range  $75$ – $200^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

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

$\log (P/mmHg) = 7.21287 - 1644.083/(214.585 + t/^{\circ}C)$ ; temp range  $32$ – $112.4^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log (P/atm) = (1 - 443.504/(T/K) \times 10^4[0.890379 - 7.17666 \times 10^4 \cdot (T/K) + 5.97058 \times 10^7 \cdot (T/K)^2])$ ; temp range  $305.16$ – $385.5 K$  (Cox vapor pressure eq., Chao et al. 1983)

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

$\log (P/kPa) = 6.33107 - 1660.041/(214.219 + t/^{\circ}C)$ ; temp range  $32$ – $112.4^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/mmHg) = 7.2129 - 1644.08/(214.59 + t/^{\circ}C)$ ; temp range  $32$ – $112^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.88461 - 1485.41/(200.0 + t/^{\circ}C)$ ; temp range  $75$ – $255^{\circ}C$  (Antoine eq., Dean 1985, 1992)

$\log (P_L/kPa) = 6.27762 - 1628.405/(-61.764 + T/K)$ ; temp range  $305$ – $385 K$  (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 36.8413 - 3.7269 \times 10^3/(T/K) - 9.7997 \cdot \log (T/K) + 1.4115 \times 10^{-10} \cdot (T/K) + 1.9658 \times 10^{-6} \cdot (T/K)^2$ , temp range  $205$ – $659 K$  (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  $K_B$ :

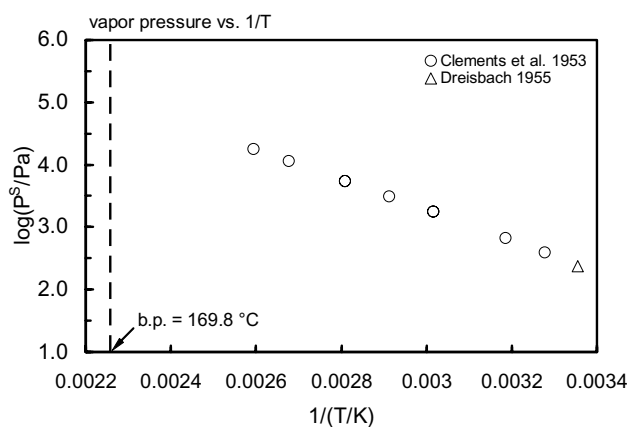
Sorption Partition Coefficient, log  $K_{OC}$ :

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

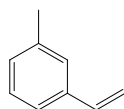
Half-Lives in the Environment:

**TABLE 3.1.1.38.1**  
**Reported vapor pressures of *o*-methylstyrene at various temperatures**

Clements et al. 1953	
differential manometer	
$t/^{\circ}\text{C}$	$P/\text{Pa}$
32.01	387
40.85	663
58.51	1753
58.54	1765
70.2	3113
82.8	5529
82.83	5534
100.35	11310
112.35	17698
mp/ $^{\circ}\text{C}$	-68.57
bp/ $^{\circ}\text{C}$	169.8
$\Delta H_v = 35.54 \text{ kJ/mol}$	
$\log P = A - B/(C + t/^{\circ}\text{C})$	
eq. 2	mmHg
A	7.15272
B	1628.405
C	211.386



**FIGURE 3.1.1.38.1** Logarithm of vapor pressure versus reciprocal temperature for *o*-methylstyrene.

3.1.1.39 *m*-MethylstyreneCommon Name: *m*-MethylstyreneSynonym: methylvinylbenzene, 3-vinyl toluene, *m*-methylvinylbenzene

Chemical Name: 3-methylstyrene

CAS Registry No: 100-42-1

Molecular Formula: C<sub>9</sub>H<sub>10</sub>, 3-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CH=CH<sub>2</sub>

Molecular Weight: 118.175

Melting Point (°C):

-86.3 (Lide 2003)

Boiling Point (°C):

164 (Lide 2003)

Density (g/cm<sup>3</sup> at 20°C):

0.9028 (20°C, Weast 1982-83)

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

130.9 ((20°C, calculated-density)

155.2 (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, F: 1.0

Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):89.0 (*m*- and *p*-methylstyrene commercial product, Dreisbach 1955)89.0, 100 (quoted, *m*- and *p*-methylstyrene, calculated-group contribution, Irmann 1965)

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):

2693\* (67.6°C, mercury manometer, measured range 67.6-169.1°C, Buck et al. 1949)

log (P/mmHg) = -3563/(T/K) - 7.553·log (T/K) + 30.90; temp range 80-120°C (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)

687\* (41.48°C, differential manometer, Clements et al. 1953)

log (P/mmHg) = 6.95079 - 1520.412/(210.967 + t/°C); temp range 41.48-111.8°C (Antoine eq. from differential manometer measurements, measured range 41.48-111.8°C, Clements et al. 1953)

257 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.99468 - 1553.4/(206.0 + t/°C); temp range 75-225°C (Antoine eq. for liquid state, Dreisbach 1955)

228, 244 (extrapolated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 7.06423 - 1564.74/(204.083 + t/°C); temp range 67.6-169°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/mmHg) = 7.11224 - 1615.091/(210.809 + t/°C); temp range 41.7-111.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/atm) = (1 - 442.985/T) × 10<sup>4</sup>/(0.885861 - 7.19653 × 10<sup>4</sup>·T + 6.75359 × 10<sup>7</sup>·T<sup>2</sup>); T in K, temp range 314.93-442.15 K (Cox vapor pressure eq., Chao et al. 1983)

227, 244 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.17253 - 1553.744/(202.922 + t/°C); temp range 67.6-169.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.22823 - 1609.825/(210.331 + t/°C); temp range 41.7-111.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 7.27534 - 1695.4/(220.0 + t/°C); temp range 10-72°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.87928 - 1471.28/(200.0 + t/°C); temp range 72-250°C (Antoine eq., Dean 1985, 1992)



245 (Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.07569 - 1520.412/(-71.183 + T/\text{K})$ ; temp range 314–385 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 11.6959 - 2.9912 \times 10^3/(T/\text{K}) + 0.33334 \cdot \log (T/\text{K}) - 8.8935 \times 10^{-3} \cdot (T/\text{K}) + 4.9793 \times 10^{-6} \cdot (T/\text{K})^2$ , temp range 187–657 K (Yaws 1994)

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

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

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

3.35 (Leo et al. 1971)

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

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

1.50 (gold fish, flow-through method, Ogata et al. 1984)

1.50, 1.63 (gold fish, quoted, calculated-MCI  $\chi$ , Ogata et al. 1984)

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

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

Half-Lives in the Environment:

**TABLE 3.1.1.39.1**

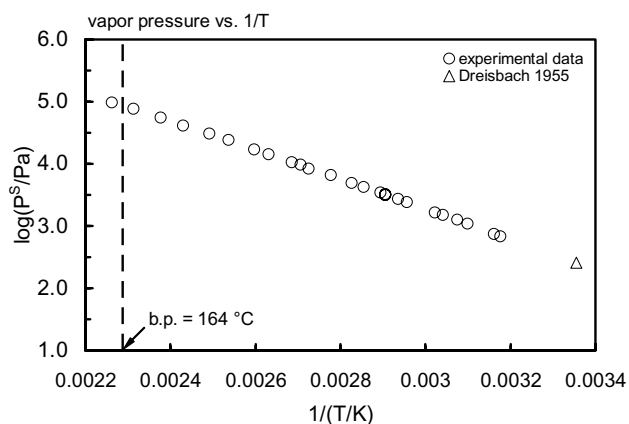
**Reported vapor pressures of *m*-methylstyrene at various temperatures and the coefficients for the vapor pressure equations**

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

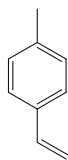
**Buck et al. 1949**

**Clements et al. 1953**

<b>Hg manometer</b>				<b>differential manometer</b>			
$t/^\circ\text{C}$	$P/\text{Pa}$	$t/^\circ\text{C}$	$P/\text{Pa}$	$t/^\circ\text{C}$	$P/\text{Pa}$	$t/^\circ\text{C}$	$P/\text{Pa}$
67.6	2693	eq. 4 $t/^\circ\text{C}$	$P/\text{mmHg}$	41.48	687	99.33	10696
72.3	3440	A	30.9	43.22	744	111.8	17020
80.7	4933	B	3563	49.49	1104		
87	6533	C	7.553	52.12	1261	mp/ $^\circ\text{C}$	−86.34
93.8	8373			55.73	1499	bp/ $^\circ\text{C}$	171.6
96.6	9733			57.8	1673		
106.9	14399			65.2	2445	$\Delta H_V = 38.79 \text{ kJ/mol}$	
121	12998			70.95	3192		
128.3	30398			71.01	3202	eq. 2	mmHg
138.5	41597			71.02	3204	A	6.95079
147.6	54795			71.1	3248	B	1520.412
159.2	75727			77.12	4234	C	201.967
169.1	98392						



**FIGURE 3.1.1.39.1** Logarithm of vapor pressure versus reciprocal temperature for *m*-methylstyrene.

3.1.1.40 *p*-Methylstyrene

Common Name: *p*-Methylstyrene

Synonym: methylvinylbenzene, 4-vinyl toluene, *p*-methylvinylbenzene

Chemical Name: 4-methylstyrene

CAS Registry No: 622-97-9

Molecular Formula:  $C_9H_{10}$ ,  $4-CH_3C_6H_4CH=CH_2$

Molecular Weight: 118.17

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

−34.1 (Lide 2003)

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

172.8 (Lide 2003)

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

0.9016, 0.9060 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Dreisbach 1955)

0.8760 ( $20^{\circ}C$ , Weast 1982–83)

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

129.8 ( $20^{\circ}C$ , calculated-density)

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

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

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

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

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

89.0 (quoted, *m*- and *p*-methylstyrene commercial product, Dreisbach 1955)

89.0, 100 (quoted, *m*- and *p*-methylstyrene, calculated-group contribution, Irrmann 1965)

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\* ( $16^{\circ}C$ , summary of literature data, temp range  $16$ – $175^{\circ}C$ , Stull 1947)

2773\* ( $68.6^{\circ}C$ , mercury manometer, measured range  $68.6$ – $170^{\circ}C$ , Buck et al. 1949)

$\log (P/mmHg) = -3476/(T/K) - 6.923 \cdot \log (T/K) + 29.03$ ; temp range  $80$ – $120^{\circ}C$  (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)

$\log (P/mmHg) = 7.34046 - 1791.0/(230 + t/^{\circ}C)$  (Antoine eq., Dreisbach & Martin 1949)

4954\* ( $90.98^{\circ}C$ , ebulliometry, measured range  $90.98$ – $171.06^{\circ}C$ , Dreisbach & Shrader 1949)

376\* ( $31.82^{\circ}C$ , differential manometer, measured range  $31.8$ – $96.9^{\circ}C$ , Clements et al. 1953)

$\log (P/mmHg) = 7.0483 - 1594.747/(209.889 + t/^{\circ}C)$ ; temp range  $31.8$ – $96.9^{\circ}C$  (Antoine eq. from differential manometer measurements, Clements et al. 1953)

241.5 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 7.35420 - 1765.6/(223.8 + t/^{\circ}C)$ ; temp range  $75$ – $205^{\circ}C$  (Antoine eq. for liquid state, Dreisbach 1955)

$\log (P/mmHg) = [-0.2185 \times 10724.2/(T/K)] + 8.130903$ ; temp range  $16.0$ – $175^{\circ}C$  (Antoine eq., Weast 1972–73)

216.6, 241 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 7.01119 - 1535.073/(200.732 + t/^{\circ}C)$ ; temp range  $68.6$ – $170^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log (P/mmHg) = 6.11531 - 1591.082/(209.441 + t/^{\circ}C)$ ; temp range  $31.8$ – $96.93^{\circ}C$  (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log (P/atm) = (1 - 443.748/(T/K) \times 10^4[0.875061 - 7.08160 \times 10^{-4} \cdot (T/K) + 7.33467 \times 10^{-7} \cdot (T/K)^2])$ ; temp range:  $289.15$ – $443.15$  K, (Cox vapor pressure eq., Chao et al. 1983)

215, 241 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.11531 - 1521.514/(199.299 + t/^{\circ}\text{C})$ ; temp range 68.6–170°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.16144 - 1586.596/(209.046 + t/^{\circ}\text{C})$ ; temp range 31.8–96.93°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.0112 - 1535.1/(200.7 + t/^{\circ}\text{C})$ ; temp range 68–170°C (Antoine eq., Dean 1985, 1992)  
242 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1732 - 1594.147/(-63.261 + T/\text{K})$ ; temp range 304–370 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 50.6506 - 4.0628 \times 10^3/(T/\text{K}) - 15.524 \cdot \log (T/\text{K}) + 5.5381 \times 10^{-3} \cdot (T/\text{K}) - 1.1313 \times 10^{-13} \cdot (T/\text{K})^2$ ,  
temp range 239–665 K (Yaws 1994)

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

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

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

3.35 (Leo et al. 1971; quoted, Ogata et al. 1984)

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

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

1.55 (gold fish, flow-through method, Ogata et al. 1984)

1.55, 1.62 (gold fish, quoted, calculated-MCI  $\chi$ , Ogata et al. 1984)

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

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

Half-Lives in the Environment:

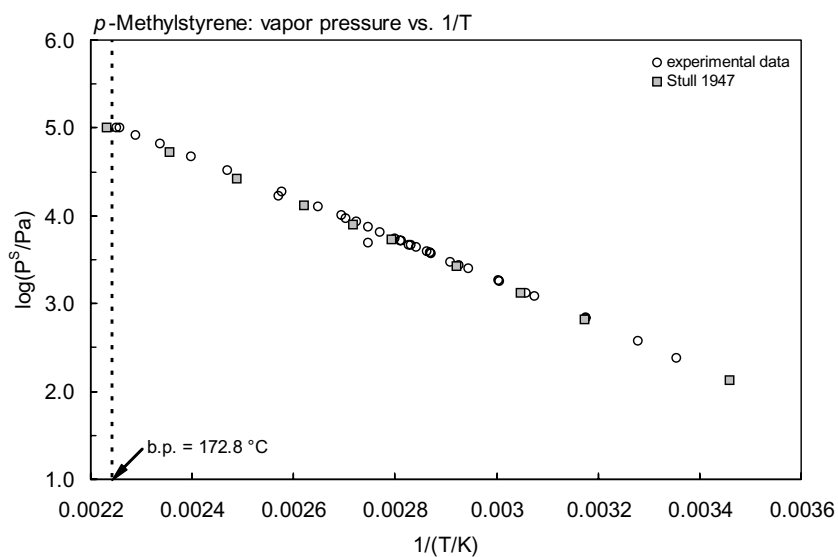
**TABLE 3.1.1.40.1**

**Reported vapor pressures of *p*-methylstyrene at various temperatures and the coefficients for the vapor pressure equations**

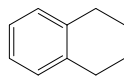
$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}C)$		(2)		$\ln P = A - B/(C + t/^{\circ}C)$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Buck et al. 1949		Dreisbach & Shrader 1949		Clements et al. 1953	
summary of literature data		Hg manometer		ebulliometry		differential manometer	
t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa
16	133.3	68.6	2773	90.98	4954	31.82	376
42	666.6	70.6	2986	98.13	10351	41.76	689
55.1	1333	75.1	3733	116.06	16959	41.83	693
6.2	2666	78.8	4400	171.06	101325	52.17	1207
85	5333	80.6	4720			53.94	1331
95	7999	82.7	5200	mp/^{\circ}C	-70.3	59.56	1797
108.6	13332	84.2	5573	bp/^{\circ}C	171.06	59.91	1855
128.7	26664	87	6559			66.62	2538
151.2	53329	94.1	8559			75.4	3858
175	101325	104.4	12826			76.19	3974
		115.1	18958			80.2	4718

TABLE 3.1.1.40.1 (Continued)

Stull 1947		Buck et al. 1949		Dreisbach & Shrader 1949		Clements et al. 1953	
summary of literature data		Hg manometer		ebulliometry		differential manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
mp/°C	—	131.9	33197			82.44	5208
		144	47996			90.9	7439
		154.7	65728			96.93	9466
		163.7	83193				
		170	99725			mp/°C	−34.15
						bp/°C	172.78
		mp/°C	−37.8			$\Delta H_v = 38.95$ kJ/mol	
		eq. 4	P/mmHg			eq. 2	P/mmHg
		A	29.03			A	7.0483
		B	3476			B	1594.747
		C	6.923			C	209.889

FIGURE 3.1.1.40.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-methylstyrene.

## 3.1.1.41 Tetralin



Common Name: Tetralin

Synonym: naphthalene-1,2,3,4-tetrahydride

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

CAS Registry No: 119-64-2

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

Molecular Weight: 132.202

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

−35.7 (Lide 2003)

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

207.6 (Weast 1982–83; Lide 2003)

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

0.9702 ( $20^{\circ}C$ , Weast 1982–83; Dean 1985)

0.9695, 0.9660 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Riddick et al. 1986)

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

136.4 ( $20^{\circ}C$ , calculated- density)

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

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

12.477 (Riddick et al. 1986)

12.45 (Chickos et al. 1999)

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

52.44, 49.6 (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  $25^{\circ}C$ ):

14.94 (calculated-QSAR Data base, Passino & Smith 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):

2666\* ( $93.8^{\circ}C$ , temp range  $93.8$ – $171.06^{\circ}C$ , Herz & Schuftan 1922)

53.3\* (mercury manometer, measured range  $-2.4$ – $65^{\circ}C$ , Linder 1931)

66.66\* ( $39.3^{\circ}C$ , ebulliometry, measured range  $39.3$ – $148.6^{\circ}C$ , Gardner & Brewer 1937)

133.3\* ( $38^{\circ}C$ , summary of literature data, temp range  $38$ – $207^{\circ}C$ , Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11613.0/(T/K)] + 8.194951$ ; temp range  $38$ – $207.2^{\circ}C$  (Antoine eq., Weast 1972–73)

1737\* ( $82.3^{\circ}C$ , diaphragm gauge, measured range  $82.3$ – $276.21^{\circ}C$ , Nasir et al. 1980)

$\log(P/mmHg) = [1 - 480.364/(T/K)] \times 10^{\{0.85916 - 5.75417 \times 10^{-4} \cdot (T/K) + 4.41971 \times 10^{-7} \cdot (T/K)^2\}}$ ; temp range  $311.15$ – $710.93 K$ , (Cox eq., Chao et al. 1983)

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

$\log(P/mmHg) = 7.07055 - 1741.30/(208.26 + t/^{\circ}C)$ ; temp range  $94$ – $206^{\circ}C$  (Antoine eq., Dean 1985, 1992)

53.0 (selected lit. average, Riddick et al. 1986)

$\log(P/kPa) = 11.079 - 2797.90/(T/K) + 1.187 \cdot \log(T/K)$ , temp range not specified (Antoine eq., Riddick et al. 1986)

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

$\log(P_L/kPa) = 6.35719 - 1854.82/(-54.237 + T/K)$ ; temp range  $311$ – $481 K$  (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 39.9174 - 4.132 \times 10^3/(T/K) - 10.78 \cdot \log(T/K) + 1.9691 \times 10^{-10} \cdot (T/K) + 2.0405 \times 10^{-6} \cdot (T/K)^2$ , temp range  $237$ – $720 K$  (Yaws 1994)

38.35\* ( $20.26^{\circ}C$ , static method, measured range  $253.8$ – $442.8 K$ , Mokbel et al. 1998)

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):

76.0, 106.4, 137.8, 189.5, 271.6 (0, 15, 20, 25,  $30^\circ\text{C}$ , EPICS-GC, Ashworth et al. 1988)

$\ln [H/(\text{atm m}^3 \text{ mol}^{-1})] = 11.83 - 5392/(T/K)$ ; temp range  $10\text{--}30^\circ\text{C}$  (EPICS-GC, Ashworth et al. 1988)

142.8 ( $20^\circ\text{C}$ , selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.332 - 2215/(T/K)$  (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

3.83 (calculated-fragment const., Rekker 1977)

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

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

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

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

Volatilization:

Photolysis:

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

$k_{\text{OH}} = (3.43 \pm 0.06) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{NO}_3} = (8.6 \pm 1.3) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at room temp. (relative rate method, Atkinson & Aschmann 1988)

$k_{\text{OH}} = 3.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (recommended, Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 11.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\text{OH}}(\text{exptl}) = 34.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

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

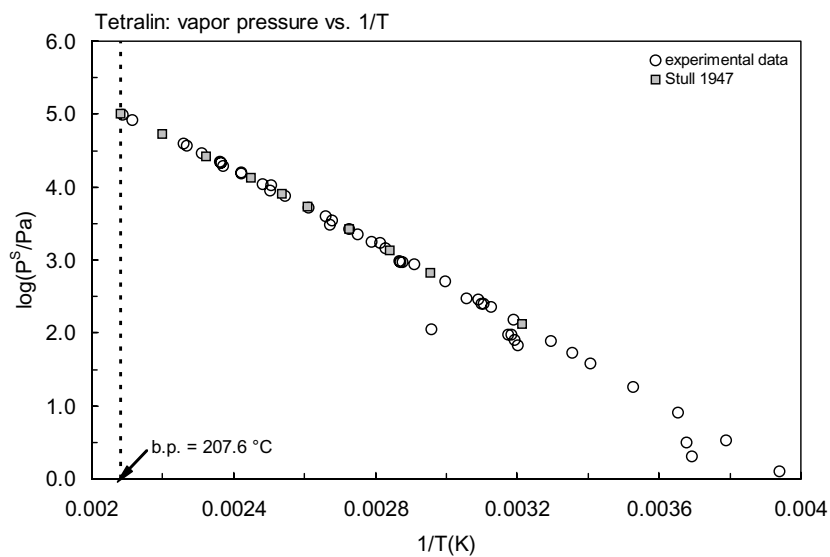
Half-Lives in the Environment:

TABLE 3.1.1.41.1

Reported vapor pressures of tetralin 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)					
Herz & Schuftan 1922		Stull 1947		Gardner & Brewer 1937		Mokbel et al. 1998	
		summary of literature data		ebulliometry		static method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
93.8	2666	38	133	39.3	66.66	253.8	1.279
103	4000	65.3	666.6	40.1	79.99	264.01	3.349
140	15732	79	1333	40.8	93.33	273.65	7.984
150	21598	93.8	2666	41.8	93.33	283.54	17.94
167.5	36397	110	5333	46.6	226.7	293.51	38.35
206.2	98658	121.3	7999	48.9	253.3	303.52	78.52
		135.3	13332	49.4	253.3	313.51	153.0
		157.2	26664	54	293.3	323.55	284.0
Linder 1931		181.8	53329	74.4	946.6	333.57	506.0
mercury manometer		207.2	101325	75.1	959.9	343.62	868.0
t/°C	P/Pa			101.1	3040	353.66	1443
		mp/°C	−31.0	126.6	9040	358.64	1801
−2.4	2			148.6	19625	363.62	2254
−1.2	3.133					373.66	3508
25	53.33			bp/°C	210.5	383.00	5179
65	110.7					392.95	7617
						402.89	10948
				Nasir et al. 1980		412.86	15444
				diaphragm gauge		422.82	21388
				t/°C	P/Pa	432.84	29254
						442.80	39128
				82.3	1737		
				125.81	10500		data fitted to Wagner eq.
				150.15	22419		
				200.11	84002		
				250.66	257307		
				276.21	348091		





**FIGURE 3.1.1.41.1** Logarithm of vapor pressure versus reciprocal temperature for tetralin.

## 3.2 SUMMARY TABLES AND QSPR PLOTS

**TABLE 3.2.1**  
**Summary of the physical properties of mononuclear aromatic hydrocarbons**

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	mp °C	bp °C	Fugacity ratio, F at 25 °C*	Density, $\rho$ g/cm <sup>3</sup> at 20°C	Molar volume, $V_M$ cm <sup>3</sup> /mol	
								MW/p at 20°C	Le Bas
Benzene	71-43-2	C <sub>6</sub> H <sub>6</sub>	78.112	5.49	80.09	1	0.8765	89.12	96.0
Toluene	108-88-3	C <sub>7</sub> H <sub>8</sub>	92.139	-94.95	110.63	1	0.8668	106.30	118.2
Ethylbenzene	100-41-4	C <sub>8</sub> H <sub>10</sub>	106.165	-94.96	136.19	1	0.867	122.45	140.4
<i>o</i> -Xylene	95-47-6	C <sub>8</sub> H <sub>10</sub>	106.165	-25.2	144.5	1	0.8802	120.61	140.4
<i>m</i> -Xylene	108-38-3	C <sub>8</sub> H <sub>10</sub>	106.165	-47.8	139.12	1	0.8842	120.07	140.4
<i>p</i> -Xylene	106-42-3	C <sub>8</sub> H <sub>10</sub>	106.165	13.25	138.37	1	0.8611	123.29	140.4
1,2,3-Trimethylbenzene	526-73-8	C <sub>9</sub> H <sub>12</sub>	120.191	-25.4	176.12	1	0.8944	134.38	162.6
1,2,4-Trimethylbenzene	95-63-6	C <sub>9</sub> H <sub>12</sub>	120.191	-43.77	169.38	1	0.8758	137.24	162.6
1,3,5-Trimethylbenzene	108-67-8	C <sub>9</sub> H <sub>12</sub>	120.191	-44.72	164.74	1	0.8800	136.58	162.6
<i>n</i> -Propylbenzene	103-65-1	C <sub>9</sub> H <sub>12</sub>	120.191	-99.6	159.24	1	0.862	139.43	162.6
Isopropylbenzene	98-82-8	C <sub>9</sub> H <sub>12</sub>	120.191	-96.02	152.41	1	0.8618	139.47	162.6
1-Ethyl-2-methylbenzene ( <i>o</i> -Ethyltoluene)	611-14-3	C <sub>9</sub> H <sub>12</sub>	120.191	-79.83	165.2	1	0.8807	136.47	162.6
1-Ethyl-3-methylbenzene ( <i>m</i> -Ethyltoluene)	620-14-4	C <sub>9</sub> H <sub>12</sub>	120.191	-95.6	161.3	1	0.8645	139.03	162.6
1-Ethyl-4-methylbenzene ( <i>p</i> -Ethyltoluene)	622-96-8	C <sub>9</sub> H <sub>12</sub>	120.191	-62.35	162	1	0.8614	139.53	162.6
Isopropyl-4-methylbenzene ( <i>p</i> -Cymene)	99-87-6	C <sub>10</sub> H <sub>14</sub>	134.218	-67.94	177.1	1	0.8573	156.56	184.8
<i>n</i> -Butylbenzene	104-51-8	C <sub>10</sub> H <sub>14</sub>	134.218	-87.85	183.31	1	0.8601	156.05	184.8
Isobutylbenzene	538-93-2	C <sub>10</sub> H <sub>14</sub>	134.218	-51.4	172.79	1	0.8532	157.31	184.8
<i>sec</i> -Butylbenzene	135-98-8	C <sub>10</sub> H <sub>14</sub>	134.218	-82.7	173.3	1	0.8621	155.69	184.4
<i>tert</i> -Butylbenzene	98-06-6	C <sub>10</sub> H <sub>14</sub>	134.218	-57.8	169.1	1	0.8665	154.90	184.8
1,2,3,4-Tetramethylbenzene	488-23-3	C <sub>10</sub> H <sub>14</sub>	134.218	-6.2	205	1	0.9052	148.27	184.8
1,2,3,5-Tetramethylbenzene	527-53-7	C <sub>10</sub> H <sub>14</sub>	134.218	-23.7	198	1	0.8903	150.76	184.8
1,2,4,5-Tetramethylbenzene	95-93-2	C <sub>10</sub> H <sub>14</sub>	134.218	79.3	196.8	0.293	0.8380	160.16	184.8
<i>n</i> -Pentylbenzene	538-68-1	C <sub>11</sub> H <sub>16</sub>	148.245	-75	205.4	1	0.8585	172.68	207.0

Pentamethylbenzene	700-12-9	C <sub>11</sub> H <sub>16</sub>	148.245	54.5	232	0.514	0.917	161.66	207.0
<i>n</i> -Hexylbenzene	1077-16-3	C <sub>12</sub> H <sub>18</sub>	162.271	-61	226.1	1	0.8613	188.40	229.2
Hexamethylbenzene	87-85-4	C <sub>12</sub> H <sub>18</sub>	162.271	165.5	263.4	0.0418	1.063	152.65#	229.2
Heptylbenzene	1078-71-3	C <sub>13</sub> H <sub>20</sub>	176.298	-48	240	1	0.8567	205.79	251.4
Octylbenzene	2189-60-8	C <sub>14</sub> H <sub>22</sub>	190.325	-36	264	1	0.8562	222.29	273.6
Nonylbenzene	1081-77-2	C <sub>15</sub> H <sub>24</sub>	204.352	-24	280.5	1	0.8584	238.06	295.8
Decylbenzene	104-72-3	C <sub>16</sub> H <sub>26</sub>	218.377	-14.4	293	1	0.8555	255.26	318.0
Undecylbenzene	6742-54-7	C <sub>17</sub> H <sub>28</sub>	232.404	-5	316	1	0.8553	271.72	340.2
Dodecylbenzene	123-01-3	C <sub>18</sub> H <sub>30</sub>	246.431	3	328	1	0.8551	288.19	362.4
Tridecylbenzene	123-02-4	C <sub>19</sub> H <sub>32</sub>	260.457	10	346	1	0.8550	304.63	384.6
Tetradecylbenzene	1459-10-5	C <sub>20</sub> H <sub>34</sub>	274.484	16	359	1	0.8549	321.07	406.8
Styrene	100-42-5	C <sub>8</sub> H <sub>8</sub>	104.150	-30.65	145	1	0.9060	114.96	133.0
<i>o</i> -Methylstyrene	611-15-4	C <sub>9</sub> H <sub>10</sub>	118.175	-68.5	169.8	1	0.9106	129.78	155.2
<i>m</i> -Methylstyrene	100-80-1	C <sub>9</sub> H <sub>10</sub>	118.175	-86.3	164	1	0.9028	130.90	155.2
<i>p</i> -Methylstyrene	622-97-9	C <sub>9</sub> H <sub>10</sub>	118.175	-34.1	172.8	1	0.9016	131.07	155.2
$\alpha$ -Methylstyrene	98-83-9	C <sub>9</sub> H <sub>10</sub>	118.175	-23.2	165.4	1	0.9106	129.78	155.2
$\beta$ -Methylstyrene, <i>cis</i> -	766-90-5	C <sub>9</sub> H <sub>10</sub>	118.175	-61.6	167.5	1	0.9088	130.03	155.2
$\beta$ -Methylstyrene, <i>trans</i> -	873-66-5	C <sub>9</sub> H <sub>10</sub>	118.175	-29.3	178.3	1	0.9023	130.97#	155.2
Tetralin	119-64-2	C <sub>10</sub> H <sub>12</sub>	132.202	-35.7	207.6	1	0.9695	136.36	177.4

\* Assuming  $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$ .

# at 25°C.

**TABLE 3.2.2**  
**Summary of selected physical-chemical properties of mononuclear aromatic hydrocarbons at 25°C**

Compound	Selected properties:						Henry's law constant
	Vapor pressure		Aqueous solubility			log $K_{OW}$	H/( Pa·m <sup>3</sup> /mol) calculated P/C
	P <sup>s</sup> /Pa	P <sub>L</sub> /Pa	S/(g/m <sup>3</sup> )	C <sup>s</sup> /(mol/m <sup>3</sup> )	C <sub>L</sub> /(mol/m <sup>3</sup> )		
Benzene	12700	12700	1780	22.788	22.788	2.13	557
Toluene	3800	3800	515	5.590	5.590	2.69	680
Ethylbenzene	1270	1270	152	1.431	1.431	3.13	887
<i>o</i> -Xylene	1170	1170	220	2.072	2.072	3.15	565
<i>m</i> -Xylene	1100	1100	160	1.507	1.507	3.20	730
<i>p</i> -Xylene	1170	1170	215	2.024	2.024	3.18	578
1,2,3-Trimethylbenzene	200	200	70	0.582	0.582	3.55	343
1,2,4-Trimethylbenzene	270	270	57	0.474	0.474	3.60	569
1,3,5-Trimethylbenzene	325	325	50	0.416	0.416	3.58	781
<i>n</i> -Propylbenzene	450	450	52	0.433	0.433	3.69	1040
Isopropylbenzene	610	610	50	0.416	0.416	3.63	1466
1-Ethyl-2-methylbenzene	330	330	75	0.624	0.624	3.63	529
1-Ethyl-3-methylbenzene	391	391					
1-Ethyl-4-methylbenzene	395	395	95	0.790	0.790	3.63	500
Isopropyl-4-methylbenzene	204	204	34	0.253	0.253	4.10	805
<i>n</i> -Butylbenzene	137	137	13.8	0.103	0.103	4.26	1332
Isobutylbenzene	250	250	10.1	0.075	0.075	4.01	3322
<i>sec</i> -Butylbenzene	240	240	17	0.127	0.127		1890
<i>tert</i> -Butylbenzene	286	286	30	0.224	0.224	4.11	1280
1,2,3,4-Tetramethylbenzene	45	45				3.90	
1,2,3,5-Tetramethylbenzene	62	62				4.04	
1,2,4,5-Tetramethylbenzene	66	66	3.48	0.026	0.026	4.10	2546
<i>n</i> -Pentylbenzene	44	44	3.85	0.026	0.026	4.90	1694
Pentamethylbenzene	9.52	18.63	15.5	0.105	0.205		
<i>n</i> -Hexylbenzene	13.61	13.61	1.02	0.006	0.006	5.52	2165
Hexamethylbenzene	0.155	3.90	0.235	0.001	0.036	4.61	
Heptylbenzene	3.95	3.95				5.37	
Octylbenzene	2.03	2.03				6.30	
Nonylbenzene	0.30	0.30				6.82	
Decylbenzene	0.077	0.077				7.37	

Undecylbenzene	0.045	0.045				8.14
Dodecylbenzene	0.017	0.017				8.65
Tridecylbenzene	0.00070	0.0007				9.36
Tetradecylbenzene	0.000113	0.000113				9.95
Styrene	880	880	250	2.40	2.40	2.95
<i>o</i> -Methylstyrene	245	245				
<i>m</i> -Methylstyrene	250	250				3.35
<i>p</i> -Methylstyrene	242	242				3.35
$\alpha$ -Methylstyrene	324	324				3.48
$\beta$ -Methylstyrene, <i>cis</i> -	258	258				3.35
$\beta$ -Methylstyrene, <i>trans</i> -	216.6	216.6				
Tetralin	54	54				3.83

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TABLE 3.2.3

Suggested half-life classes of mononuclear aromatic hydrocarbons in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Benzene	3	4	5	6
Toluene	2	5	6	7
Ethyl benzene	2	5	6	7
<i>o</i> -Xylene	2	5	6	7
<i>m</i> -Xylene	2	5	6	7
<i>p</i> -Xylene	2	5	6	7
1,2,3-Trimethylbenzene	2	5	6	7
1,2,4-Trimethylbenzene	2	5	6	7
1,3,5-Trimethylbenzene	2	5	6	7
<i>n</i> -Propylbenzene	2	5	6	7
Isopropylbenzene	2	5	6	7
1-Isopropyl-4-methylbenzene ( <i>p</i> -Cymene)	2	5	6	7
1,2,4,5-Tetramethylbenzene	2	5	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

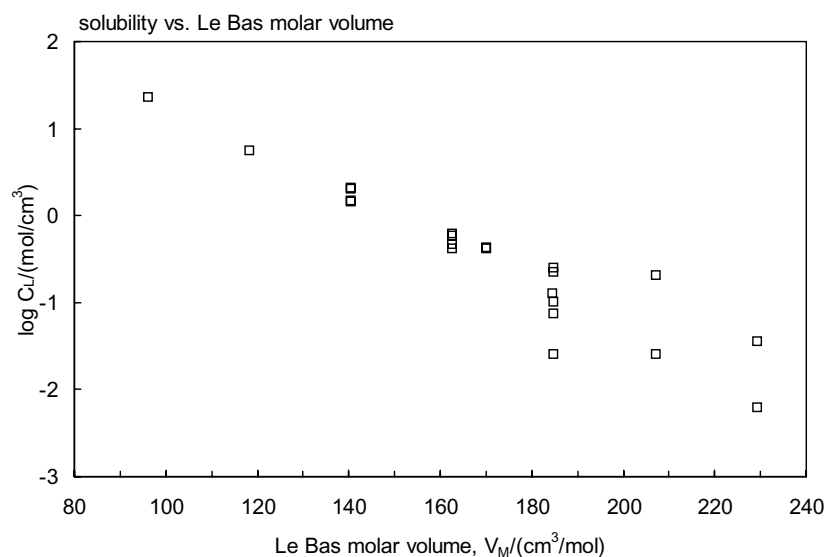
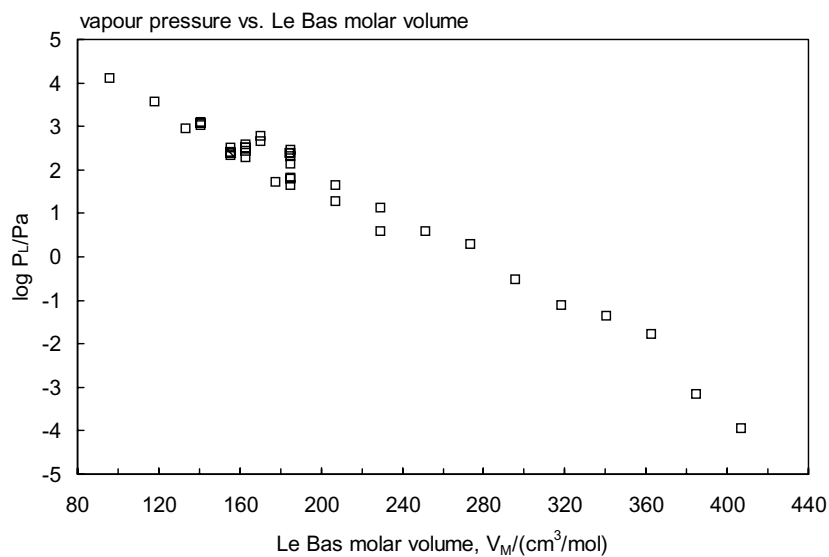
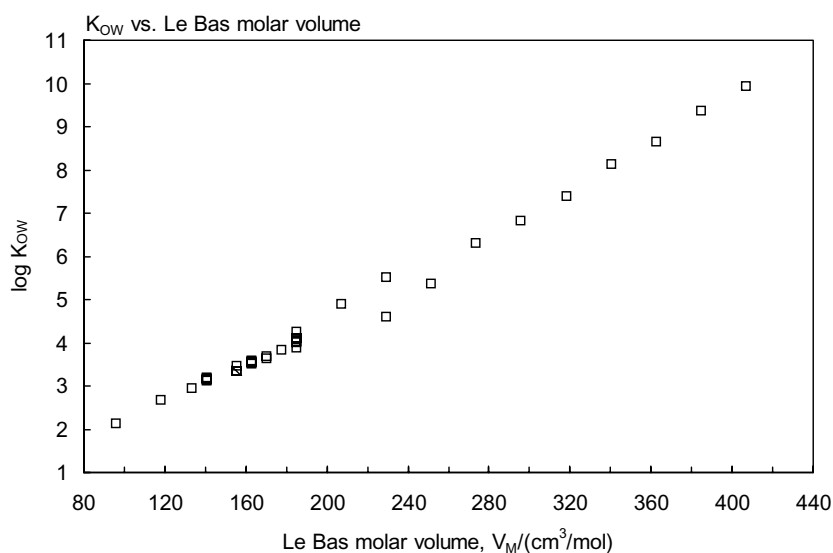


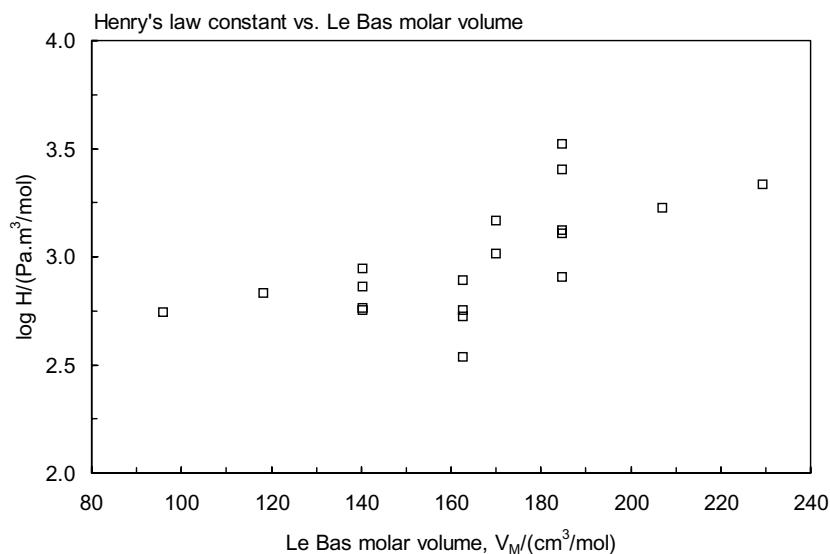
FIGURE 3.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.



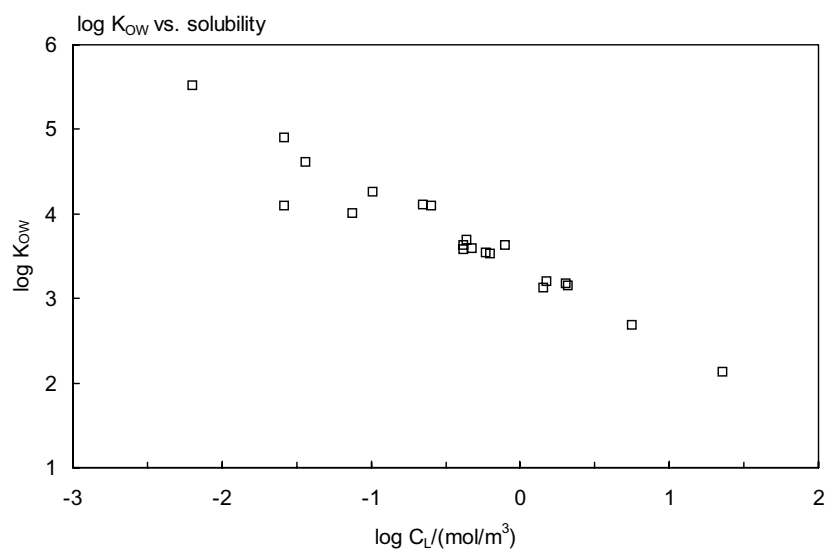
**FIGURE 3.2.2** Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.



**FIGURE 3.2.3** Octanol-water partition coefficient versus Le Bas molar volume for mononuclear aromatic hydrocarbons.



**FIGURE 3.2.4** Henry's law constant versus Le Bas molar volume for mononuclear aromatic hydrocarbons.



**FIGURE 3.2.5** Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for mononuclear aromatic hydrocarbons.



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