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ILLUSTRATED HANDBOOK

OF

PHYSICAL - CHEMICAL
PROPERTIES

AND

ENVIRONMENTAL FATE

FOR

ORGANIC CHEMICALS

Volume I
 Monoaromatic Hydrocarbons,
 Chlorobenzenes,
 and PCBs

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 Kuo Ching Ma

LOS ALAMOS
 NATIONAL LABORATORY
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 Boca Raton Ann Arbor London

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Common Name: Toluene

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

Chemical Name: toluene

CAS Registry No: 108-88-3

Molecular Formula: $C_6H_5CH_3$

Molecular Weight: 92.13

Melting Point (°C): -95

Boiling Point (°C): 110.6

Density (g/cm³ at 20°C): 0.8669

Molar Volume (cm³/mol):

106.3 (20 °C, calculated-density, McAuliffe 1966)

106.86 (Windholz 1983; Budavari 1989)

106.3 (25°C, calculated-density, Miller et al. 1985)

106.0 (calculated-density, Klevens 1950; Lande & Banerjee 1981; Chiou 1985)

85.74 (characteristic molecular volume, McGowen & Mellors 1986)

118.0 (LeBas method, Abernethy & Mackay 1987)

106.9 (20°C, calculated-density, Stephenson & Malanowski 1987)

0.591 (intrinsic volume: $V_i/100$, Leahy 1986; Kamlet et al. 1987, 1988)

Molecular Volume (A³):

99.98 (Pearlman 1986)

Total Surface Area, TSA (A²):

126.5 (Yalkowsky & Valvani 1976, Whitehouse & Cooke 1982)

286.5 (calculated-hydration shell, Amidon & Anik 1981)

128.3 (calculated- χ , Sabljic 1987a)

129.70 (Doucette & Andren 1988)

131.2 (Warne et al. 1990)

Heat of Fusion, kcal/mol:

Fugacity Ratio, F: 1.0

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

470 (Fühner, 1924; quoted, Chiou et al. 1977; Freed et al. 1977)

570 (30°C, shake flask-interferometer, Gross & Saylor 1931; quoted, Vesala 1974)

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

530 (shake flask-UV, Andrews & Keffer 1949; quoted, Chey & Calder 1972; Vesala 1974; Shiu et al. 1990)

500 (flask flask-UV, Klevens 1950; quoted, Suntio et al. 1988; Shiu et al. 1990)

627 (shake flask-UV, Bohon & Claussen 1951; quoted, Chey & Calder 1972; Vesala 1974; API 1985; Suntio et al. 1988; Shiu et al. 1990)

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

550 (Dreisbach 1955; quoted, Chey & Calder 1972; Vesala 1974)

595 (quoted, Deno & Berkheimer 1960)

538 (shake flask-GC, McAuliffe 1963)

- 515 (shake flask-GC, McAuliffe 1966; quoted, Hermann 1972; Vesala 1974; Mackay & Leinonen 1975; Mackay & Shiu 1975; 1981; 1990; Mackay et al. 1975; Hutchinson et al. 1980; Mackay et al. 1980; Chiou 1981; 1985; Mackay 1981; Chiou et al. 1982; Geyer et al. 1982; API 1985; Garbarnini & Lion 1985; Abernethy et al. 1986; Suntio et al. 1988; Shiu et al. 1988; 1990)
- 470 (quoted, Hansch et al. 1968)
- 354 (calculated- K_{ow} , Hansch et al. 1968)
- 479 (21°C, extraction by nonpolar resins/evolution, Chey & Calder 1972)
- 573 (shake flask-GC, Polak & Lu 1973; quoted, API 1985)
- 517 (shake flask-GC, Mackay & Wolkoff 1973)
- 627 (shake flask-UV, Vesala 1974)
- 517 (quoted, Hine & Moorkerjee 1975; Kõnemann 1981; Kamlet et al. 1987)
- 517 (shake flask-GC, Mackay et al. 1975; Shiu et al. 1990)
- 520 (shake flask-GC, Mackay & Shiu 1975; quoted, API 1985; Suntio et al. 1988; Shiu et al. 1990)
- 534.8 (shake flask-GC, Sutton & Calder 1975; quoted, API 1985; Howard 1990)
- 524, 512 (selected, calcd. - χ , reported as ln S, should be -log S in molar concn., Kier & Hall 1976)
- 554 (shake flask-GC, Price 1976; quoted, API 1985; Suntio et al. 1988; Shiu et al. 1990)
- 488 (shake flask-titration, Sada et al. 1975)
- 534 (shake flask-Fluo., Schwarz 1977; quoted, Shiu et al. 1990)
- 515 (quoted, Verschueren, 1977 & 1983)
- 535 (quoted, Callahan et al. 1979; Mabey et al. 1982)
- 470 (quoted, Neely 1980)
- 623, 660 (quoted, elution chromatography, Schwarz 1980)
- 732, 739 (20 °C, exptl.-elution chromatography, shake flask-UV, Schwarz & Miller 1980)
- 566, 735 (20°C, quoted, average exptl. value, Schwarz & Miller 1980)
- 1548 (shake flask-LSC, Banerjee et al. 1980)
- 581 (quoted, Lande & Banerjee 1981)
- 507 (shake flask-GC, Rossi & Thomas 1981)
- 542 (quoted lit. mean, Amidon & Anik 1981)
- 530, 715 (quoted exptl. average, calculated- K_{ow} , Valvani et al. 1981)
- 585 (gen. col.-HPLC/UV, Teweri et al. 1982b; quoted, Doucette & Andren 1988)
- 578 (gen. col.-HPLC/UV, Teweri et al. 1982c)
- 514, 535, 507; 520 (quoted, quoted lit. average, Whitehouse & Cooke 1982)
- 534 (calculated-HPLC- k' , converted from reported γ_w , Hakenscheid & Tomlinson 1983a)
- 555 (calculated- K_{ow} , Yalkowsky et al. 1983)
- 580 (gen. col.-HPLC/UV, Wasik et al. 1983)
- 524 (shake flask-HPLC/UV, Banerjee 1984)
- 561, 428 (quoted, calculated-UNIFAC, Banerjee 1985)

- 578 (quoted, Miller et al. 1985; Vowles & Mantoura 1987; Eastcott et al. 1988)
- 530 (quoted, Brookman et al. 1985; Cline et al. 1991)
- 529 (quoted, Leahy 1986)
- 272 (calculated- V_p , solvatochromic parameters, Leahy 1986)
- 575, 1581 (quoted, calculated- K_{ow} & HPLC-RT, Chin et al. 1986)
- 515, 265 (quoted, calculated-characteristic volume, McGowen & Mellors 1986)
- 461 (calculated- V_p , solvatochromic parameters, Kamlet et al. 1987)
- 707 (calculated- χ , Nirmalakhandan & Speece 1988a)
- 580 (shake flask-GC, Keeley et al. 1988)
- 538 (purge and trap-GC, Coutant & Keigley 1988)
- 525 (quoted, Mackay 1988)
- 440 (calculated-UNIFAC, Banerjee & Howard 1988)
- 525 (quoted, Isnard & Lambert 1988, 1989)
- 515, 530 (quoted, calculated-UNIFAC, Al-Sahhaf 1989)
- 535 (quoted, Abdul et al. 1990)
- 545 (quoted, Warne et al. 1990)

Vapor Pressure (Pa at 25 °C):

- 3800 (interpolated, Antoine eqn., Zwolinski & Wilhoit 1971; quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay & Shiu 1975; 1981; 1990, Mackay 1981; Eastcott et al. 1988; Suntio et al. 1988)
- 3792 (quoted, Hine & Mookerjee 1975)
- 4000 (quoted, Verschueren, 1977 & 1983)
- 3826 (quoted, Callahan et al. 1979)
- 30 torr — 4000 (quoted, Neely 1980)
- 3749, 3881 (quoted, calculated-B.P., Mackay et al. 1982)
- 26 torr — 3560 (gas saturation, Politzki et al. 1982)
- 3786 (Daubert & Danner 1985; quoted, Howard 1990)
- 3792 (extrapolated, Antoine eqn., Dean 1985)
- 3800 (extrapolated, Antoine eqn., Stephenson & Malanowski 1987)
- 3786, 855 (quoted, calculated-UNIFAC, Banerjee et al. 1990)

Henry's Law Constant (Pa m³/mol):

- 677 (calculated, Mackay & Leinonen 1975; Mackay 1981)
- 518 (calculated-bond contribution, Hine & Mookerjee 1975)
- 682 (calculated as $1/K_{Aw}$, C_w/C_A , reported as exptl., Hine & Mookerjee 1975; Nirmalakhandan & Speece 1988b)
- 673, 675 (batch stripping, calculated-P/C, Mackay et al. 1979; quoted, Suntio et al. 1988)
- 673 (quoted exptl., Mackay & Shiu 1981)
- 680 (calculated-P/C, Mackay & Shiu 1981; quoted, Pankow et al. 1984; Pankow 1986; Pankow & Rosen 1988; Pankow 1990; Olsen & Davis 1990)
- 647 (concentration ratio, Leighton & Calo 1981)

t al. 1988)

- 620 (C_A/C_w , Matter-Müller et al. 1981)
- 675 (calculated, Mabey et al. 1982)
- 602 (Shen 1982; quoted, Howard 1990)
- 824 (calculated-UNIFAC, Gmehling et al. 1982)
- 825 (calculated-UNIFAC, Arbuckle 1983)
- 647 (EPICS, Garbarnini & Lion 1985)
- 594 (20°C, EPICS, Yurteri et al. 1987)
- 519 (20°C, calculated-P/C, Yurteri et al. 1987)
- 651 (EPICS, Ashworth et al. 1988)
- 604 (calculated- C_A/C_w , Eastcott et al. 1988)
- 605 (concentration ratio, Keeley et al. 1988)
- 637 (calculated-QSAR, Nirmalakhandan & Speece 1988b)
- 679 (batch stripping, Suntio et al. 1988)
- 533 (calculated-P/C, Munz & Roberts 1989)
- 680 (calculated, Mackay & Shiu 1990)
- 673 (selected, Mackay & Shiu 1990)
- 694 (calculated- C_A/C_w , Jury et al. 1990)

rs 1986)

kay & Wolkoff
1990, Mackay

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

- 2.69 (shake flask-UV, Fujita et al. 1964; quoted, Hansch et al. 1968; Hansch et al. 1972; Chiou et al. 1977; 1982; Chiou 1981; 1985; Hutchinson et al. 1980; McCall 1975; Whitehouse & Cooke 1982; Garbarnini & Lion 1985; Brooke et al. 1986; Hodson & Williams 1988; Suntio et al. 1988; Jafvert 1991)
- 2.11, 1.83 (shake flask-UV, calculated-M.O. indices, Rogers & Cammarata 1969)
- 2.69, 2.73, 2.11, 2.80 (quoted, Leo et al. 1971)
- 2.73, 2.54 (quoted, calculated- χ , Kier & Hall 1976)
- 2.62 (calculated-f const., Yalkowsky & Valvani 1976)
- 2.60 (calculated-f const., Rekker 1977; quoted, Harnisch et al. 1983)
- 2.69, 2.73, 2.71, 2.80 (Hansch & Leo 1979)
- 2.69 (quoted of Hansch & Leo 1979, Callahan et al. 1979; Harnish et al. 1983; Suntio et al. 1988)
- 2.69; 2.51 (quoted; calculated-S, Mackay et al. 1980)
- 2.21 (shake flask-LSC, Banerjee et al. 1980; quoted, Suntio et al. 1988; Olsen & Davis 1990)
- 2.58, 2.68 (quoted, shake flask-HPLC, Nahum & Horvath 1980)
- 2.59 (HPLC- k' , Hanai et al. 1981)
- 2.69, 2.97 (quoted, HPLC- k' , McDuffie 1981)
- 2.59 (calculated-f const., Könemann 1981; quoted, Leegwater 1989)
- 2.58 (quoted, Valvani et al. 1981)
- 2.79 (calculated-f constants, Mabey et al. 1982)
- 2.78 (HPLC- k , Hammers et al. 1982)
- 2.59 (HPLC- k' , D'Amboise & Hanai 1982)
- 2.69, 2.65 (quoted, gen. col.-HPLC/UV, Teweri et al. 1982b,c)

ookerjee 1975;

d, Suntio et al.

; Pankow 1986;

- 2.69, 2.62 (quoted, HPLC-k', Miyake & Terada 1982)
- 2.77, 2.65 (quoted of HPLC methods, Harnisch et al. 1983)
- 2.69 (quoted, Verschueren 1983)
- 2.63 (calculated-f constants, Yalkowsky et al. 1983)
- 2.65 (gen. col.-HPLC/UV, Wasik et al. 1983)
- 2.74 (HPLC-k', Hafkanschaid & Tomlinson 1983b)
- 2.69, 2.52, 2.76 (quoted, calculated-MR & IP, MR, Yoshida et al. 1983)
- 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 (Platford 1979,1983)
- 2.11-2.80, 2.69 (range, quoted, Garst & Wilson 1984; quoted, Sabljic 1987b)
- 2.72 (HPLC-RV, Garst & Wilson 1984)
- 2.89 (HPLC-RT, Rapaport & Eisenreich 1984)
- 2.58, 2.78, 2.79 (quoted, HPLC/MS, calculated, Burkhard et al. 1985)
- 2.73 (quoted, Campbell & Luthy 1985)
- 2.65 (quoted, Miller et al. 1985; Vowles & Mantoura 1987; Szabo et al. 1990a,b)
- 2.66 (calculated-V₁, solvatochromic parameters, Taft et al. 1985)
- 2.73 (Hansch & Leo 1985; quoted, Howard 1990)
- 2.63 (quoted, Burkhard & Kuehl 1986)
- 2.78 (quoted, Tomlinson & Hafkanschaid 1986)
- 2.92 (calculated-V₁, solvatochromic parameters, Leahy 1986)
- 3.00 (HPLC-k', De Kock & Lord 1987)
- 2.65, 2.64 (gen. col.-RPLC, calculated-activity coeff., Schantz & Martire 1987)
- 2.69 (quoted, Ryan et al. 1988; Lee et al. 1989)
- 2.65 (quoted exptl., Doucette & Andren 1988)
- 2.60, 2.93, 2.81, 2.75, 3.01 (calculated- π , f const., HPLC-RT, MW, TSA, Doucette & Andren 1988)
- 2.11-2.94 (quoted range, Dearden & Bresnen 1988)
- 2.73, 2.39 (quoted, calculated-UNIFAC, Banerjee & Howard 1988)
- 2.73 (recommended, Sangster 1989)
- 2.63 (quoted, Isnard & Lambert 1988; 1989)
- 2.786 (slow stirring-GC, De Bruijn et al. 1989)
- 2.74, 2.73 (quoted, calculated-MO calculation, Bodor et al. 1989)
- 2.73, 2.791 (quoted, calculated-f constants, Bodor et al. 1989)
- 2.11-2.94 (quoted from the Medchem Data-base, Dearden 1990)
- 2.65 (quoted, Szabo et al. 1990a,b)
- 2.687 (quoted, Warne et al. 1990)

Bioconcentration Factor, log BCF:

- 1.12 (eels, Ogata & Miyake 1978)
- 0.22 (Manila clam, Nunes & Benville 1979)
- 0.62 (mussels, Geyer et al. 1982)
- 2.17 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

- 0.92 (goldfish, Ogata et al. 1984),
- 3.28, 2.58, 1.95 (activated sludge, algae, fish, Freitag et al. 1985)
- 0.89, 0.92 (fish, calculated, correlated, Sabljic 1987b)
- 1.12, 0.22, 0.72, 2.58, 1.95 (quoted: eels, Manila clam, mussels, algae, fish, Howard 1990)
- 1.99 (s. capricornutum, Herman et al. 1991)

3)
1983)
3)
1987b)

Sorption Partition Coefficient, log K_{oc} :

- 2.49 (soil, calculated- K_{ow} , Karickhoff et al. 1979)
- 2.43 (soil, calculated- K_{ow} , Means et al. 1980)
- 2.25 (Wilson et al. 1981)
- 2.39 (soil, Schwarzenbach & Westall 1981)
- 2.48 (sediment, calcd.- K_{ow} , Mabey et al. 1982)
- 1.89-2.28 (soil, headspace equilibrium technique, Garbarnini & Lion 1985)
- 1.93, 2.43, 2.49 (soil: calculated-S, K_{ow} , Garbarnini & Lion 1985)
- 2.32 (soil, calculated- χ , Sabljic 1987a & b)
- 1.12-2.85 (soil, calculated- K_{ow} , Sabljic 1987b)
- 2.58, 1.77, 3.28 (quoted: algae, fish, activated sludge, Halfon & Reggiani 1986)
- 2.00, 2.18 (quoted, Hodson & Williams 1988)
- 2.0, 2.18, 2.25 (quoted, Howard 1990)
- 2.18, 2.26 (quoted, HPLC-k', Szabo et al. 1990a,b)
- 1.99 (soil, Jury et al. 1990)

al. 1990a,b)

Sorption Partition Coefficient, log K_{om} :

- 1.29, 1.39 (untreated soil, Lee et al. 1989)
- 2.16-2.89 (organic cations treated soil, Lee et al. 1989)

ire 1987)

TSA, Doucette

Half-Lives in the Environment:

- Air: 4.6 hours (Doyle et al. 1975) and 2.4-24 hours (Darnall et al. 1976) based on rate of disappearance for the reaction with hydroxy radicals; 10-104 hours, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991).
- Surface Water: 5.55 hours, based on evaporative loss at 25°C and 1 m depth of water (calculated, Mackay & Leinonen 1975; Haque et al. 1980); 96-528 hours, based on estimated aqueous aerobic biodegradation half-life (Wakeham et al. 1983; Howard et al. 1991).
- Groundwater: estimated half-life from observed persistence in groundwater of Netherlands, 0.3 year (Zoeteman et al. 1981); 168-672 hours, 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: 96-528 hours, based on estimated aqueous aerobic biodegradation half-life (Wakeham et al. 1983; Howard et al. 1991); < 10 days (Ryan et al. 1988); 5 days assumed first-order biological/chemical degradation in soil (Jury et al. 1990); disappearance half-life from test soils, < 2.0 days (Anderson et al. 1991).

Biota: 10 hours clearance from fish (Neely 1980).

Environmental Fate Rate Constants or Half-Lives:

Volatilization: $t_{1/2} = 5.18$ hours from water depth of 1 m (Mackay & Leinonen 1975; Haque et al. 1980); half-lives from marine mesocosm: 16 days at 8-16°C in the spring, 1.5 days at 20-22°C in the summer and 13 days at 3-7°C in the winter (Wakeham et al. 1983); estimated evaporation half-life from a river of 1 m depth with wind speed of 3 m/sec and water current of 1 m/s to be 2.9 h at 20°C (Lyman et al. 1982); estimated half-life for evaporation from a river and lake to be 1 and 4 days (Howard 1990).

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

Oxidation: photooxidation half-life in water: 321-1284 hours, based on measured rate data for hydroxy radicals in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991); calculated rate constant for the reaction with OH radicals in ambient LA basin air at 300°K was 2.5×10^9 liter mole⁻¹ sec⁻¹ with an initial concentration of 9.8×10^{10} mole liter⁻¹ (Doyle et al. 1975); absolute room temperature rate constant for the reaction with OH radicals determined by flash photolysis-resonance fluorescence was 5.78×10^{12} cm³ molecule⁻¹ sec⁻¹ (Hansen et al. 1975); rate constant for reaction in gas phase with hydroxyl radicals = 3.6×10^9 L mol⁻¹ s⁻¹ and $t_{1/2} = 2.4-24$ h (Darnall et al. 1976); half-life about 15 hours, probably not an important aquatic fate (Callahan et al. 1979); k (singlet oxygen) $\ll 360$ M⁻¹ h⁻¹ & k (RO₂) = 144 M⁻¹ h⁻¹ (Mabey et al. 1982); reaction with ozone at 300°K having a rate constant of 160 cm³ mol⁻¹ sec⁻¹ (Lyman et al. 1982); rate constant $k = 3.5 \times 10^9$ M⁻¹ sec⁻¹, $t_{1/2} = 1.6$ days, oxidation by OH radicals in the atmosphere (Mill 1982); photooxidation half-life in air: 10-104 hours, based on measured room temperature rate constant of 5.7×10^{12} cm³ molecule⁻¹ sec⁻¹ for the vapor phase reaction with hydroxy radicals in air (Atkinson 1985; Howard et al. 1991); rate constant for the gas phase reaction with OH radicals at 25°C, 6.03×10^{12} cm³ molecule⁻¹ sec⁻¹ (Ohta & Ohyama 1985).

Hydrolysis: not aquatically significant (Callahan et al. 1979); $k_h = 0$, no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation: 100% biodegraded after 192 hours at 13°C with an initial concentration of 2.22×10^{-6} l/l (Jamison et al. 1976); half-life in uncontaminated estuarine water estimated to be 90 days and in oil polluted water estimated to be 30 days (Lee 1977); significant degradation in aerobic environment, $k_b = 0.5$ day⁻¹ (Tabak et al. 1981; Mills et al. 1982); aqueous aerobic biodegradation half-life: 96-528 hours, based on an acclimated seawater dieaway test (Wakeham et al. 1983; Howard et al. 1991); anaerobic aqueous biodegradation half-life: 1344-5040 hours, based on anaerobic screening test data and anaerobic sediment grab sample data (Horowitz et al. 1982; Howard et al. 1991); first-order rate constant 0.07 year⁻¹ with a half-life of 39 days (Zoeteman et al. 1981; Olsen & Davis 1990).

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

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives: half-life of elimination from eels in seawater estimated to be 1.4 days (Ogata & Miyake 1978).

Leinonen 1975;
s at 8-16°C in the
7°C in the winter
n a river of 1 m
i/s to be 2.9 h at
from a river and

982).

on measured rate
ms 1973; Howard
1 OH radicals in
e⁻¹ with an initial
) ; absolute room
terminated by flash
le⁻¹ sec⁻¹ (Hansen
droxyl radicals =
half-life about 15
1979); k (singlet
oy et al. 1982);
0 cm³ mol⁻¹ sec⁻¹
, $t_{1/2} = 1.6$ days,
oxidation half-life
rate constant of
hydroxy radicals
for gas phase
e⁻¹ (Ohta &

, no hydrolyzable

itial concentration
ed estuarine water
be 30 days (Lee
.5 day⁻¹ (Tabak et
half-life: 96-528
ham et al. 1983;
f-life: 1344-5040
ic sediment grab
order rate constant
l; Olsen & Davis

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ILLUSTRATED HANDBOOK

OF
PHYSICAL-CHEMICAL
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ENVIRONMENTAL FATE

FOR
ORGANIC CHEMICALS

Volume IV
Oxygen, Nitrogen, and
Sulfur Containing Compounds

Donald Mackay
Wan-Ying Shiu
Kuo-Ching Ma

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Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals

Volume I

Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs

Monoaromatic Hydrocarbons
Chlorobenzenes
Polychlorinated Biphenyls (PCBs)

Volume II

Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, Dibenzofurans

Polynuclear Aromatic Hydrocarbons (PAHs)
Chlorinated Dibenzo-*p*-Dioxins
Chlorinated Dibenzofurans

Volume III

Volatile Organic Chemicals

Hydrocarbons
Halogenated Hydrocarbons
Ethers

Volume IV

Oxygen, Nitrogen, and Sulfur Containing Compounds

Alcohols
Aldehydes and Ketones
Phenolic Compounds
Carboxylic Acids
Esters
Nitrogen and Sulfur Compounds

als.

omatic hydrocarbons,
trogen, and sulfur

che —

91-33888

material is quoted with
e been made to publish
validity of all materials

ectronic or mechanical,
system, without prior

creating new works, or

l.

Common Name: Acetone
Synonym: 2-propanone, dimethylketone, DMK
Chemical Name: acetone, 2-propanone
CAS Registry No: 67-64-1
Molecular Formula: CH_3COCH_3
Molecular Weight: 58.08
Melting Point ($^{\circ}\text{C}$):
-94.6 (Stull 1947; Verschueren 1983)
-95.35 (Weast 1982-83; Dean 1985; Howard 1990)
-94.7 (Riddick et al. 1986)
Boiling Point ($^{\circ}\text{C}$):
56.5 (Stull 1947)
56.20 (Weast 1982-83; Verschueren 1983; Howard 1990)
56.06 (Boublik et al. 1984; Riddick et al. 1986)
56.24 (Dean 1985)
56.00 (Banerjee et al. 1990)
Density (g/cm^3 at 20°C):
0.7899 (Weast 1982-83)
0.7910 (Verschueren 1983)
0.7908 (Dean 1985)
0.78998 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
77.5 (exptl. at normal B.P., Lee et al. 1972; quoted, Reid et al. 1977)
73.8 (Rohrschneider 1973)
74.0 (LeBas method, Reid et al. 1977; Abernethy et al. 1988)
73.4 (Taft et al. 1985; Kamlet et al. 1986,87; Leahy 1986)
38.0 (intrinsic volume V_i , Leahy 1986; Kamlet et al. 1987; Abernethy et al. 1988)
59.3 (calculated-density, Jarworska & Schultz 1993)
Molecular Volume (\AA^3):
Total Surface Area, TSA (\AA^2):
Heat of Fusion ΔH_{fus} , kcal/mol:
1.360 (Riddick et al. 1986)
Entropy of Fusion ΔS_{fus} , cal/mol·K (e.u.):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 13.5$ e.u.), F: 1.0
Water Solubility (g/m^3 or mg/L at 25°C):
infinite (20°C , Palit 1947)
485610 (calculated-activity coefficient of Perry 1950, Rathbun et al. 1982)
miscible (Dean 1985; Pinal et al. 1991)
infinite (Riddick et al. 1986; Howard 1990)
483090, 483090 (quoted, calculated- V_i and solvatochromic p., Taft et al. 1986)
440580, 698275 (quoted, calculated- V_i and solvatochromic p., Leahy 1986)
440580, 748215 (quoted, calculated- V_i and solvatochromic p., Kamlet et al. 1987)
miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C):

- 199 — 29613 (interpolated-regression of tabulated data, Stull 1947)
26660 (22.7°C, Stull 1947)
30494 (Perry 1950; quoted, Rathbun et al. 1982)
30792 (Buttery et al. 1969; quoted, Howard 1990)
30812 (Hoy 1970)
30806 (ebulliometry, fitted to Antoine eqn., Ambrose et al. 1975)
30867, 31522 (quoted exptl., calculated-Antoine eqn., Boublik et al. 1984)
30780 (calculated-Antoine eqn., Dean 1985)
232 — 30926 (Howard et al. 1986; quoted, Banerjee et al. 1990)
30806 (Riddick et al. 1986)
19330 (calculated-solvatochromic p., Banerjee et al. 1990)

Henry's Law Constant (Pa·m³/mol):

- 3.342 (partial pressure, Butler & Ramchandani 1935)
3.960 (shake flask, partial vapor pressure-GC, Burnett 1963; quoted, Betterton 1991)
3.25 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
3.97 (shake flask, partial vapor pressure-GC, Buttery et al. 1969; quoted, Betterton 1991)
4.140 (quoted, calculated-K_{AW}, Buttery et al. 1969)
4.020 (quoted, exptl., Hine & Mookerjee 1975)
3.929 (calculated-group contribution, Hine & Mookerjee 1975)
2.912 (calculated-bond contribution, Hine & Mookerjee 1975)
4.104 (calculated-γ·P, Rathbun & Tai 1982)
3.334 (calculated-MW, Rathbun & Tai 1982)
3.648 (calculated-P/C from Perry 1950 data, Rathbun et al. 1982)
3.93 (headspace-GC, Snider & Dawson 1985; quoted, Howard 1990)
3.378 (quoted, Gaffney et al. 1987)
2.93 (gas stripping-HPLC, Zhou & Mopper 1990)
3.070 (gas stripping-GC, Betterton 1991)
3.27, 3.90, 3.75, 3.96 (quoted literature values, Betterton)
4.331 (computed, Yaws et al. 1991)

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

- 0.24 (shake flask-CR, Collander 1951; quoted, Leo et al. 1971; Sangster 1989)
-0.73 (calculated, Iwasa et al. 1965)
-0.21 (Leo et al. 1969)
-0.24 (quoted, shake flask at pH 7, Unger et al. 1978)
-0.30 (calculated-f const., Könemann 1981)
-0.24 (calculated-f const. as per Hansch & Leo 1979, Veith et al. 1983)
-0.24 (Verschueren 1983; quoted, Pinal et al. 1991)
-0.24 (Hansch & Leo 1985; quoted, Howard 1990)
0.38 (computed, Klopman et al. 1985; quoted, Pangrekar et al. 1994)
-0.24, -0.13 (quoted, calculated-V₁ and solvatochromic p., Taft et al. 1985)
-0.24 (measured, GEMS 1986; quoted, Vaishnav et al. 1987)

- 0.24, -0.24 (quoted, calculated-V₁ and solvatochromic p., Leahy 1986)
- 0.48 (shake flask-GC, Tani et al. 1986; quoted, Sangster 1989)
- 0.24 (quoted, Abernethy et al. 1988)
- 0.24, -0.24 (quoted from Hansch & Leo 1979, quoted from CLOGP, Bodor et al. 1989)
- 0.027, -0.07 (calculated from CLOGP, calculated-MO, Bodor et al. 1989)
- 0.24 (recommended, Sangster 1989)
- 0.24 (quoted, Verhaar et al. 1992)
- 0.24 (calculated as per Hansch & Leo 1979, Dallos et al. 1993)
- 0.37 (calculated-UNIFAC, Dallos et al. 1993)
- 0.24 (quoted from CLOGP 3.15, Jaworska & Schultz 1993)
- 0.266 (calculated-QSAR, Kollig 1993)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

- 0.586 (calculated-K_{ow}, Kollig 1993)

Half-Lives in the Environment:

Air: half-life of >9.9 days for the gas-phase reaction with hydroxyl radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976); photooxidation half-life of 279-2790 hours, based on measured data for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991).

Surface water: photooxidation half-life of 11.3-453 years, based on measured data for the reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991); 24-168 hours, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: 48-336 hours, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: 24-168 hours, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

Environmental Fate Rate Constants or Half-Lives:

Volatilization: using Henry's law constant, a half-life of 20 hours was estimated for a model river 1 m deep flowing at 1 m/sec with a wind velocity of 3 m/sec (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: photooxidation half-life of 11.3-453 years, based on measured data for the reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991); photooxidation half-life of >9.9 days for the gas-phase reaction with hydroxyl radicals in air, based on the rate of disappearance

of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976); rate constant of $(0.23 \pm 0.03) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{sec}^{-1}$ by flash photolysis-resonance fluorescence for the gas-phase reaction with OH radicals at 300 K in air (Zetzsch 1982; quoted, Atkinson 1985); rate constant of $(0.62 \pm 0.09) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{sec}^{-1}$ by relative rate technique to *n*-hexane for the gas-phase reaction with OH radicals at 298 K in air (Chiorboli et al. 1983; quoted, Atkinson 1985); photooxidation half-life of 279-2790 hours, based on measured data for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1985; selected, Howard et al. 1991); rate constant of $2.16 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{sec}^{-1}$ for the gas-phase reaction with hydroxyl radicals in air and $1.80 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{sec}^{-1}$ for the aqueous-phase reaction with hydroxyl radicals in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988).

Hydrolysis:

Biodegradation: biodegradation rate constants of 0.016-0.020 h⁻¹ in 30 mg/L activated sludge after a time lag of 20-25 hours (Urano & Kato 1986b); aqueous aerobic half-life of 24-168 hours, based on unacclimated aqueous screening test data (Bridie et al. 1979; Dore et al. 1975; selected, Howard et al. 1991); aqueous anaerobic half-life of 96-672 hours, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); experimental rate constant of 0.0440 h⁻¹ compared to group contribution method predicted rate constants of 0.0433 h⁻¹ (nonlinear) and 0.043 h⁻¹ (linear) (Tabak & Govind 1993).

Biotransformation:

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