

Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry

<http://www.mpch-mainz.mpg.de/~sander/res/henry.html>

Rolf Sander
Air Chemistry Department
Max-Planck Institute of Chemistry
PO Box 3060
55020 Mainz
Germany
e-mail: sander@mpch-mainz.mpg.de

Version 3 (April 8, 1999)

© Rolf Sander (non-commercial reproduction permitted)

Contents

1	Introduction	3
2	The physical quantity of solubility	3
3	Temperature dependence	3
4	Unit conversions	3
5	How to use the Tables	4
6	Further Sources of Information	4
7	Data Table (Inorganic)	6
	oxygen (O)	6
	hydrogen (H)	6
	nitrogen (N)	7
	fluorine (F)	8
	chlorine (Cl)	9
	bromine (Br)	10
	iodine (I)	11
	sulfur (S)	12
	rare gases	13
	other elements	13

8 Data Table (Organic)	14
alkanes (C and H only)	14
cycloalkanes (C and H only)	27
aliphatic alkenes and cycloalkenes (C and H only)	28
aliphatic alkynes (C and H only)	30
mononuclear aromatics (C and H only)	31
terpenes and polynuclear aromatics (C and H only)	35
alcohols (ROH) (C, H, and O only)	37
polyols (R(OH) _n) (C, H, and O only)	41
peroxides (ROOH) and peroxy radicals (ROO) (C, H, and O only)	43
aldehydes (RCHO) (C, H, and O only)	44
ketones (RCOR) (C, H, and O only)	46
carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (C, H, and O only)	48
esters (RCOOR) (C, H, and O only)	50
ethers (ROR) (C, H, and O only)	54
miscellaneous, e.g. multiple functional groups (C, H, and O only)	55
compounds with nitrogen: amines (RNH ₂) (C, H, O, and N only)	58
compounds with nitrogen: amino acids (RCHNH ₂ COOH)	59
compounds with nitrogen: heterocycles (C, H, O, and N only)	59
compounds with nitrogen: nitrates (RONO ₂) (C, H, O, and N only)	61
compounds with nitrogen: nitriles (RCN) (C, H, O, and N only)	65
compounds with nitrogen: nitro (RNO ₂) (C, H, O, and N only)	66
compounds with fluorine	68
aliphatic compounds with chlorine	71
aromatic compounds with chlorine	82
compounds with chlorine and fluorine	84
compounds with bromine	86
compounds with iodine	89
compounds with sulfur	90
polychlorobiphenyls (PCB's), pesticides, etc.	92
9 Notes	96
10 Acknowledgements	99
References	99

1 Introduction

Henry's law constants (solubilities) of trace gases of potential importance in environmental chemistry (atmospheric chemistry, waste water treatment, ...) have been collected and converted into a uniform format.

Disclaimer: Although this compilation has been edited with greatest care the possibility of errors cannot be excluded. If you use data from this table it is recommended that you also check the original literature. If you find an error in this table, please tell me about it!

2 The physical quantity of solubility

There are several ways of describing the solubility of a gas in water. Usually the Henry's law constant k_H is defined as:

$$k_H \stackrel{\text{def}}{=} c_a/p_g \quad (1)$$

Here, c_a is the concentration of a species in the aqueous phase and p_g is the partial pressure of that species in the gas phase. If k_H refers to standard conditions ($T^\ominus = 298.15$ K) it will be denoted as k_H^\ominus .

Henry's law constant can also be expressed as the dimensionless ratio between the aqueous-phase concentration c_a of a species and its gas-phase concentration c_g :

$$k_H^{cc} \stackrel{\text{def}}{=} c_a/c_g = k_H \times RT \quad (2)$$

where R = gas constant and T = temperature. To distinguish these different physical quantities, this constant has been named k_H^{cc} here.

Sometimes the reciprocal value $k_{H,\text{inv}}^{px}$ is used, representing the volatility instead of the solubility. The usual definition is:

$$k_{H,\text{inv}}^{px} \stackrel{\text{def}}{=} p_g/x_a = \frac{\varrho_{\text{H}_2\text{O}}}{M_{\text{H}_2\text{O}} \times k_H} \quad (3)$$

where x_a = molar mixing ratio in the aqueous phase, $\varrho_{\text{H}_2\text{O}}$ = density of water, and $M_{\text{H}_2\text{O}}$ = molar mass of water.

3 Temperature dependence

A simple way to describe Henry's law as a function of temperature is:

$$k_H = k_H^\ominus \times \exp\left(\frac{-\Delta_{\text{soln}}H}{R} \left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \quad (4)$$

where $\Delta_{\text{soln}}H$ = enthalpy of solution. Here, the temperature dependence is:

$$\frac{-d \ln k_H}{d(1/T)} = \frac{\Delta_{\text{soln}}H}{R} \quad (5)$$

4 Unit conversions

Detailed information about the conversion between different units and definitions of Henry's law constants is given by Sander [1999]. Here is a short summary:

The commonly used unit for k_H is $[\text{M}/\text{atm}] = \left[\frac{\text{mol}_{\text{aq}}/\text{dm}_{\text{aq}}^3}{\text{atm}}\right]$. The official SI unit is $\left[\frac{\text{mol}_{\text{aq}}/\text{m}_{\text{aq}}^3}{\text{Pa}}\right]$. The conversion is:

$$\frac{k_H}{[\text{M}/\text{atm}]} = 101.325 \times \frac{k_H}{[(\text{mol}_{\text{aq}}/\text{m}_{\text{aq}}^3)/\text{Pa}]} \quad (6)$$

The relation between k_H and k_H^{cc} is:

$$\frac{T}{[\text{K}]} \times \frac{k_H}{[\text{M}/\text{atm}]} = 12.2 \times k_H^{cc} \quad (7)$$

At $T = 298.15$ K this leads to:

$$\frac{k_{\text{H}}}{[\text{M}/\text{atm}]} = 0.0409 \times k_{\text{H}}^{\text{cc}} \quad (8)$$

The commonly used unit for $k_{\text{H,inv}}^{\text{px}}$ is [atm]. The product of k_{H} and $k_{\text{H,inv}}^{\text{px}}$ is constant:

$$\frac{k_{\text{H}}}{[\text{M}/\text{atm}]} \times \frac{k_{\text{H,inv}}^{\text{px}}}{[\text{atm}]} = 55.3 \quad (9)$$

5 How to use the Tables

Inorganic substances are sorted according to the elements they contain. The order chosen is: O, H, N, F, Cl, Br, I, S, rare gases, others.

Organic substances (i.e. everything with carbon, including CO and CO₂) are sorted somewhat arbitrarily by increasing chain length and complexity. Hetero atoms (N, F, Cl, Br, I, and S) are sorted in the same way as for inorganic compounds.

The column labeled 'substance' gives the systematic name, the chemical formula, trivial names (if any), and in several cases the CAS registry number (in square brackets).

The column labeled ' k_{H}^{\ominus} ' contains the Henry's law constants as defined in equation (1), rounded to two significant digits and given in the unit [M/atm].

The column labeled ' $-\text{d} \ln k_{\text{H}}/\text{d}(1/T)$ ' contains the temperature dependence of the Henry's law constants as defined in equations (4) and (5), rounded to two significant digits and given in the unit [K].

For each table entry the column labeled 'type' denotes how the Henry's law constant was obtained in the given reference. Literature reviews are usually most reliable, followed by original publications of experimental determinations of k_{H} . Other data has to be treated more carefully. The types listed here are roughly ordered by decreasing reliability:

'L'	The cited paper is a literature review.
'M'	Original publication of a measured value (e.g. head-space or bubble column technique as explained by <i>Betterton</i> [1992]).
'V'	Vapor pressure of the pure substance is used to determine the Henry's law constant (c/p for a saturated solution).
'R'	The cited paper presents a recalculation of previously published material (e.g. extrapolation to a different temperature or concentration range).
'T'	Thermodynamical calculation ($\Delta_{\text{soln}}G = -RT \ln k_{\text{H}}$, see <i>Sander</i> [1999] for details).
'C'	The paper that is cited here refers to another reference which I could not obtain (e.g. personal communication, Ph.D. theses, internal papers etc.).
'X'	I haven't seen the paper that I cite here. I found it referenced by another paper or I know about it through others.
'?'	The cited paper doesn't clearly state how the value was obtained.
'E'	The value is estimated. Estimates are only listed if no reliable measurements are available for that compound.

In some cases there might be good agreement between different authors. However, if the original work they refer to is not known one has to be careful when evaluating the reliability. It is possible that they were recalculating data from the same source. The similarity in that case would not be due to independent investigations.

6 Further Sources of Information

Further important references:

- monoaromatic hydrocarbons, chlorobenzenes, and PCBs: *Mackay et al.* [1992a]

- polynuclear aromatic hydrocarbons, polychlorinated dioxins, and dibenzofuranes: *Mackay et al.* [1992b]
- volatile organic chemicals: *Mackay et al.* [1993]
- oxygen, nitrogen, and sulfur containing compounds: *Mackay et al.* [1995]
- pestizides, PCB's, etc.: *Westcott et al.* [1981]; *Burkhard et al.* [1985]; *Hassett and Milicic* [1985]; *Yin and Hassett* [1986]; *Murphy et al.* [1987]; *Shiu et al.* [1988]; *Rice et al.* [1997]; *Fendinger and Glotfelty* [1988]; *Fendinger et al.* [1989]; *De Maagd et al.* [1998]; *Duce et al.* [1991]
- additional references that are not (yet) included: *Lide and Frederikse* [1995]; *Shiu et al.* [1994]; *Watts and Brimblecombe* [1987]; *Wright et al.* [1992a]; *Tse et al.* [1992]; *Kolb et al.* [1992]; *Ettre et al.* [1993]; *Gan and Yates* [1996]; *Peng and Wan* [1997]; *Roberts and Dändliker* [1983]; *Economou et al.* [1997]; *Wong and Wang* [1997]; *Suleimenov and Krupp* [1994]; *Heron et al.* [1998]; *Becker et al.* [1998]; *Leuenberger et al.* [1985]
- predictive methods for Henrys law coefficients (QSPRs): *Russell et al.* [1992]; *Nirmalakhandan et al.* [1997]; *Brennan et al.* [1998]

On the Internet:

- The NIST Chemistry WebBook at <http://webbook.nist.gov/chemistry>
- The Pesticide Properties Database (PPD) at <http://www.arsusda.gov/rsml/ppdb2.html>

7 Data Table (Inorganic)

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
oxygen (O)					
oxygen	1.3×10^{-3}	1700	<i>Loomis</i> [1928]	X	1
O ₂	1.2×10^{-3}	1800	<i>Carpenter</i> [1966]	M	
[7782-44-7]	1.3×10^{-3}	1500	<i>Wilhelm et al.</i> [1977]	L	
	1.3×10^{-3}	1700	<i>Dean</i> [1992]	?	2
	1.3×10^{-3}	1500	<i>Lide and Frederikse</i> [1995]	L	
	1.2×10^{-3}	1700	<i>Kavanaugh and Trussell</i> [1980]	X	3
ozone	1.2×10^{-2}	2300	<i>Loomis</i> [1928]	X	1
O ₃	1.3×10^{-2}	2000	<i>Briner and Perrottet</i> [1939]	M	
[10028-15-6]	1.3×10^{-2}	2000	<i>Wilhelm et al.</i> [1977]	L	
	1.2×10^{-2}		<i>Durham et al.</i> [1981]	C	
	1.1×10^{-2}	2300	<i>Kosak-Channing and Helz</i> [1983]	M	
	1.2×10^{-2}	2700	<i>Chameides</i> [1984]	T	
	9.4×10^{-3}	2500	<i>Hoffmann and Jacob</i> [1984]	?	4
	1.1×10^{-2}	2400	<i>Jacob</i> [1986]	C	
	9.4×10^{-3}	2400	<i>Seinfeld</i> [1986]	C	
	8.9×10^{-3}	2900	<i>Kavanaugh and Trussell</i> [1980]	X	3
hydrogen (H)					
hydrogen	7.8×10^{-4}		<i>Hine and Weimar</i> [1965]	R	
H ₂	7.8×10^{-4}	490	<i>Wilhelm et al.</i> [1977]	L	
[1333-74-0]	7.8×10^{-4}	640	<i>Dean</i> [1992]	?	2
	7.8×10^{-4}	500	<i>Lide and Frederikse</i> [1995]	L	
hydroxyl radical	2.9×10^1	3100	<i>Berdnikov and Bazhin</i> [1970]	T	5
OH	3.2×10^1		<i>Mozurkewich</i> [1986]	T	
[3352-57-6]	2.5×10^1	5300	<i>Jacob</i> [1986]	C	6
	2.5×10^1		<i>Lelieveld and Crutzen</i> [1991]	C	
	2.0×10^2		<i>Lelieveld and Crutzen</i> [1991]	C	
	9.0×10^3		<i>Lelieveld and Crutzen</i> [1991]	C	
	3.0×10^1	4500	<i>Hanson et al.</i> [1992]	T	
hydroperoxy radical	4.6×10^3	4800	<i>Berdnikov and Bazhin</i> [1970]	T	5
HO ₂	9.0×10^3		<i>Chameides</i> [1984]	T	
[3170-83-0]	1.2×10^3		<i>Schwartz</i> [1984]	T	7
		6600	<i>Jacob</i> [1986]	E	
	9.0×10^3		<i>Weinstein-Lloyd and Schwartz</i> [1991]	T	
	4.0×10^3	5900	<i>Hanson et al.</i> [1992]	T	
	5.7×10^3		<i>Régimbal and Mozurkewich</i> [1997]	R	
hydrogen peroxide	7.1×10^4	7000	<i>Martin and Damschen</i> [1981]	T	
H ₂ O ₂	7.1×10^4	7300	<i>Hoffmann and Jacob</i> [1984]	?	4
[7722-84-1]	1.4×10^5		<i>Yoshizumi et al.</i> [1984]	M	8
	9.7×10^4	6600	<i>Chameides</i> [1984]	T	
	6.9×10^4	7900	<i>Hwang and Dasgupta</i> [1985]	M	
	1.0×10^5	6300	<i>Lind and Kok</i> [1994]	M	9
	8.3×10^4	7400	<i>O'Sullivan et al.</i> [1996]	M	
	1.1×10^5	7500	<i>Staffelbach and Kok</i> [1993]	M	10
	8.6×10^4	6500	<i>Zhou and Lee</i> [1992]	M	

substance	$\frac{k_H^\ominus}{[M/atm]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
nitrogen (N)					
ammonia NH ₃ [7664-41-7]	5.9×10 ¹ 5.7×10 ¹ 1.0×10 ¹ 6.1×10 ¹ 7.6×10 ¹ 5.8×10 ¹ 7.8×10 ¹ 5.8×10 ¹ 5.6×10 ¹ 5.6×10 ¹ 6.1×10 ¹ 2.7×10 ¹ 6.2×10 ¹ 5.4×10 ¹ 6.0×10 ¹	4100 4100 1500 4200 3400 4100 4100 4100 4100 4200 4200 2100 4100 4200 4400	<i>Sillen and Martell</i> [1964] <i>Robinson and Stokes</i> [1970] <i>Wilhelm et al.</i> [1977] <i>Edwards et al.</i> [1978] <i>Hales and Drewes</i> [1979] <i>Chameides</i> [1984] <i>Holzwarth et al.</i> [1984] <i>Hoffmann and Jacob</i> [1984] <i>Dasgupta and Dong</i> [1986] <i>Dasgupta and Dong</i> [1986] <i>Clegg and Brimblecombe</i> [1989] <i>Dean</i> [1992] <i>Van Krevelen et al.</i> [1949] <i>Bone et al.</i> [1983] <i>Kavanaugh and Trussell</i> [1980]	X X L L M T M ? M T M ? X ? X	1 1 2 11 12 3
hydrazoic acid HN ₃ [7782-79-8]	9.9	3100	<i>Wilhelm et al.</i> [1977]	L	
dinitrogen monoxide N ₂ O (nitrous oxide, laughing gas) [10024-97-2]	2.5×10 ⁻² 2.6×10 ⁻² 2.4×10 ⁻² 2.5×10 ⁻² 2.4×10 ⁻² 2.5×10 ⁻² 2.4×10 ⁻²	2600 2800 2600 2700	<i>Loomis</i> [1928] <i>Liss and Slater</i> [1974] <i>Wilhelm et al.</i> [1977] <i>Seinfeld</i> [1986] <i>Dean</i> [1992] <i>Lide and Frederikse</i> [1995] <i>Perry</i> [1963]	X ? L ? ? L X	1 13 2 14
nitrogen N ₂ [7727-37-9]	6.5×10 ⁻⁴ 6.1×10 ⁻⁴	1300 1300	<i>Wilhelm et al.</i> [1977] <i>Kavanaugh and Trussell</i> [1980]	L X	3
nitrogen monoxide NO (nitric oxide) [10102-43-9]	7.9×10 ⁻⁷ 1.4×10 ⁻³ 1.9×10 ⁻³ 1.9×10 ⁻³ 1.9×10 ⁻³ 1.9×10 ⁻³	3800 1500 1700 1400	<i>Wilhelm et al.</i> [1977] <i>Zafirion and McFarland</i> [1980] <i>Schwartz and White</i> [1981] <i>Durham et al.</i> [1981] <i>Dean</i> [1992] <i>Lide and Frederikse</i> [1995]	L M L C ? L	2
nitrogen dioxide NO ₂ [10102-44-0]	3.4×10 ⁻² 7.0×10 ⁻³ 4.0×10 ⁻² 2.4×10 ⁻² 1.2×10 ⁻² 4.1×10 ⁻² 1.2×10 ⁻²	1800 2500	<i>Berdnikov and Bazhin</i> [1970] <i>Lee and Schwartz</i> [1981] <i>Lee and Schwartz</i> [1981] <i>Lee and Schwartz</i> [1981] <i>Schwartz and White</i> [1981] <i>Durham et al.</i> [1981] <i>Chameides</i> [1984]	T M C C L C T	5 15
nitrogen trioxide NO ₃ (nitrate radical) [12033-49-7]	3.4×10 ⁻² 1.2×10 ¹ 2.0 6.0×10 ⁻¹ see note 1.8	2000 1900 2000	<i>Berdnikov and Bazhin</i> [1970] <i>Chameides</i> [1986] <i>Thomas et al.</i> [1993] <i>Rudich et al.</i> [1996] <i>Seinfeld and Pandis</i> [1998] <i>Thomas et al.</i> [1998]	T T M M M M	5 16 17

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
dinitrogen trioxide N ₂ O ₃ [10544-73-7]	6.0×10 ⁻¹ 2.6×10 ¹		<i>Schwartz and White</i> [1981] <i>Durham et al.</i> [1981]	L C	
dinitrogen tetroxide N ₂ O ₄ [10544-72-6]	1.4 1.6		<i>Schwartz and White</i> [1981] <i>Durham et al.</i> [1981]	L C	
dinitrogen pentoxide N ₂ O ₅ (nitric anhydride) [10102-03-1]	∞ 2.1 ∞	3400	<i>Jacob</i> [1986] <i>Fried et al.</i> [1994] <i>Sander and Crutzen</i> [1996]	E E E	18 19 18
nitrous acid HNO ₂ [7782-77-6]	4.9×10 ¹ 3.7×10 ¹ 4.9×10 ¹ 4.8×10 ¹ 4.9×10 ¹ 5.0×10 ¹	4800 4800 4700 4900 4900	<i>Schwartz and White</i> [1981] <i>Durham et al.</i> [1981] <i>Chameides</i> [1984] <i>Martin</i> [1984] <i>Park and Lee</i> [1988] <i>Becker et al.</i> [1996]	L C T T M M	
nitric acid HNO ₃ [7697-37-2]	2.1×10 ⁵ 8.9×10 ⁴ 2.6×10 ⁶ 3.5×10 ⁵ /K _A 2.4×10 ⁶ /K _A 2.1×10 ⁵	8700 8700 8700 8700 8700	<i>Schwartz and White</i> [1981] <i>Durham et al.</i> [1981] <i>Chameides</i> [1984] <i>Hoffmann and Jacob</i> [1984] <i>Brimblecombe and Clegg</i> [1989] <i>Lelieveld and Crutzen</i> [1991]	T C T ? T R	20, 4 20, 21 22
pernitric acid HNO ₄ [26404-66-0]	2.0×10 ⁴ 1.0×10 ⁵ 1.2×10 ⁴ 4.0×10 ³	0 6900	<i>Jacob et al.</i> [1989] <i>Möller and Mauersberger</i> [1992] <i>Régimbal and Mozurkewich</i> [1997] <i>Amels et al.</i> [1996]	C E T M	23
fluorine (F)					
fluorine atom F [14762-94-8]	2.1×10 ⁻²	400	<i>Berdnikov and Bazhin</i> [1970]	T	5
hydrogen fluoride HF [7664-39-3]	9.6/K _A	7400	<i>Brimblecombe and Clegg</i> [1989]	T	20, 21
nitrogen trifluoride NF ₃ [7783-54-2]	7.9×10 ⁻⁴	1900	<i>Wilhelm et al.</i> [1977]	L	
dinitrogen tetrafluoride N ₂ F ₄ (tetrafluorohydrazine) [10036-47-2]	8.5×10 ⁻⁴	2500	<i>Wilhelm et al.</i> [1977]	L	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
chlorine (Cl)					
hydrogen chloride HCl [7647-01-0]	1.9×10 ¹ 1.7×10 ⁵ / <i>K</i> _A 1.5×10 ³ 2.0×10 ¹ 1.1 2.5×10 ³ 2.0×10 ⁶ / <i>K</i> _A 1.9×10 ¹ 2.0×10 ⁶ / <i>K</i> _A	9000 2000 9000 600 9000	<i>Loomis</i> [1928] <i>Loomis</i> [1928] <i>Chen et al.</i> [1979] <i>Graedel and Goldberg</i> [1983] <i>Marsh and McElroy</i> [1985] <i>Seinfeld</i> [1986] <i>Brimblecombe and Clegg</i> [1989] <i>Dean</i> [1992] <i>Wagman et al.</i> [1982]	X X X C T ? T ? T	1 1,20 1 13 20, 21 2
hypochlorous acid HOCl [7790-92-3]	7.3×10 ² 4.8×10 ² 9.3×10 ² 6.6×10 ² 2.6×10 ²	 5900 5100	<i>Holzwarth et al.</i> [1984] <i>Hanson and Ravishankara</i> [1991] <i>Blatchley et al.</i> [1992] <i>Huthwelker et al.</i> [1995] <i>Wagman et al.</i> [1982]	M M M L T	24
nitrosyl chloride NOCl [2696-92-6]	> 0.05		<i>Scheer et al.</i> [1997]	M	
nitryl chloride ClNO ₂ [13444-90-1]	2.4×10 ⁻² 4.6×10 ⁻²		<i>Behnke et al.</i> [1997] <i>Frenzel et al.</i> [1998]	E E	25
chlorine nitrate ClNO ₃ [14545-72-3]	∞		<i>Sander and Crutzen</i> [1996]	E	18
molecular chlorine Cl ₂ [7782-50-5]	see note 9.1×10 ⁻² 6.2×10 ⁻² 9.3×10 ⁻² 6.3×10 ⁻² 9.5×10 ⁻² 8.6×10 ⁻²	2500 2800 2300 3200 2100 2000	<i>Kruis and May</i> [1962] <i>Wilhelm et al.</i> [1977] <i>Wagman et al.</i> [1982] <i>Dean</i> [1992] <i>Brian et al.</i> [1962] <i>Lide and Frederikse</i> [1995] <i>Kavanaugh and Trussell</i> [1980]	? L T ? L L X	26 2 3
dichlorine monoxide Cl ₂ O [7791-21-1]	1.7×10 ¹ 1.7×10 ¹	1800 1700	<i>Wilhelm et al.</i> [1977] <i>Lide and Frederikse</i> [1995]	L L	
chlorine dioxide ClO ₂ [10049-04-4]	1.0 1.0 8.5×10 ⁻¹	3300 3300 3400	<i>Wilhelm et al.</i> [1977] <i>Lide and Frederikse</i> [1995] <i>Kavanaugh and Trussell</i> [1980]	L L X	14 3
chlorine atom Cl [22537-15-1]	1.5×10 ⁻² 2.0×10 ⁻¹	1500	<i>Berdnikov and Bazhin</i> [1970] <i>Mozurkewich</i> [1986]	T T	5
chloramide NH ₂ Cl [10599-90-3]	9.4×10 ¹	4800	<i>Holzwarth et al.</i> [1984]	M	
dichloroamine NHCl ₂ (chlorimide) [3400-09-7]	2.9×10 ¹	4200	<i>Holzwarth et al.</i> [1984]	M	
nitrogen trichloride NCl ₃ [10025-85-1]	1.0×10 ⁻¹	4100	<i>Holzwarth et al.</i> [1984]	M	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-\text{d} \ln k_{\text{H}}}{\text{d}(1/T)}$ [K]	reference	type	note
bromine (Br)					
hydrogen bromide HBr [10035-10-6]	$1.3 \times 10^9 / K_{\text{A}}$ 7.2×10^{-1} 2.5×10^1 $7.2 \times 10^8 / K_{\text{A}}$	10000 6100 370 10000	<i>Brimblecombe and Clegg</i> [1989] <i>Chameides and Stelson</i> [1992] <i>Dean</i> [1992] <i>Wagman et al.</i> [1982]	T C ? T	20, 21 27 2
hypobromous acid HOBr [13517-11-8]	$>1.9 \times 10^3$ 1.8 9.3×10^1 see note 6.1×10^3		<i>Blatchley et al.</i> [1992] <i>Mozurkewich</i> [1995] <i>Vogt et al.</i> [1996] <i>Fickert</i> [1998] <i>Frenzel et al.</i> [1998]	M T E M E	28 29
nitryl bromide BrNO ₂ [13536-70-4]	3.0×10^{-1}		<i>Frenzel et al.</i> [1998]	E	
bromine nitrate BrNO ₃ [40423-14-1]	∞		<i>Sander and Crutzen</i> [1996]	E	18
molecular bromine Br ₂ [7726-95-6]	7.9×10^{-1} 7.1×10^{-1} 9.7×10^{-1} 8.0×10^{-1} 6.9×10^{-1} 7.3×10^{-1} 7.6×10^{-1} 1.8	3600 4100 3900 4000 4100 3300	<i>Winkler</i> [1899] <i>Kelley and Tartar</i> [1956] <i>Jenkins and King</i> [1965] <i>Jenkins and King</i> [1965] <i>Hill et al.</i> [1968] <i>Wagman et al.</i> [1982] <i>Dean</i> [1992] <i>Dubik et al.</i> [1987]	X M M R M T ? M	30 8 31
bromine chloride BrCl [13863-41-7]	4.2 1.1 7.4×10^{-1} 5.2 9.4×10^{-1} 5.9×10^{-1}	3700 5600	<i>Dubik et al.</i> [1987] see note see note <i>Disselkamp et al.</i> [1998] <i>Bartlett and Margerum</i> [1998] <i>Frenzel et al.</i> [1998]	M T T M M E	31 32 33 34
bromine atom Br [10097-32-2]	3.4×10^{-2} 1.2	1800	<i>Berdnikov and Bazhin</i> [1970] <i>Mozurkewich</i> [1986]	T T	5

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
iodine (I)					
hydrogen iodide HI [10034-85-2]	$2.5 \times 10^9 / K_{\text{A}}$ $2.2 \times 10^9 / K_{\text{A}}$	9800 9800	<i>Brimblecombe and Clegg</i> [1989] <i>Wagman et al.</i> [1982]	T T	20, 21
hypoiodous acid HOI [14332-21-9]	$>4.5 \times 10^1$ $<4.5 \times 10^4$ $>4.1 \times 10^2$		<i>Thompson and Zafiriou</i> [1983] <i>Thompson and Zafiriou</i> [1983] <i>Palmer et al.</i> [1985]	E E C	
molecular iodine I ₂ [7553-56-2]	3.1 3.3 1.1 3.0	4600 4800 4400	<i>Berdnikov and Bazhin</i> [1970] <i>Wagman et al.</i> [1982] <i>Thompson and Zafiriou</i> [1983] <i>Palmer et al.</i> [1985]	R T C R	35
iodine atom I [14362-44-8]	6.3×10^{-3} 8.0×10^{-2}	2300	<i>Berdnikov and Bazhin</i> [1970] <i>Mozurkewich</i> [1986]	T T	5
iodine chloride ICl [7790-99-0]	1.1×10^2		<i>Wagman et al.</i> [1982]	T	
iodine bromide IBr [7789-33-5]	2.4×10^1		<i>Wagman et al.</i> [1982]	T	

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
sulfur (S)					
hydrogen sulfide H ₂ S [7783-06-4]	1.0×10 ⁻³ 1.0×10 ⁻¹ 1.0×10 ⁻¹ 1.0×10 ⁻¹ 1.0×10 ⁻¹ 1.0×10 ⁻¹ 8.7×10 ⁻² 9.8×10 ⁻²	2300 2100 2100 2200 2300 2000 2100 2200	<i>Loomis</i> [1928] <i>Hine and Weimar</i> [1965] <i>Wilhelm et al.</i> [1977] <i>Edwards et al.</i> [1978] <i>Carroll and Mather</i> [1989] <i>Dean</i> [1992] <i>Lide and Frederikse</i> [1995] <i>De Bruyn et al.</i> [1995] <i>Kavanaugh and Trussell</i> [1980]	X R L L L ? L M X	1 2 3
sulfur dioxide SO ₂ [7446-09-5]	1.2 1.2 1.1 1.2 1.4 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.5 1.2 1.2 1.4 1.3	3200 3100 3100 2800 3000 3100 3100 3200 3100 2900 3200 2900 2800	<i>Sillen and Martell</i> [1964] <i>Hales and Sutter</i> [1973] <i>Liss and Slater</i> [1974] <i>Smith and Martell</i> [1976] <i>Wilhelm et al.</i> [1977] <i>Edwards et al.</i> [1978] <i>Durham et al.</i> [1981] <i>Chameides</i> [1984] <i>Hoffmann and Jacob</i> [1984] <i>Jacob</i> [1986] <i>Pandis and Seinfeld</i> [1989] <i>Dean</i> [1992] <i>Maahs</i> [1982] <i>Maahs</i> [1982] <i>Lide and Frederikse</i> [1995] <i>Kavanaugh and Trussell</i> [1980]	X c c X L L C T ? C C ? X X L X	1 1 4 2 11 1 3
sulfur trioxide SO ₃ [7446-11-9]	∞		<i>Sander and Crutzen</i> [1996]	E	18
sulfuric acid H ₂ SO ₄ [7664-93-9]	see note		<i>Gmitro and Vermeulen</i> [1964]	M	36
sulfur hexafluoride SF ₆ [2551-62-4]	2.4×10 ⁻⁴	2400	<i>Wilhelm et al.</i> [1977]	L	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
rare gases					
helium He [7440-59-7]	3.7×10^{-4} 3.8×10^{-4}	360 92	<i>Morrison and Johnstone</i> [1954] <i>Wilhelm et al.</i> [1977]	M L	37
neon Ne [7440-01-9]	4.5×10^{-4} 4.5×10^{-4}	530 450	<i>Morrison and Johnstone</i> [1954] <i>Wilhelm et al.</i> [1977]	M L	37
argon Ar [7440-37-1]	1.4×10^{-3} 1.4×10^{-3}	1100 1500	<i>Morrison and Johnstone</i> [1954] <i>Wilhelm et al.</i> [1977]	M L	
krypton Kr [7439-90-9]	2.4×10^{-3} 2.5×10^{-3}	1500 1900	<i>Morrison and Johnstone</i> [1954] <i>Wilhelm et al.</i> [1977]	M L	
xenon Xe [7440-63-3]	4.3×10^{-3} 4.3×10^{-3}	1900 2200	<i>Morrison and Johnstone</i> [1954] <i>Wilhelm et al.</i> [1977]	M L	
radon Rn [10043-92-2]	9.3×10^{-3}	2600	<i>Wilhelm et al.</i> [1977]	L	
other elements					
selenium hydride H ₂ Se [7783-07-5]	8.4×10^{-2}	1900	<i>Wilhelm et al.</i> [1977]	L	
phosphorus trihydride PH ₃ (phosphine) [7803-51-2]	8.1×10^{-3}	2000	<i>Wilhelm et al.</i> [1977]	L	
arsenic hydride AsH ₃ (arsine) [7784-42-1]	8.9×10^{-3}	2100	<i>Wilhelm et al.</i> [1977]	L	
mercury Hg [7439-97-6]	9.3×10^{-2}		<i>Brimblecombe</i> [1986]	?	38

8 Data Table (Organic)

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
alkanes (C and H only)					
methane CH ₄	9.2×10 ⁻³		<i>Butler and Ramchandani</i> [1935]	V	
	1.4×10 ⁻³		<i>Hine and Weimar</i> [1965]	R	
	9.7×10 ⁻⁴		<i>Liss and Slater</i> [1974]	C	
	1.5×10 ⁻³		<i>Hine and Mookerjee</i> [1975]	V	
	1.4×10 ⁻³	1700	<i>Wilhelm et al.</i> [1977]	L	
	1.3×10 ⁻³		<i>Mackay and Shiu</i> [1981]	L	
	1.3×10 ⁻³	1900	<i>Dean</i> [1992]	?	2
	1.4×10 ⁻³	1600	<i>Lide and Frederikse</i> [1995]	L	14
	1.5×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
1.3×10 ⁻³	1800	<i>Kavanaugh and Trussell</i> [1980]	X	3	
ethane C ₂ H ₆	1.1×10 ⁻²		<i>Butler and Ramchandani</i> [1935]	V	
	2.0×10 ⁻³		<i>Hine and Mookerjee</i> [1975]	V	
	1.8×10 ⁻³	2400	<i>Wilhelm et al.</i> [1977]	L	
	2.0×10 ⁻³		<i>Mackay and Shiu</i> [1981]	L	
	1.9×10 ⁻³	2300	<i>Lide and Frederikse</i> [1995]	L	
	2.0×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
propane C ₃ H ₈	1.4×10 ⁻³		<i>Hine and Mookerjee</i> [1975]	V	
	1.5×10 ⁻³	2700	<i>Wilhelm et al.</i> [1977]	L	
	1.4×10 ⁻³		<i>Mackay and Shiu</i> [1981]	L	
	1.5×10 ⁻³	2700	<i>Lide and Frederikse</i> [1995]	L	
	1.4×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
butane C ₄ H ₁₀	4.9×10 ⁻³		<i>Butler and Ramchandani</i> [1935]	V	
	1.1×10 ⁻³		<i>Hine and Mookerjee</i> [1975]	V	
	1.2×10 ⁻³	3100	<i>Wilhelm et al.</i> [1977]	L	
	1.1×10 ⁻³		<i>Mackay and Shiu</i> [1981]	L	
	1.1×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
2-methylpropane HC(CH ₃) ₃ (isobutane)	8.5×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975]	V	
	8.1×10 ⁻⁴	2700	<i>Wilhelm et al.</i> [1977]	L	
	8.4×10 ⁻⁴		<i>Mackay and Shiu</i> [1981]	L	
	8.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
dimethylpropane C(CH ₃) ₄ (neopentane)	4.6×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975]	V	
	5.9×10 ⁻⁴	3400	<i>Wilhelm et al.</i> [1977]	L	
	2.7×10 ⁻⁴		<i>Mackay and Shiu</i> [1981]	L	
pentane C ₅ H ₁₂	8.0×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975]	V	
	8.1×10 ⁻⁴		<i>Mackay and Shiu</i> [1981]	L	
	7.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2-methylbutane C ₅ H ₁₂ (isopentane)	7.3×10 ⁻⁴		<i>Mackay and Shiu</i> [1981]	L	
	7.3×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2-dimethylpropane C ₅ H ₁₂	4.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
hexane C ₆ H ₁₄	5.5×10 ⁻⁴ 6.0×10 ⁻⁴ 7.7×10 ⁻⁴ 1.0×10 ⁻³	7500	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988]	V L ? X	 39 3
2-methylpentane C ₆ H ₁₄ (isohexane) [107-83-5]	5.8×10 ⁻⁴ 6.0×10 ⁻⁴ 5.8×10 ⁻⁴ 1.3×10 ⁻¹	960	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988]	V L ? X	 39 3
3-methylpentane C ₆ H ₁₄	5.9×10 ⁻⁴ 5.9×10 ⁻⁴ 8.9×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	 39
2,2-dimethylbutane C ₆ H ₁₄	5.1×10 ⁻⁴ 5.9×10 ⁻⁴ 6.6×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	 39
2,3-dimethylbutane C ₆ H ₁₄	7.8×10 ⁻⁴ 7.7×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
heptane C ₇ H ₁₆	4.9×10 ⁻⁴ 4.4×10 ⁻⁴ 1.2×10 ⁻³ 3.7×10 ⁻⁴ 1.2×10 ⁻³	3700 3700	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Hansen et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	V L L ? X	 39 3
2-methylhexane C ₇ H ₁₆	2.9×10 ⁻⁴ 1.9×10 ⁻³ 2.9×10 ⁻⁴ 1.9×10 ⁻³	-3600 -3500	<i>Mackay and Shiu</i> [1981] <i>Hansen et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	L M ? X	 40 39 3
3-methylhexane C ₇ H ₁₆	4.2×10 ⁻⁴ 3.2×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
2,2-dimethylpentane C ₇ H ₁₆	3.2×10 ⁻⁴ 3.1×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
2,3-dimethylpentane C ₇ H ₁₆	5.8×10 ⁻⁴ 5.8×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
2,4-dimethylpentane C ₇ H ₁₆	3.2×10 ⁻⁴ 3.4×10 ⁻⁴ 3.4×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	 39
3,3-dimethylpentane C ₇ H ₁₆	5.4×10 ⁻⁴ 5.5×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
3-ethylpentane C ₇ H ₁₆	3.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,3-trimethylbutane C ₇ H ₁₆	4.1×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
octane C_8H_{18}	3.1×10^{-4} 3.4×10^{-4} 2.0×10^{-4} 2.9×10^{-3}	7800	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	V L ? X	 39 3
2-methylheptane C_8H_{18}	2.7×10^{-4} 2.7×10^{-4}		<i>Hoff et al.</i> [1993] <i>Yaws and Yang</i> [1992]	? ?	13 39
3-methylheptane C_8H_{18}	2.7×10^{-4} 2.7×10^{-4}		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
4-methylheptane C_8H_{18}	2.7×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2-dimethylhexane C_8H_{18}	2.9×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3-dimethylhexane C_8H_{18}	2.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,4-dimethylhexane C_8H_{18}	2.8×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,5-dimethylhexane C_8H_{18}	3.0×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,3-dimethylhexane C_8H_{18}	2.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,4-dimethylhexane C_8H_{18}	2.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
3-ethylhexane C ₈ H ₁₈	2.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,3-trimethylpentane C ₈ H ₁₈	2.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,4-trimethylpentane C ₈ H ₁₈	3.3×10 ⁻⁴ 3.1×10 ⁻⁴ 3.0×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
2,3,3-trimethylpentane C ₈ H ₁₈	2.4×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,3,4-trimethylpentane C ₈ H ₁₈	5.3×10 ⁻⁴ 5.7×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
3-ethyl-2-methylpentane C ₈ H ₁₈	2.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-3-methylpentane C ₈ H ₁₈	2.3×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,3,3-tetramethylbutane C ₈ H ₁₈	2.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
nonane C ₉ H ₂₀	2.0×10 ⁻⁴ 1.7×10 ⁻⁴ 2.4×10 ⁻³	210	<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988]	L ? X	 39 3
2-methyloctane C ₉ H ₂₀	2.1×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-methyloctane C ₉ H ₂₀	2.0×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
4-methyloctane C ₉ H ₂₀	1.0×10 ⁻⁴ 1.0×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
2,3-dimethylheptane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2-dimethylheptane C ₉ H ₂₀	2.1×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,4-dimethylheptane C ₉ H ₂₀	2.1×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,5-dimethylheptane C ₉ H ₂₀	2.0×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,6-dimethylheptane C ₉ H ₂₀	2.1×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3,3-dimethylheptane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3,4-dimethylheptane C ₉ H ₂₀	1.8×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3,5-dimethylheptane C ₉ H ₂₀	2.0×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
4,4-dimethylheptane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-ethylheptane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
4-ethylheptane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-\text{d} \ln k_{\text{H}}}{\text{d}(1/T)}$ [K]	reference	type	note
2,2,3-trimethylhexane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,4-trimethylhexane C ₉ H ₂₀	2.1×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,5-trimethylhexane C ₉ H ₂₀	2.9×10 ⁻⁴ 1.9×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
2,3,3-trimethylhexane C ₉ H ₂₀	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,3,4-trimethylhexane C ₉ H ₂₀	1.8×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,3,5-trimethylhexane C ₉ H ₂₀	2.0×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,4,4-trimethylhexane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3,3,4-trimethylhexane C ₉ H ₂₀	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2-methylhexane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
4-ethyl-2-methylhexane C ₉ H ₂₀	2.1×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-3-methylhexane C ₉ H ₂₀	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-4-methylhexane C ₉ H ₂₀	1.8×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,3,3-tetramethylpentane C ₉ H ₂₀	1.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,3,4-tetramethylpentane C ₉ H ₂₀	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2,4,4-tetramethylpentane C ₉ H ₂₀	1.9×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,3,3,4-tetramethylpentane C ₉ H ₂₀	1.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
3-ethyl-2,2-dimethylpentane C ₉ H ₂₀	1.8×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,3-dimethylpentane C ₉ H ₂₀	1.5×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,4-dimethylpentane C ₉ H ₂₀	1.8×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3,3-diethylpentane C ₉ H ₂₀	1.5×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
decane C ₁₀ H ₂₂	1.4×10 ⁻⁴ 2.1×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
2-methylnonane C ₁₀ H ₂₂	1.8×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
3-methylnonane C ₁₀ H ₂₂	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
4-methylnonane C ₁₀ H ₂₂	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
5-methylnonane C ₁₀ H ₂₂	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,2-dimethyloctane C ₁₀ H ₂₂	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,3-dimethyloctane C ₁₀ H ₂₂	1.5×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,4-dimethyloctane C ₁₀ H ₂₂	1.7×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,5-dimethyloctane C ₁₀ H ₂₂	1.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
2,6-dimethyloctane C ₁₀ H ₂₂	1.6×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
2,7-dimethyloctane C ₁₀ H ₂₂	1.7×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,3-dimethyloctane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,4-dimethyloctane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,5-dimethyloctane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,6-dimethyloctane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4,4-dimethyloctane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4,5-dimethyloctane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyloctane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-ethyloctane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,3-trimethylheptane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,4-trimethylheptane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
2,2,5-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,6-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.7×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,3-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,4-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,5-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,6-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,4,4-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,4,5-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,4,6-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.8×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,5,5-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,3,4-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,3,5-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,4,4-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,4,5-trimethylheptane $\text{C}_{10}\text{H}_{22}$	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
3-ethyl-2-methylheptane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-ethyl-2-methylheptane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
5-ethyl-2-methylheptane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-3-methylheptane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-ethyl-3-methylheptane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-5-methylheptane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-4-methylheptane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-ethyl-4-methylheptane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-propylheptane C ₁₀ H ₂₂	1.7×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-isopropylheptane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,3,3-tetramethylhexane C ₁₀ H ₂₂	1.2×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,3,4-tetramethylhexane C ₁₀ H ₂₂	1.2×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
2,2,3,5-tetramethylhexane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,4,4-tetramethylhexane C ₁₀ H ₂₂	1.2×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,4,5-tetramethylhexane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,5,5-tetramethylhexane C ₁₀ H ₂₂	1.8×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,3,4-tetramethylhexane C ₁₀ H ₂₂	1.2×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,3,5-tetramethylhexane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,4,4-tetramethylhexane C ₁₀ H ₂₂	1.2×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,3,4,5-tetramethylhexane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,3,4,4-tetramethylhexane C ₁₀ H ₂₂	1.0×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,2-dimethylhexane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-ethyl-2,2-dimethylhexane C ₁₀ H ₂₂	1.6×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,3-dimethylhexane C ₁₀ H ₂₂	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-ethyl-2,3-dimethylhexane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,4-dimethylhexane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
4-ethyl-2,4-dimethylhexane C ₁₀ H ₂₂	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,5-dimethylhexane C ₁₀ H ₂₂	1.5×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-\text{d} \ln k_{\text{H}}}{\text{d}(1/T)}$ [K]	reference	type	note
4-ethyl-3,3-dimethylhexane C ₁₀ H ₂₂	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-3,4-dimethylhexane C ₁₀ H ₂₂	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,3-diethylhexane C ₁₀ H ₂₂	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,4-diethylhexane C ₁₀ H ₂₂	1.4×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-isopropyl-2-methylhexane C ₁₀ H ₂₂	1.1×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,3,3,4-pentamethylpentane C ₁₀ H ₂₂	1.0×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,2,3,4,4-pentamethylpentane C ₁₀ H ₂₂	1.0×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,2,3-trimethylpentane C ₁₀ H ₂₂	1.0×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,2,4-trimethylpentane C ₁₀ H ₂₂	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3-ethyl-2,3,4-trimethylpentane C ₁₀ H ₂₂	1.1×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
3,3-diethyl-2-methylpentane C ₁₀ H ₂₂	1.1×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39
2,4-dimethyl-3-isopropylpentane C ₁₀ H ₂₂	1.3×10^{-4}		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
undecane C ₁₁ H ₂₄	5.5×10 ⁻⁵ 5.5×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
dodecane C ₁₂ H ₂₆	1.4×10 ⁻⁴ 1.4×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
tridecane C ₁₃ H ₂₈	4.3×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
tetradecane C ₁₄ H ₃₀	8.8×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
pentadecane C ₁₅ H ₃₂	2.1×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
hexadecane C ₁₆ H ₃₄	4.3×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
heptadecane C ₁₇ H ₃₆	1.8×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
octadecane C ₁₈ H ₃₈	1.1×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
nonadecane C ₁₉ H ₄₀	3.4×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
eicosane C ₂₀ H ₄₂	3.1		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
cycloalkanes (C and H only)					
cyclopropane C ₃ H ₆	1.1×10 ⁻² 1.3×10 ⁻²	1700	<i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992]	L ?	39, 41
cyclopentane C ₅ H ₁₀	5.4×10 ⁻³ 5.5×10 ⁻³ 6.6×10 ⁻³ 5.4×10 ⁻³ 6.6×10 ⁻³	3400 3300	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Hansen et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	V L M ? X	39 3
cyclohexane C ₆ H ₁₂	5.1×10 ⁻³ 5.6×10 ⁻³ 5.2×10 ⁻³ 5.6×10 ⁻³ 6.3×10 ⁻³	3200 710	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988] <i>USEPA</i> [1982]	V L ? X X	39 3 3
cycloheptane C ₇ H ₁₄	1.6×10 ⁻¹ 1.1×10 ⁻²		<i>Hoff et al.</i> [1993] <i>Yaws and Yang</i> [1992]	? ?	13 39
cyclooctane C ₈ H ₁₆	9.9×10 ⁻³ 9.6×10 ⁻³		<i>Hoff et al.</i> [1993] <i>Yaws and Yang</i> [1992]	? ?	13 39
methylcyclopentane C ₅ H ₉ CH ₃	2.8×10 ⁻³ 2.8×10 ⁻³ 2.8×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
methylcyclohexane C ₆ H ₁₁ CH ₃	2.3×10 ⁻³ 2.5×10 ⁻³ 9.7×10 ⁻³ 2.3×10 ⁻³ 9.4×10 ⁻³	9400 9100	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Hansen et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	V L M ? X	39 3
<i>cis</i> -1,2-dimethylcyclohexane C ₆ H ₁₀ (CH ₃) ₂	2.8×10 ⁻³ 2.8×10 ⁻³ 2.8×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
<i>trans</i> -1,2-dimethylcyclohexane C ₆ H ₁₀ (CH ₃) ₂	2.1×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
<i>trans</i> -1,4-dimethylcyclohexane C ₆ H ₁₀ (CH ₃) ₂	1.1×10 ⁻³ 1.1×10 ⁻³		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
1,1,3-trimethylcyclopentane C ₅ H ₇ (CH ₃) ₃	6.4×10 ⁻⁴		<i>Mackay and Shiu</i> [1981]	L	
propylcyclopentane C ₅ H ₉ C ₃ H ₇	1.1×10 ⁻³ 1.1×10 ⁻³		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
pentylcyclopentane C ₅ H ₉ C ₅ H ₁₁	5.5×10 ⁻⁴ 5.5×10 ⁻⁴		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
decahydronaphthalene C ₁₀ H ₁₈ (decalin) [91-17-8]	7.3×10 ⁻³	4100	<i>Ashworth et al.</i> [1988]	X	3

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
aliphatic alkenes and cycloalkenes (C and H only)					
ethene C ₂ H ₄ (ethylene)	4.9×10 ⁻³ 4.7×10 ⁻³ 4.7×10 ⁻³ 4.7×10 ⁻³ 4.9×10 ⁻³ 4.8×10 ⁻³	1800	<i>Loomis</i> [1928] <i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Seinfeld</i> [1986] <i>Yaws and Yang</i> [1992]	X V L L ? ?	1 13 39
propene C ₃ H ₆ (propylene)	4.8×10 ⁻³ 7.4×10 ⁻³ 4.8×10 ⁻³ 4.8×10 ⁻³	3400	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L L ?	 39
1-butene C ₄ H ₈	4.0×10 ⁻³ 1.3×10 ⁻² 1.4×10 ⁻³ 4.0×10 ⁻³	6400	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L L ?	 39
<i>cis</i> -2-butene C ₄ H ₈	4.3×10 ⁻³		<i>Irrmann</i> [1965]	X	42
<i>trans</i> -2-butene C ₄ H ₈	4.4×10 ⁻³		<i>Irrmann</i> [1965]	X	42
2-methylpropene C ₄ H ₈ (isobutene)	4.7×10 ⁻³ 5.7×10 ⁻³ 1.6×10 ⁻³ 4.8×10 ⁻³	3000	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L L ?	 39
1-pentene C ₅ H ₁₀	2.5×10 ⁻³ 2.5×10 ⁻³ 2.5×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	 39
<i>cis</i> -2-pentene C ₅ H ₁₀	4.4×10 ⁻³ 4.4×10 ⁻³		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
<i>trans</i> -2-pentene C ₅ H ₁₀	4.3×10 ⁻³ 4.3×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	 39
2-methyl-2-butene C ₅ H ₁₀	4.5×10 ⁻³		<i>Hine and Mookerjee</i> [1975]	V	
3-methyl-1-butene C ₅ H ₁₀	1.9×10 ⁻³ 1.9×10 ⁻³ 1.9×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	 39

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1-hexene C ₆ H ₁₂	2.4×10 ⁻³ 2.4×10 ⁻³ 3.3×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
2-methyl-1-pentene C ₆ H ₁₂	3.6×10 ⁻³ 3.6×10 ⁻³		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
4-methyl-1-pentene C ₆ H ₁₂	1.6×10 ⁻³ 1.6×10 ⁻³ 1.6×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
1-heptene C ₇ H ₁₄	2.5×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
<i>trans</i> -2-heptene C ₇ H ₁₄	2.5×10 ⁻³ 2.4×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981]	V L	
1-octene C ₈ H ₁₆	1.1×10 ⁻³ 1.1×10 ⁻³ 1.6×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
1-nonene C ₉ H ₁₈	1.2×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
1,3-butadiene C ₄ H ₆	1.6×10 ⁻² 1.4×10 ⁻² 1.4×10 ⁻² 1.4×10 ⁻²	4500	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L L ?	39
methylbutadiene C ₅ H ₈ (isoprene)	1.3×10 ⁻² 1.3×10 ⁻² 2.8×10 ⁻² 1.3×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Karl and Lindinger</i> [1997] <i>Yaws and Yang</i> [1992]	V L M ?	43 39
1,4-pentadiene C ₅ H ₈	8.3×10 ⁻³ 8.4×10 ⁻³ 8.5×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
1,5-hexadiene C ₆ H ₁₀	7.4×10 ⁻³		<i>Hine and Mookerjee</i> [1975]	V	
2,3-dimethyl-1,3-butadiene C ₆ H ₁₀	2.1×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
cyclopentene C ₅ H ₈	1.6×10 ⁻² 1.5×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
cyclohexene C ₆ H ₁₀	2.2×10 ⁻² 2.6×10 ⁻² 2.2×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Nielsen et al.</i> [1994] <i>Yaws and Yang</i> [1992]	V M ?	39
1-methylcyclohexene C ₆ H ₉ CH ₃	1.3×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
1,3,5-cycloheptatriene C ₇ H ₈	2.1×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
aliphatic alkynes (C and H only)					
ethyne C ₂ H ₂ (acetylene)	4.2×10 ⁻² 4.1×10 ⁻² 3.9×10 ⁻²	1800	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992]	V L ?	39
propyne CH ₃ CCH (methylacetylene)	9.2×10 ⁻² 9.1×10 ⁻² 9.4×10 ⁻² see note		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Wilhelm et al.</i> [1977]	V L ? ?	39 44
1-butyne C ₂ H ₅ CCH (ethylacetylene)	5.4×10 ⁻² 7.6×10 ⁻² 5.3×10 ⁻² 5.5×10 ⁻²	1900	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L L ?	39
1-pentyne C ₃ H ₇ CCH	4.0×10 ⁻² 4.1×10 ⁻² 2.0×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	39
1-hexyne C ₄ H ₉ CCH	2.5×10 ⁻² 4.6×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
1-heptyne C ₅ H ₁₁ CCH	1.5×10 ⁻² 1.4×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
1-octyne C ₆ H ₁₃ CCH	1.2×10 ⁻² 1.2×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
1-nonyne C ₇ H ₁₅ CCH	6.9×10 ⁻³ 7.0×10 ⁻³		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
3-buten-1-yne CH ₂ CHCCH (vinylacetylene)	3.8×10 ⁻²	1700	<i>Wilhelm et al.</i> [1977]	L	
butadiyne C ₄ H ₂ (biacetylene)	1.9×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[M/atm]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
mononuclear aromatics (C and H only)					
benzene C ₆ H ₆ [71-43-2]	1.8×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
	1.8×10 ⁻¹		<i>Mackay et al.</i> [1979]	M	
	1.8×10 ⁻¹		<i>Mackay et al.</i> [1979]	T	
	1.8×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	1.8×10 ⁻¹		<i>Ettre et al.</i> [1993]	X	45
	1.9×10 ⁻¹	3800	<i>Robbins et al.</i> [1993]	M	
	2.1×10 ⁻¹		<i>Nielsen et al.</i> [1994]	M	
	2.1×10 ⁻¹	3600	<i>Dewulf et al.</i> [1995]	M	
	1.8×10 ⁻¹		<i>Vitenberg et al.</i> [1975]	M	
	1.6×10 ⁻¹	4500	<i>Wasik and Tsang</i> [1970]	M	
	1.8×10 ⁻¹		<i>Bohon and Claussen</i> [1951]	V	
	1.7×10 ⁻¹		<i>Hoff et al.</i> [1993]	M	
	2.2×10 ⁻¹	4200	<i>Hartkopf and Karger</i> [1973]	M	
	1.8×10 ⁻¹		<i>Karl and Lindinger</i> [1997]	M	43
	1.8×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
	1.7×10 ⁻¹	3900	<i>Cooling et al.</i> [1992]	X	3
	1.8×10 ⁻¹	2200	<i>USEPA</i> [1982]	X	3
	1.9×10 ⁻¹	4300	<i>Kavanaugh and Trussell</i> [1980]	X	3
	1.2×10 ⁻¹	5300	<i>Ervin et al.</i> [1980]	X	3
	1.6×10 ⁻¹	4100	<i>Staudinger and Roberts</i> [1996]	L	
1.6×10 ⁻¹	4300	<i>Bissonette et al.</i> [1990]	X	3	
1.8×10 ⁻¹	3200	<i>Ashworth et al.</i> [1988]	X	3	
1.8×10 ⁻¹	4000	<i>Leighton and Calo</i> [1981]	X	3	
1.8×10 ⁻¹		<i>Allen et al.</i> [1998]	E		
methylbenzene C ₆ H ₅ CH ₃ (toluene) [108-88-3]	1.5×10 ⁻¹		<i>McAuliffe</i> [1971]	X	45
	1.5×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
	1.5×10 ⁻¹		<i>Mackay et al.</i> [1979]	M	
	1.5×10 ⁻¹		<i>Mackay et al.</i> [1979]	T	
	1.5×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	1.6×10 ⁻¹		<i>Kolb et al.</i> [1992]	X	45
	1.6×10 ⁻¹		<i>Ettre et al.</i> [1993]	X	45
	1.5×10 ⁻¹	3400	<i>Robbins et al.</i> [1993]	M	
	1.6×10 ⁻¹		<i>Nielsen et al.</i> [1994]	M	
	1.8×10 ⁻¹	4100	<i>Dewulf et al.</i> [1995]	M	
	1.9×10 ⁻¹		<i>Vitenberg et al.</i> [1975]	M	
	1.7×10 ⁻¹	5900	<i>Wasik and Tsang</i> [1970]	M	
	1.8×10 ⁻¹		<i>Bohon and Claussen</i> [1951]	V	
	1.3×10 ⁻¹		<i>Hoff et al.</i> [1993]	M	
	2.1×10 ⁻¹	4600	<i>Hartkopf and Karger</i> [1973]	M	
	1.6×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
	1.5×10 ⁻¹	1900	<i>USEPA</i> [1982]	X	3
	1.5×10 ⁻¹	4000	<i>Staudinger and Roberts</i> [1996]	L	
	1.4×10 ⁻¹	5000	<i>Bissonette et al.</i> [1990]	X	3
	1.5×10 ⁻¹	3000	<i>Ashworth et al.</i> [1988]	X	3
1.5×10 ⁻¹	3700	<i>Leighton and Calo</i> [1981]	X	3	
1.5×10 ⁻¹	4900	<i>Ervin et al.</i> [1980]	X	3	
1.7×10 ⁻¹	8400	<i>Lamarche and Droste</i> [1989]	X	3	
1.6×10 ⁻¹		<i>Allen et al.</i> [1998]	E		

substance	k_{H}^{\ominus} [M/atm]	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
1,2-dimethylbenzene $\text{C}_6\text{H}_4(\text{CH}_3)_2$ (o-xylene) [95-47-6]	1.9×10^{-1} 2.0×10^{-1} 1.9×10^{-1} 2.5×10^{-1} 2.9×10^{-1} 2.4×10^{-1} 1.9×10^{-1} 1.9×10^{-1} 2.1×10^{-1}	 3400 4200 5400 3200 4000 5600	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Robbins et al.</i> [1993] <i>Dewulf et al.</i> [1995] <i>Wasik and Tsang</i> [1970] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988] <i>Staudinger and Roberts</i> [1996] <i>Bissonette et al.</i> [1990]	V L M M M ? X L X	 39 3 3
1,3-dimethylbenzene $\text{C}_6\text{H}_4(\text{CH}_3)_2$ (m-xylene) [108-38-3]	1.6×10^{-1} 1.4×10^{-1} 1.6×10^{-1} 1.7×10^{-1} 1.5×10^{-1} 1.3×10^{-1} 1.3×10^{-1} 1.4×10^{-1}	 4000 3300 4200 6000	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Dewulf et al.</i> [1995] <i>Bohon and Claussen</i> [1951] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988] <i>Staudinger and Roberts</i> [1996] <i>Bissonette et al.</i> [1990]	V L M V ? X L X	 39 3 3
1,4-dimethylbenzene $\text{C}_6\text{H}_4(\text{CH}_3)_2$ (p-xylene) [106-42-3]	1.6×10^{-1} 1.4×10^{-1} 1.7×10^{-1} 1.6×10^{-1} 2.3×10^{-1} 1.6×10^{-1} 1.2×10^{-1} 1.2×10^{-1} 1.3×10^{-1} 1.3×10^{-1}	 4500 5400 3000 5300 3500 3800	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Dewulf et al.</i> [1995] <i>Bohon and Claussen</i> [1951] <i>Wasik and Tsang</i> [1970] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993] <i>Bissonette et al.</i> [1990] <i>Ashworth et al.</i> [1988] <i>Staudinger and Roberts</i> [1996]	V L M V M ? X X X L	 39 3 3 3
1,2,3-trimethylbenzene $\text{C}_6\text{H}_3(\text{CH}_3)_3$ [526-73-8]	3.1×10^{-1} 2.7×10^{-1}		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
1,2,4-trimethylbenzene $\text{C}_6\text{H}_3(\text{CH}_3)_3$ [95-63-6]	1.7×10^{-1} 1.7×10^{-1} 1.5×10^{-1} 1.8×10^{-1} 1.5×10^{-1}	 4300 4200	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Hansen et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	V L M ? X	 39 3
1,3,5-trimethylbenzene $\text{C}_6\text{H}_3(\text{CH}_3)_3$ (mesitylene) [108-67-8]	1.7×10^{-1} 1.2×10^{-1} 1.4×10^{-1}	 3600	<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988]	L ? X	39 3
1,2,4,5-tetramethylbenzene $\text{C}_6\text{H}_2(\text{CH}_3)_4$	4.0×10^{-2} 3.9×10^{-2}		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
ethylbenzene C ₆ H ₅ C ₂ H ₅ [100-41-4]	1.2×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
	1.2×10 ⁻¹		<i>Mackay et al.</i> [1979]	M	
	1.1×10 ⁻¹		<i>Mackay et al.</i> [1979]	T	
	1.3×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	1.3×10 ⁻¹	4600	<i>Robbins et al.</i> [1993]	M	
	1.5×10 ⁻¹	4600	<i>Dewulf et al.</i> [1995]	M	
	1.5×10 ⁻¹		<i>Bohon and Claussen</i> [1951]	V	
	1.1×10 ⁻¹		<i>Hoff et al.</i> [1993]	?	13
	1.7×10 ⁻¹	6100	<i>Hartkopf and Karger</i> [1973]	M	
	1.2×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
	1.2×10 ⁻¹	5100	<i>Staudinger and Roberts</i> [1996]	L	
	1.6×10 ⁻¹	1700	<i>USEPA</i> [1982]	X	3
	1.1×10 ⁻¹	5500	<i>Bissonette et al.</i> [1990]	X	3
	1.2×10 ⁻¹	5000	<i>Ashworth et al.</i> [1988]	X	3
1.4×10 ⁻¹	5500	<i>Ervin et al.</i> [1980]	X	3	
1.3×10 ⁻¹		<i>Allen et al.</i> [1998]	E		
propylbenzene C ₆ H ₅ C ₃ H ₇ [103-65-1]	1.0×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
	1.4×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	9.8×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
	9.1×10 ⁻²	3700	<i>Ashworth et al.</i> [1988]	X	3
(2-propyl)-benzene C ₆ H ₅ C ₃ H ₇ (isopropylbenzene, cumene) [98-82-8]	6.8×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
	7.8×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	6.9×10 ⁻²		<i>Hoff et al.</i> [1993]	?	13
	6.9×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
	8.8×10 ⁻²	3200	<i>Hansen et al.</i> [1993]	X	3
1-ethyl-2-methylbenzene C ₆ H ₄ CH ₃ C ₂ H ₅ (o-ethyltoluene) [611-14-3]	2.4×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	2.3×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
1-ethyl-4-methylbenzene C ₆ H ₄ CH ₃ C ₂ H ₅ (p-ethyltoluene) [622-96-8]	2.0×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	2.0×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
butylbenzene C ₆ H ₅ C ₄ H ₉ [104-51-8]	8.0×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
	7.8×10 ⁻²		<i>Mackay and Shiu</i> [1981]	L	
	7.6×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
2-methylpropylbenzene C ₆ H ₅ C ₄ H ₉ [538-93-2]	3.1×10 ⁻²		<i>Mackay and Shiu</i> [1981]	L	
<i>sec</i> -butylbenzene C ₆ H ₅ C ₄ H ₉ [135-98-8]	8.7×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
	7.2×10 ⁻²		<i>Mackay and Shiu</i> [1981]	L	
<i>tert</i> -butylbenzene C ₆ H ₅ C ₄ H ₉ [98-06-6]	8.5×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
	8.4×10 ⁻²		<i>Mackay and Shiu</i> [1981]	L	
1-isopropyl-4-methylbenzene C ₆ H ₄ CH ₃ C ₃ H ₇	1.3×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
pentylbenzene $C_6H_5C_5H_{11}$	1.7×10^{-1} 6.0×10^{-2}		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
hexylbenzene $C_6H_5C_6H_{13}$	4.6×10^{-2}		<i>Yaws and Yang</i> [1992]	?	39
$C_6H_5C_5H_{11}$ (<i>tert</i> -amylbenzene)	5.5×10^{-2}		<i>Hine and Mookerjee</i> [1975]	V	
ethenylbenzene C_8H_8 (styrene)	3.7×10^{-1} 2.9×10^{-1} 3.8×10^{-1}	4800 4200	<i>Yaws and Yang</i> [1992] <i>Bissonette et al.</i> [1990] <i>USEPA</i> [1982]	? X X	39 3 3
1-ethenyl-3-methylbenzene C_9H_{10} (<i>m</i> -methylstyrene)	2.6×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
1-ethenyl-4-methylbenzene C_9H_{10} (<i>p</i> -methylstyrene)	3.5×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
terpenes and polynuclear aromatics (C and H only)					
pinene C ₁₀ H ₁₆ [127-91-3]	4.9×10 ⁻²		<i>Karl and Lindinger</i> [1997]	M	43
naphthalene C ₁₀ H ₈	2.4 2.1 2.1 2.4 1.9 8.1×10 ⁻¹ 2.0 2.1		<i>Hine and Mookerjee</i> [1975] <i>Mackay et al.</i> [1979] <i>Mackay et al.</i> [1979] <i>Mackay and Shiu</i> [1981] <i>Bohon and Claussen</i> [1951] <i>Yaws and Yang</i> [1992] <i>Meylan and Howard</i> [1991] <i>USEPA</i> [1982]	V M T L V ? X X	 39 3 3
1-methylnaphthalene C ₁₀ H ₇ CH ₃	2.3 3.9 2.7		<i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L M ?	 39
2-methylnaphthalene C ₁₀ H ₇ CH ₃	2.5 5.1×10 ⁻³ 2.0 5.1×10 ⁻³	1200 1200	<i>Mackay and Shiu</i> [1981] <i>Hansen et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	L M ? X	 39 3
1-ethylnaphthalene C ₁₀ H ₇ C ₂ H ₅	2.7 2.7		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
2-ethylnaphthalene C ₁₀ H ₇ C ₂ H ₅	1.2 1.6		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39
1,3-dimethylnaphthalene C ₁₂ H ₁₂	1.4		<i>Yaws and Yang</i> [1992]	?	39
1,4-dimethylnaphthalene C ₁₂ H ₁₂	2.0		<i>Yaws and Yang</i> [1992]	?	39
1,5-dimethylnaphthalene C ₁₂ H ₁₂	1.6		<i>Yaws and Yang</i> [1992]	?	39
2,3-dimethylnaphthalene C ₁₂ H ₁₂	1.7		<i>Yaws and Yang</i> [1992]	?	39
2,6-dimethylnaphthalene C ₁₂ H ₁₂	8.3×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
biphenyl (C ₆ H ₅) ₂	2.5 3.6 3.3 1.2 1.2		<i>Mackay et al.</i> [1979] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Bohon and Claussen</i> [1951] <i>Yaws and Yang</i> [1992]	M L M V ?	 39

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
acenaphthene C ₁₂ H ₁₀ [83-32-9]	1.3×10 ¹ 6.8 4.2 6.5×10 ⁻¹ 4.1 6.5	2800	<i>Hine and Mookerjee</i> [1975] <i>Mackay et al.</i> [1979] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>USEPA</i> [1982] <i>Meylan and Howard</i> [1991]	V M L M X X	 3 3
phenanthrene C ₁₄ H ₁₀	3.9×10 ¹ 2.5×10 ¹ 2.5×10 ¹ 2.8×10 ¹ 2.8×10 ¹ 9.5	4700	<i>Hine and Mookerjee</i> [1975] <i>Mackay et al.</i> [1979] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Meylan and Howard</i> [1991] <i>USEPA</i> [1982]	V M L M X X	 3 3
2,3-benzindene C ₁₃ H ₁₀ (fluorene) [86-73-7]	1.2×10 ¹ 1.0×10 ¹ 8.5 1.0×10 ¹	3000	<i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>USEPA</i> [1982] <i>Meylan and Howard</i> [1991]	L M X X	 3 3
anthracene C ₁₄ H ₁₀ [120-12-7]	5.6×10 ¹ 1.7×10 ¹ 1.4 1.5×10 ¹ 3.5×10 ¹	4000	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Meylan and Howard</i> [1991] <i>USEPA</i> [1982]	V L M X X	 3 3
pyrene C ₁₆ H ₁₀ [129-00-0]	8.4×10 ¹ 9.2×10 ¹		<i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981]	L M	
fluoranthene C ₁₆ H ₁₀ [206-44-0]	4.6×10 ⁻¹ 1.1×10 ²	6900	<i>Mackay and Shiu</i> [1981] <i>tenHulscher et al.</i> [1992]	L X	3
benzo[a]fluoranthene	1.7×10 ³ 9.7×10 ⁻¹	5900 1900	<i>tenHulscher et al.</i> [1992] <i>USEPA</i> [1982]	X X	3 3
benzo[b]fluoranthene	1.5×10 ³	5500	<i>tenHulscher et al.</i> [1992]	X	3
benzo[k]fluoranthene	1.7×10 ³	5900	<i>tenHulscher et al.</i> [1992]	X	3
indeno[1,2,3-cd]pyrene	2.9×10 ³	3600	<i>tenHulscher et al.</i> [1992]	X	3
benzo[a]pyrene C ₂₀ H ₁₂ [50-32-8]	1.6×10 ⁻¹ 2.2×10 ³	110 4700	<i>USEPA</i> [1982] <i>tenHulscher et al.</i> [1992]	X X	3 3
benzo[ghi]perylene C ₂₂ H ₁₂ [191-24-2]	3.0×10 ³	3200	<i>tenHulscher et al.</i> [1992]	X	3
1,2,3,4-tetrahydronaphthalene C ₁₀ H ₁₂ (tetralin) [119-64-2]	5.3×10 ⁻¹	5400	<i>Ashworth et al.</i> [1988]	X	3

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
alcohols (ROH) (C, H, and O only)					
methanol CH ₃ OH	2.3×10 ² 2.3×10 ² 2.1×10 ² 2.2×10 ² 2.2×10 ² 1.4×10 ² 1.6×10 ² 2.2×10 ²	5200 5600	<i>Butler et al.</i> [1935] <i>Burnett</i> [1963] <i>Timmermans</i> [1960] <i>Gaffney and Senum</i> [1984] <i>Snider and Dawson</i> [1985] <i>Yaws and Yang</i> [1992] <i>Schaffer and Daubert</i> [1969] <i>Meylan and Howard</i> [1991]	M M M,X X M ? X X	46 47 48 39 3 3
ethanol C ₂ H ₅ OH	1.9×10 ² 2.2×10 ² 1.6×10 ² 2.0×10 ² 1.9×10 ² 2.3×10 ² 1.2×10 ² 1.5×10 ² 2.0×10 ²	6600 6400	<i>Butler et al.</i> [1935] <i>Burnett</i> [1963] <i>Timmermans</i> [1960] <i>Gaffney and Senum</i> [1984] <i>Snider and Dawson</i> [1985] <i>Rohrschneider</i> [1973] <i>Yaws and Yang</i> [1992] <i>Schaffer and Daubert</i> [1969] <i>Meylan and Howard</i> [1991]	M M M,X X M M ? X X	47 48 39 3 3
1-propanol C ₃ H ₇ OH [71-23-8]	1.4×10 ² 1.6×10 ² 1.3×10 ² 1.5×10 ² 1.1×10 ²	7500	<i>Butler et al.</i> [1935] <i>Burnett</i> [1963] <i>Snider and Dawson</i> [1985] <i>Snider and Dawson</i> [1985] <i>Yaws and Yang</i> [1992]	M M M C ?	46 39
2-propanol C ₃ H ₇ OH (isopropanol) [67-63-0]	1.2×10 ² 1.7×10 ² 1.3×10 ² 8.9×10 ¹	7500	<i>Butler et al.</i> [1935] <i>Hine and Weimar</i> [1965] <i>Snider and Dawson</i> [1985] <i>Yaws and Yang</i> [1992]	M R M ?	39
1-butanol C ₄ H ₉ OH [71-36-3]	1.2×10 ² 1.1×10 ² 1.4×10 ² 1.3×10 ² 1.2×10 ² 5.4×10 ¹	7200	<i>Butler et al.</i> [1935] <i>Buttery et al.</i> [1969] <i>Burnett</i> [1963] <i>Snider and Dawson</i> [1985] <i>Snider and Dawson</i> [1985] <i>Friant and Suffet</i> [1979]	M M M M C M	46 49
2-butanol C ₄ H ₁₀ O (<i>sec</i> -butanol) [78-92-2]	9.8×10 ¹ 9.8×10 ¹ 1.1×10 ²	7300	<i>Butler et al.</i> [1935] <i>Butler et al.</i> [1935] <i>Snider and Dawson</i> [1985]	M V M	
2-methyl-1-propanol C ₄ H ₁₀ O (isobutanol) [78-83-1]	8.4×10 ¹ 1.0×10 ²		<i>Butler et al.</i> [1935] <i>Snider and Dawson</i> [1985]	M M	
2-methyl-2-propanol C ₄ H ₁₀ O (<i>tert</i> -butanol) [75-65-0]	8.4×10 ¹ 7.0×10 ¹ see note	8300	<i>Butler et al.</i> [1935] <i>Snider and Dawson</i> [1985] <i>Koga</i> [1995]	M M M	50

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
1-pentanol C ₅ H ₁₁ OH (amylalcohol) [71-41-0]	7.7×10 ¹ 7.9×10 ¹ 8.2×10 ¹		<i>Butler et al.</i> [1935] <i>Butler et al.</i> [1935] <i>Yaws and Yang</i> [1992]	M V ?	39
2-pentanol C ₅ H ₁₂ O (<i>sec</i> -pentanol) [6032-29-7]	6.8×10 ¹		<i>Butler et al.</i> [1935]	M	
2-methyl-1-butanol C ₅ H ₁₂ O (isopentanol) [137-32-6]	7.1×10 ¹		<i>Butler et al.</i> [1935]	M	
2-methyl-2-butanol C ₅ H ₁₂ O (<i>tert</i> -pentanol) [75-85-4]	7.3×10 ¹		<i>Butler et al.</i> [1935]	M	
2,2-dimethyl-1-propanol C ₅ H ₁₂ O [75-84-3]	5.0×10 ¹		<i>Saxena and Hildemann</i> [1996]	E	51
1-hexanol C ₆ H ₁₃ OH [111-27-3]	6.5×10 ¹ 5.9×10 ¹ 6.5×10 ¹ 5.4×10 ¹		<i>Butler et al.</i> [1935] <i>Buttery et al.</i> [1969] <i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V M V ?	39
3-hexanol C ₆ H ₁₄ O [623-37-0]	2.0×10 ¹		<i>Hine and Mookerjee</i> [1975]	V	
2-methyl-2-pentanol C ₆ H ₁₄ O [590-36-3]	3.1×10 ¹		<i>Hine and Mookerjee</i> [1975]	V	
4-methyl-2-pentanol C ₆ H ₁₄ O [108-11-2]	2.2×10 ¹		<i>Hine and Mookerjee</i> [1975]	V	
2-methyl-3-pentanol C ₆ H ₁₄ O [565-67-3]	2.9×10 ¹		<i>Hine and Mookerjee</i> [1975]	V	
2,3-dimethyl-2-butanol C ₆ H ₁₄ O [594-60-5]	3.0×10 ¹		<i>Hine and Mookerjee</i> [1975]	V	
1-heptanol C ₇ H ₁₅ OH [110-70-6]	5.3×10 ¹ 5.4×10 ¹ 8.6×10 ¹		<i>Butler et al.</i> [1935] <i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V V ?	39
1-octanol C ₈ H ₁₇ OH [111-87-5]	4.1×10 ¹ 4.2×10 ¹ 4.0×10 ¹ 6.3×10 ¹		<i>Butler et al.</i> [1935] <i>Hine and Mookerjee</i> [1975] <i>Buttery et al.</i> [1969] <i>Yaws and Yang</i> [1992]	V V M ?	39

substance	$\frac{k_H^\ominus}{[M/atm]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1-nonanol C ₉ H ₁₉ OH	6.1×10 ¹		<i>Yaws and Yang</i> [1992]	?	39
1-decanol C ₁₀ H ₂₁ OH	3.7×10 ¹		<i>Yaws and Yang</i> [1992]	?	39
1-dodecanol C ₁₂ H ₂₅ OH	1.1×10 ¹		<i>Yaws and Yang</i> [1992]	?	39
1-tetradecanol C ₁₄ H ₂₉ OH	3.9×10 ⁵		<i>Yaws and Yang</i> [1992]	?	39
1-pentadecanol C ₁₅ H ₃₁ OH	3.0×10 ⁵		<i>Yaws and Yang</i> [1992]	?	39
1-hexadecanol C ₁₆ H ₃₃ OH	6.0×10 ¹		<i>Yaws and Yang</i> [1992]	?	39
1-heptadecanol C ₁₇ H ₃₅ OH	1.2×10 ³		<i>Yaws and Yang</i> [1992]	?	39
1-octadecanol C ₁₈ H ₃₇ OH	9.2×10 ¹		<i>Yaws and Yang</i> [1992]	?	39, 52
cyclohexanol C ₆ H ₁₁ OH [108-93-0]	1.7×10 ²		<i>Hine and Mookerjee</i> [1975]	V	
2-propen-1-ol C ₃ H ₅ OH (allyl alcohol) [107-18-6]	2.0×10 ² 1.8×10 ² 2.0×10 ² 4.4×10 ²	7200	<i>Pierotti et al.</i> [1957] <i>Yaws and Yang</i> [1992] <i>Meylan and Howard</i> [1991] <i>USEPA</i> [1982]	X ? X X	53 39 3 3
2-buten-1-ol CH ₃ CHCHCH ₂ OH	3.0×10 ²		<i>Saxena and Hildemann</i> [1996]	E	51
2-methyl-3-buten-2-ol [115-18-4]	6.5×10 ¹		<i>Iraci et al.</i> [1998]	M	49

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
hydroxybenzene C ₆ H ₅ OH (phenol)	4.9×10 ² 3.0×10 ³ 2.9×10 ³ 7.8×10 ⁻² 1.9×10 ² 3.0×10 ³ 1.9×10 ³ 1.6×10 ³	6800 3600 7300	<i>Hine and Weimar</i> [1965] <i>Gaffney and Senum</i> [1984] <i>Parsons et al.</i> [1971] <i>Howe et al.</i> [1987] <i>Janini and Quaddora</i> [1986] <i>Meylan and Howard</i> [1991] <i>USEPA</i> [1982] <i>Tremp et al.</i> [1993]	R X M X X X X X	48 54 11 3 3 3 55,8
(hydroxymethyl)benzene C ₆ H ₅ CH ₂ OH (benzyl alcohol) [100-51-6]	9.0×10 ³		<i>Saxena and Hildemann</i> [1996]	E	51
4- <i>tert</i> -butylphenol (CH ₃) ₃ CC ₆ H ₄ OH	9.0×10 ²	7700	<i>Parsons et al.</i> [1972]	M	56
1-hydroxy-2-methylbenzene HOC ₆ H ₄ CH ₃ (2-cresol, <i>o</i> -cresol) [95-48-7]	8.3×10 ² 8.3×10 ² 1.2×10 ³ 2.6×10 ² 8.3×10 ²	7300 4600	<i>Gaffney and Senum</i> [1984] <i>Parsons et al.</i> [1972] <i>Yaws and Yang</i> [1992] <i>Janini and Quaddora</i> [1986] <i>Meylan and Howard</i> [1991]	X M ? X X	48 56 39, 8 3 3
1-hydroxy-3-methylbenzene HOC ₆ H ₄ CH ₃ (3-cresol, <i>m</i> -cresol) [108-39-4]	1.4×10 ³ 6.3×10 ²	7700	<i>Yaws and Yang</i> [1992] <i>Janini and Quaddora</i> [1986]	? X	39, 8 3
1-hydroxy-4-methylbenzene HOC ₆ H ₄ CH ₃ (4-cresol, <i>p</i> -cresol) [106-44-5]	1.0×10 ³ 1.3×10 ³ 2.5×10 ³ 1.1×10 ³ 5.3×10 ²	7200 4600	<i>Gaffney and Senum</i> [1984] <i>Parsons et al.</i> [1972] <i>Yaws and Yang</i> [1992] <i>Meylan and Howard</i> [1991] <i>Janini and Quaddora</i> [1986]	X M ? X X	48 56 39, 8 3 3
1,3-dimethyl-4-hydroxybenzene C ₈ H ₁₀ O (2,4-dimethylphenol) [105-67-9]	1.9×10 ⁻¹ 4.1×10 ²	-3300 6600	<i>Ashworth et al.</i> [1988] <i>USEPA</i> [1982]	X X	3 3

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
polyols (R(OH)_n) (C, H, and O only)					
1,2-ethanediol HO(CH ₂) ₂ OH (ethylene glycol) [107-21-1]	1.7×10 ⁴ 4.0×10 ⁶		<i>Butler and Ramchandani</i> [1935] <i>Bone et al.</i> [1983]	M M	57 8
1,2-propanediol C ₃ H ₈ O ₂	> 1.0×10 ⁵ < 6.0×10 ⁶		<i>Saxena and Hildemann</i> [1996] <i>Saxena and Hildemann</i> [1996]	E E	51 51
1,3-propanediol C ₃ H ₈ O ₂	9.2×10 ⁵		<i>Bone et al.</i> [1983]	M	8
1,2,3-propanetriol C ₃ H ₈ O ₃ (glycerol)	6.0×10 ⁴ > 6.0×10 ⁸ < 4.0×10 ¹¹		<i>Butler and Ramchandani</i> [1935] <i>Saxena and Hildemann</i> [1996] <i>Saxena and Hildemann</i> [1996]	M E E	57 51 51
1,3-butanediol C ₄ H ₁₀ O ₂	5.0×10 ⁶		<i>Saxena and Hildemann</i> [1996]	E	51
1,4-butanediol C ₄ H ₁₀ O ₂	> 1.0×10 ⁵ < 5.0×10 ⁶		<i>Saxena and Hildemann</i> [1996] <i>Saxena and Hildemann</i> [1996]	E E	51 51
2,3-butanediol C ₄ H ₁₀ O ₂	> 4.0×10 ⁴ < 4.0×10 ⁶		<i>Saxena and Hildemann</i> [1996] <i>Saxena and Hildemann</i> [1996]	E E	51 51
1,2,3-butanetriol C ₄ H ₁₀ O ₃	3.0×10 ¹¹		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,4-butanetriol C ₄ H ₁₀ O ₃	3.0×10 ¹¹		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,4-tetrahydroxy butane C ₄ H ₁₀ O ₄	2.0×10 ¹⁶		<i>Saxena and Hildemann</i> [1996]	E	51
1,5-pentanediol C ₅ H ₁₂ O ₂	4.0×10 ⁶		<i>Saxena and Hildemann</i> [1996]	E	51
2,3-pentanediol C ₅ H ₁₂ O ₂	3.0×10 ⁶		<i>Saxena and Hildemann</i> [1996]	E	51
2,4-pentanediol C ₅ H ₁₂ O ₂	3.0×10 ⁶		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,4,5-pentahydroxy pentane C ₅ H ₁₂ O ₅	9.0×10 ²⁰		<i>Saxena and Hildemann</i> [1996]	E	51
1,6-hexanediol C ₆ H ₁₄ O ₂	3.0×10 ⁶		<i>Saxena and Hildemann</i> [1996]	E	51

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
2,5-hexanediol $\text{C}_6\text{H}_{14}\text{O}_2$	2.0×10^6		<i>Saxena and Hildemann</i> [1996]	E	51
2-methyl-1,3-pentanediol $\text{C}_6\text{H}_{14}\text{O}_2$	3.0×10^6		<i>Saxena and Hildemann</i> [1996]	E	51
2-methyl-2,4-pentanediol $\text{C}_6\text{H}_{14}\text{O}_2$	2.0×10^6		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,6-hexanetriol $\text{C}_6\text{H}_{14}\text{O}_3$	2.0×10^{11}		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,4,5,6-hexahydroxy hexane $\text{C}_6\text{H}_{14}\text{O}_6$	4.0×10^{25}		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,4,5-tetrahydroxy cyclohexane $\text{C}_6\text{H}_{12}\text{O}_4$	4.0×10^{16}		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,4,5,6-hexahydroxy cyclohexane $\text{C}_6\text{H}_{12}\text{O}_6$	1.0×10^{26}		<i>Saxena and Hildemann</i> [1996]	E	51
1,7-heptanediol $\text{C}_7\text{H}_{16}\text{O}_2$	2.0×10^6		<i>Saxena and Hildemann</i> [1996]	E	51
2,4-heptanediol $\text{C}_7\text{H}_{16}\text{O}_2$	2.0×10^6		<i>Saxena and Hildemann</i> [1996]	E	51
2,3-diethyl-1,3-propanediol $\text{C}_7\text{H}_{16}\text{O}_2$	2.0×10^6		<i>Saxena and Hildemann</i> [1996]	E	51
2-ethyl-1,3-hexanediol $\text{C}_8\text{H}_{18}\text{O}_2$	2.0×10^6		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,4,5-pentahydroxy heptane $\text{C}_7\text{H}_{16}\text{O}_5$	5.0×10^{20}		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,4,6-pentahydroxy heptane $\text{C}_7\text{H}_{16}\text{O}_5$	4.0×10^{20}		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,5,7-pentahydroxy heptane $\text{C}_7\text{H}_{16}\text{O}_5$	5.0×10^{20}		<i>Saxena and Hildemann</i> [1996]	E	51
1,2,3,4,5,6-hexahydroxy heptane $\text{C}_7\text{H}_{16}\text{O}_6$	3.0×10^{25}		<i>Saxena and Hildemann</i> [1996]	E	51

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1,2-dihydroxybenzene C ₆ H ₄ (OH) ₂ (pyrocatechol) [120-80-9]	4.6×10 ³		<i>Mackay et al.</i> [1995]	V	
1,3-dihydroxybenzene C ₆ H ₄ (OH) ₂ (resorcinol) [108-46-3]	8.3×10 ⁶	6300	<i>USEPA</i> [1982]	X	3
1,4-dihydroxybenzene C ₆ H ₄ (OH) ₂ (hydroquinone) [123-31-9]	2.6×10 ⁷ 1.7×10 ⁷ 2.5×10 ⁷		<i>Meylan and Howard</i> [1991] <i>Meylan and Howard</i> [1991] <i>Mackay et al.</i> [1995]	X X V	58 58
peroxides (ROOH) and peroxy radicals (ROO) (C, H, and O only)					
methyl hydroperoxide CH ₃ OOH (methylperoxide) [3031-73-0]	3.0×10 ² 3.1×10 ²	5300 5200	<i>Lind and Kok</i> [1994] <i>O'Sullivan et al.</i> [1996]	M M	9
ethyl hydroperoxide C ₂ H ₅ OOH (ethylperoxide)	3.4×10 ²	6000	<i>O'Sullivan et al.</i> [1996]	M	
hydroxymethyl hydroperoxide HOCH ₂ OOH (HMHP,HMP) [15932-89-5]	1.7×10 ⁶ 1.6×10 ⁶ 4.8×10 ⁵	9700 10000 1500	<i>O'Sullivan et al.</i> [1996] <i>Staffelbach and Kok</i> [1993] <i>Zhou and Lee</i> [1992]	M M M	
bis(hydroxymethyl)peroxide HOCH ₂ OOCH ₂ OH (BHMP) [17088-73-2]	>1.0×10 ⁷ 4.5×10 ⁵	8400	<i>Staffelbach and Kok</i> [1993] <i>Zhou and Lee</i> [1992]	M M	
methylperoxy radical CH ₃ OO	6.0 2.0×10 ³	5600 6600	<i>Jacob</i> [1986] <i>Lelieveld and Crutzen</i> [1991]	E E	59 60
peroxyacetyl radical CH ₃ C(O)O ₂ [36709-10-1]	< 0.1		<i>Villalta et al.</i> [1996]	M	

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
aldehydes (RCHO) (C, H, and O only)					
methanal HCHO (formaldehyde) [50-50-0]	see note 6.0×10^3 7.0×10^3 see note 6.3×10^3 3.0×10^3 1.4×10^4 3.1×10^3 3.0×10^3 3.2×10^3	6400 7200 6500 7200 6800	<i>Ledbury and Blair</i> [1925] <i>Gaffney and Senum</i> [1984] <i>Chameides</i> [1984] <i>Dong and Dasgupta</i> [1986] <i>Seinfeld</i> [1986] <i>Betterton and Hoffmann</i> [1988] <i>Warneck</i> [1988] <i>Zhou and Mopper</i> [1990] <i>Möller and Mauersberger</i> [1992] <i>Staudinger and Roberts</i> [1996]	M X T M ? M C M c L	61 48 62 13 63 64
ethanal CH ₃ CHO (acetaldehyde) [75-07-0]	1.5×10^1 1.5×10^1 1.3×10^1 1.1×10^1 1.7×10^1 1.3×10^1 1.5×10^1 9.9 1.7×10^1 1.7 1.4×10^1	5800 6300 5000 5700	<i>Buttery et al.</i> [1969] <i>Gaffney and Senum</i> [1984] <i>Snider and Dawson</i> [1985] <i>Betterton and Hoffmann</i> [1988] <i>Zhou and Mopper</i> [1990] <i>Benkelberg et al.</i> [1995] <i>Pierotti et al.</i> [1957] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Janini and Quaddora</i> [1986] <i>Staudinger and Roberts</i> [1996]	M X M M M M X ? X X L	48 63 64 65 39 3 3
propanal C ₂ H ₅ CHO (propionaldehyde) [123-38-6]	1.3×10^1 1.3×10^1 1.3×10^1 2.8 5.3	5700 2400 5600	<i>Buttery et al.</i> [1969] <i>Snider and Dawson</i> [1985] <i>Zhou and Mopper</i> [1990] <i>Janini and Quaddora</i> [1986] <i>Schaffer and Daubert</i> [1969]	M C M X X	64 3 3
butanal C ₃ H ₇ CHO (butyraldehyde) [123-72-8]	9.6 8.7 5.5	6200 4000	<i>Zhou and Mopper</i> [1990] <i>Buttery et al.</i> [1969] <i>Janini and Quaddora</i> [1986]	M M X	64 3
pentanal C ₄ H ₉ CHO (valeraldehyde) [110-62-3]	6.4 6.8 4.4	6300	<i>Zhou and Mopper</i> [1990] <i>Buttery et al.</i> [1969] <i>Yaws and Yang</i> [1992]	M M ?	64 39, 49
hexanal C ₅ H ₁₁ CHO	4.9 4.7 1.9	6500	<i>Zhou and Mopper</i> [1990] <i>Buttery et al.</i> [1969] <i>Yaws and Yang</i> [1992]	M M ?	64 39, 49
heptanal C ₆ H ₁₃ CHO	3.3 3.7 2.3	7500	<i>Zhou and Mopper</i> [1990] <i>Buttery et al.</i> [1969] <i>Yaws and Yang</i> [1992]	M M ?	64 39, 49
octanal C ₇ H ₁₅ CHO	2.1 1.9 2.1×10^2	7400	<i>Zhou and Mopper</i> [1990] <i>Buttery et al.</i> [1969] <i>Yaws and Yang</i> [1992]	M M ?	64 39, 49
nonanal C ₈ H ₁₇ CHO	1.0 1.3 7.0×10^{-1}	6700	<i>Zhou and Mopper</i> [1990] <i>Buttery et al.</i> [1969] <i>Yaws and Yang</i> [1992]	M M ?	64 39, 49
decanal C ₉ H ₁₉ CHO	6.1×10^{-1}	8700	<i>Zhou and Mopper</i> [1990]	M	64

substance	$\frac{k_H^\ominus}{[M/atm]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
propenal CH ₂ CHCHO (acrolein) [107-02-8]	8.2 7.4 1.0×10 ¹ 8.2	5100 3800	<i>Gaffney and Senum</i> [1984] <i>Snider and Dawson</i> [1985] USEPA [1982] <i>Meylan and Howard</i> [1991]	X M X X	48 3 3
2-methylpropenal C ₄ H ₆ O (methacrolein) [78-85-3]	4.3 6.5	5300	<i>Allen et al.</i> [1998] <i>Iraci et al.</i> [1998]	E M	
<i>trans</i> -2-butenal CH ₃ CHCHCHO (crotonaldehyde)	5.2×10 ¹ 5.1×10 ¹ 5.1×10 ¹ 6.0×10 ¹	3600	<i>Buttery et al.</i> [1971] <i>Gaffney and Senum</i> [1984] <i>Meylan and Howard</i> [1991] USEPA [1982]	M X X X	48 3 3
<i>trans</i> -2-hexenal C ₃ H ₇ CHCHCHO	2.0×10 ¹		<i>Buttery et al.</i> [1971]	M	
<i>trans-trans</i> -2,4-hexadienal CH ₃ CHCHCHCHO	1.0×10 ²		<i>Buttery et al.</i> [1971]	M	
<i>trans</i> -2-octenal C ₅ H ₁₁ CHCHCHO	1.3×10 ¹ see note		<i>Buttery et al.</i> [1971] see note	M ?	66
benzaldehyde C ₆ H ₅ CHO [100-52-7]	3.6×10 ¹ 3.6×10 ¹ 3.7×10 ¹ 4.2×10 ¹ 3.9×10 ¹ 3.5×10 ¹	5100 4600 4800 7000	<i>Hine and Mookerjee</i> [1975] <i>Gaffney and Senum</i> [1984] <i>Betterton and Hoffmann</i> [1988] <i>Zhou and Mopper</i> [1990] <i>Staudinger and Roberts</i> [1996] <i>Allen et al.</i> [1998]	V X M M L E	48 63 64
3-hydroxybenzaldehyde C ₆ H ₄ (OH)CHO (3-formylphenol)	4.0×10 ⁵		<i>Gaffney and Senum</i> [1984]	X	48
4-hydroxybenzaldehyde C ₆ H ₄ (OH)CHO (4-formylphenol)	1.9×10 ⁶	8600	<i>Parsons et al.</i> [1971]	M	54
generic aldehyde RCHO	4.2×10 ³		<i>Graedel and Goldberg</i> [1983]	C	
ethanedial OHCCHO (glyoxal)	>3.0×10 ⁵ 3.6×10 ⁵		<i>Betterton and Hoffmann</i> [1988] <i>Zhou and Mopper</i> [1990]	M M	63

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
ketones (RCOR) (C, H, and O only)					
propanone CH ₃ COCH ₃ (acetone) [67-64-1]	3.0×10 ¹		<i>Butler and Ramchandani</i> [1935]	R	
	2.8×10 ¹		<i>Burnett</i> [1963]	M	
	3.1		<i>Hine and Weimar</i> [1965]	R	
	2.5×10 ¹		<i>Buttery et al.</i> [1969]	M	
	3.0×10 ¹		<i>Gaffney and Senum</i> [1984]	X	48
	2.6×10 ¹	4800	<i>Snider and Dawson</i> [1985]	M	
	3.5×10 ¹	3800	<i>Zhou and Mopper</i> [1990]	M	64
	3.2×10 ¹	5800	<i>Betterton</i> [1991]	M	
	2.7×10 ¹	5300	<i>Benkelberg et al.</i> [1995]	M	
	2.5×10 ¹		<i>Vitenberg et al.</i> [1975]	M	
	2.5×10 ¹		<i>Vitenberg et al.</i> [1974]	X	67
	2.7×10 ¹		<i>Hoff et al.</i> [1993]	M	
	2.3×10 ¹		<i>Yaws and Yang</i> [1992]	?	39
	2.2×10 ¹	5000	<i>Schaffer and Daubert</i> [1969]	X	3
3.0	3300	<i>Janini and Quaddora</i> [1986]	X	3	
3.0×10 ¹	4600	<i>Staudinger and Roberts</i> [1996]	L		
2-butanone C ₂ H ₅ COCH ₃ (methyl ethyl ketone, MEK) [78-93-3]	7.1		<i>Hine and Weimar</i> [1965]	R	
	1.8×10 ¹	5700	<i>Snider and Dawson</i> [1985]	M	
	2.1×10 ¹		<i>Buttery et al.</i> [1969]	M	
	7.7		<i>Ashworth et al.</i> [1988]	X	68
	2.0×10 ¹	5000	<i>Zhou and Mopper</i> [1990]	M	64
	4.1...7.7		<i>Howe et al.</i> [1987]	X	11
	1.8×10 ¹		<i>Vitenberg et al.</i> [1975]	M	
	1.9×10 ¹		<i>Rohrschneider</i> [1973]	M	
	1.7×10 ¹		<i>Vitenberg et al.</i> [1974]	X	67
	1.0×10 ¹		<i>Friant and Suffet</i> [1979]	M	49
	2.0×10 ¹	5000	<i>Staudinger and Roberts</i> [1996]	L	
6.9	-5200	<i>Ashworth et al.</i> [1988]	X	3	
7.2	5800	<i>Janini and Quaddora</i> [1986]	X	3	
2-pentanone C ₃ H ₇ COCH ₃ [107-87-9]	1.6×10 ¹		<i>Buttery et al.</i> [1969]	M	
	1.2×10 ¹		<i>Meylan and Howard</i> [1991]	X	3
	9.2	4600	<i>Janini and Quaddora</i> [1986]	X	3
3-pentanone C ₂ H ₅ COC ₂ H ₅	2.0×10 ¹	9200	<i>Janini and Quaddora</i> [1986]	X	3
2-heptanone C ₅ H ₁₁ COCH ₃ [110-43-0]	7.0		<i>Buttery et al.</i> [1969]	M	
	3.5×10 ¹	4500	<i>Janini and Quaddora</i> [1986]	X	3
	6.3		<i>Meylan and Howard</i> [1991]	X	3

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
2-octanone <chem>C6H13COCH3</chem>	5.4		<i>Buttery et al.</i> [1969]	M	
2-nonanone <chem>C7H15COCH3</chem>	2.7		<i>Buttery et al.</i> [1969]	M	
2-undecanone <chem>C9H19COCH3</chem>	1.6		<i>Buttery et al.</i> [1969]	M	
4-methyl-2-pentanone <chem>(CH3)2CHCH2COCH3</chem> (methyl isobutyl ketone, MIBK) [108-10-1]	2.6...5.2 2.2	170	<i>Howe et al.</i> [1987] <i>Ashworth et al.</i> [1988]	X X	11 3
3-buten-2-one <chem>C4H6O</chem> (methyl vinyl ketone, MVK) [78-94-4]	2.1×10^1 4.4×10^1 4.1×10^1	7800	<i>Allen et al.</i> [1998] <i>Betterton</i> [1991] <i>Iraci et al.</i> [1998]	E ? M	
1-phenylethanone <chem>C6H5COCH3</chem> (acetophenone) [98-86-2]	9.4×10^1 1.1×10^2 9.8×10^1	6000 12000	<i>Hine and Mookerjee</i> [1975] <i>Betterton</i> [1991] <i>Allen et al.</i> [1998]	V M E	
3,5,5-trimethyl-2-cyclohexen-1-one <chem>C9H14O</chem> (isophorone) [78-59-1]	1.7×10^2	3900	<i>USEPA</i> [1982]	X	3
2,3-butanedione <chem>CH3COCOCH3</chem> (biacetyl, dimethylglycol)	1.9×10^2 5.7×10^1 7.4×10^1	5700	<i>Gaffney and Senum</i> [1984] <i>Snider and Dawson</i> [1985] <i>Betterton</i> [1991]	X M M	48

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
3-methyl butanoic acid (CH ₃) ₂ CHCH ₂ COOH	1.2×10 ³		<i>Khan et al.</i> [1995]	M	
2,2-dimethyl propanoic acid (CH ₃) ₃ CCOOH	3.5×10 ²		<i>Khan et al.</i> [1995]	M	
hexanoic acid C ₅ H ₁₁ COOH [142-62-1]	1.4×10 ³ 1.2×10 ³	6304 5900	<i>Khan et al.</i> [1995] <i>Staudinger and Roberts</i> [1996]	M ?	70
propenoic acid C ₃ H ₄ O ₂ (acrylic acid) [79-10-7]	2.4×10 ³		<i>Yaws and Yang</i> [1992]	?	39
2-Methyl-2-propenoic acid C ₄ H ₆ O ₂ (methacrylic acid) [79-41-4]	2.6×10 ³		<i>Khan et al.</i> [1992]	M	
benzoic acid C ₆ H ₅ COOH	2.4×10 ⁴ 1.4×10 ⁴	6500	<i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982]	? X	39 3
ethanedioic acid HOOC ₂ COOH (oxalic acid)	7.0×10 ⁶ 5.0×10 ⁸		<i>Gaffney and Senum</i> [1984] <i>Saxena and Hildemann</i> [1996]	X E	48 51
propanedioic acid HOOCCH ₂ COOH (malonic acid)	4.0×10 ⁸		<i>Saxena and Hildemann</i> [1996]	E	51
butanedioic acid HOOC(CH ₂) ₂ COOH (succinic acid)	3.0×10 ⁸		<i>Saxena and Hildemann</i> [1996]	E	51
pentanedioic acid HOOC(CH ₂) ₃ COOH (glutaric acid)	2.0×10 ⁸		<i>Saxena and Hildemann</i> [1996]	E	51
hexanedioic acid HOOC(CH ₂) ₄ COOH (adipic acid)	2.0×10 ⁸ 1.8×10 ⁷	11000	<i>Saxena and Hildemann</i> [1996] <i>USEPA</i> [1982]	E X	51 3
<i>cis</i> -butenedioic acid HOOC(CH) ₂ COOH (maleic acid)	1.0×10 ⁹		<i>Saxena and Hildemann</i> [1996]	E	51
ethanoic peroxyacid CH ₃ COOOH (peroxyacetic acid)	6.7×10 ² 8.4×10 ²	5900 5300	<i>Lind and Kok</i> [1994] <i>O'Sullivan et al.</i> [1996]	M M	9

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
esters (RCOOR) (C, H, and O only)					
methyl methanoate HCOOCH ₃ (methyl formate)	4.5 4.5 4.1 4.1		<i>Hine and Mookerjee</i> [1975] <i>Betterton</i> [1992] <i>Hoff et al.</i> [1993] <i>Hartkopf and Karger</i> [1973]	? ? M M	71 71
methyl ethanoate CH ₃ COOCH ₃ (methyl acetate)	1.1×10 ¹ 7.8 8.7	5000	<i>Butler and Ramchandani</i> [1935] <i>Kieckbusch and King</i> [1979] <i>Buttery et al.</i> [1969]	M M M	
methyl propanoate C ₂ H ₅ COOCH ₃ (methyl propionate)	6.2 5.8		<i>Hine and Mookerjee</i> [1975] <i>Buttery et al.</i> [1969]	V M	
methyl butanoate C ₃ H ₇ COOCH ₃ (methyl butyrate)	4.8		<i>Buttery et al.</i> [1969]	M	
methyl pentanoate C ₄ H ₉ COOCH ₃	3.1		<i>Buttery et al.</i> [1969]	M	
methyl hexanoate C ₅ H ₁₁ COOCH ₃	2.7		<i>Buttery et al.</i> [1969]	M	
methyl octanoate C ₆ H ₁₃ COOCH ₃	1.3		<i>Buttery et al.</i> [1969]	M	
methyl decanoate C ₁₁ H ₂₂ O ₂ (methyl caprate) [110-42-9]	1.4		<i>Krop et al.</i> [1997]	V	
methyl dodecanoate C ₁₃ H ₂₆ O ₂ (methyl laurate) [111-82-0]	8.4×10 ⁻¹		<i>Krop et al.</i> [1997]	V	
methyl tetradecanoate C ₁₅ H ₃₀ O ₂ (methyl myristate) [124-10-7]	5.1×10 ⁻¹		<i>Krop et al.</i> [1997]	V	
methyl hexadecanoate C ₁₇ H ₃₄ O ₂ (methyl palmitate) [112-39-0]	3.0×10 ⁻¹		<i>Krop et al.</i> [1997]	V	
methyl octadecanoate C ₁₉ H ₃₈ O ₂ (methyl stearate) [112-61-8]	1.7×10 ⁻¹		<i>Krop et al.</i> [1997]	V	

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
methyl arachidate	1.0×10^{-1}		<i>Krop et al.</i> [1997]	V	
methyl behenate	6.0×10^{-2}		<i>Krop et al.</i> [1997]	V	
(Z,Z,Z)-9,12,15-octadecatrienoic acid methyl ester C ₁₉ H ₃₂ O ₂ (methyl linolenate) [301-00-8]	2.8×10^1		<i>Krop et al.</i> [1997]	V	
(Z,Z)-9,12-octadecadienoic acid methyl ester C ₁₉ H ₃₄ O ₂ (methyl linolate) [112-63-0]	6.3		<i>Krop et al.</i> [1997]	V	
(Z)-9-octadecenoic acid methyl ester C ₁₉ H ₃₆ O ₂ (methyl oleate) [112-62-9]	1.3		<i>Krop et al.</i> [1997]	V	
(Z)-13-docosenoic acid methyl ester C ₂₃ H ₄₄ O ₂ (methyl erucate) [1120-34-9]	5.3×10^{-1}		<i>Krop et al.</i> [1997]	V	
methyl benzoate C ₆ H ₅ COOCH ₃	5.6×10^1		<i>Hine and Mookerjee</i> [1975]	V	
ethyl methanoate HCOOC ₂ H ₅ (ethyl formate)	3.6 1.4×10^{-1} 2.0×10^{-1}	4300	<i>Hine and Mookerjee</i> [1975] <i>Hoff et al.</i> [1993] <i>Hartkopf and Karger</i> [1973]	V ? M	13
ethyl ethanoate CH ₃ COOC ₂ H ₅ (ethyl acetate)	7.6 5.9 9.0 4.7 6.5	5300 5700	<i>Butler and Ramchandani</i> [1935] <i>Kieckbusch and King</i> [1979] <i>Hoff et al.</i> [1993] <i>Janini and Quaddora</i> [1986] <i>Meylan and Howard</i> [1991]	M M ? X X	13 3 3
ethyl propanoate C ₂ H ₅ COOC ₂ H ₅ (ethyl propionate)	4.6		<i>Hine and Mookerjee</i> [1975]	V	
ethyl butanoate C ₃ H ₇ COOC ₂ H ₅ (ethyl butyrate)	2.8		<i>Hine and Mookerjee</i> [1975]	V	
ethyl pentanoate C ₄ H ₉ COOC ₂ H ₅	2.9		<i>Hine and Mookerjee</i> [1975]	V	

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
ethyl heptanoate $\text{C}_6\text{H}_{13}\text{COOC}_2\text{H}_5$	2.0		<i>Hine and Mookerjee</i> [1975]	V	
ethyl dodecanoate $\text{C}_{14}\text{H}_{28}\text{O}_2$ (ethyl laurate) [106-33-2]	7.8×10^{-1}		<i>Krop et al.</i> [1997]	V	
propyl methanoate HCOOC_3H_7 (propyl formate)	2.7		<i>Hine and Mookerjee</i> [1975]	V	
propyl ethanoate $\text{CH}_3\text{COOC}_3\text{H}_7$ (propyl acetate)	5.0 5.0 4.6 4.4 4.5	5500 6000	<i>Butler and Ramchandani</i> [1935] <i>Hine and Mookerjee</i> [1975] <i>Kieckbusch and King</i> [1979] <i>Janini and Quaddora</i> [1986] <i>Meylan and Howard</i> [1991]	V V M X X	 3 3
propyl propanoate $\text{C}_2\text{H}_5\text{COOC}_3\text{H}_7$ (propyl propionate)	2.6		<i>Hine and Mookerjee</i> [1975]	V	
propyl butanoate $\text{C}_3\text{H}_7\text{COOC}_3\text{H}_7$ (propyl butyrate)	1.9		<i>Hine and Mookerjee</i> [1975]	V	
propyl dodecanoate $\text{C}_{15}\text{H}_{30}\text{O}_2$ (propyl laurate) [3681-78-5]	7.8×10^{-1}		<i>Krop et al.</i> [1997]	V	
isopropyl methanoate HCOOC_3H_7 (isopropyl formate)	1.2		<i>Hine and Mookerjee</i> [1975]	V	
isopropyl ethanoate $\text{CH}_3\text{COOC}_3\text{H}_7$ (isopropyl acetate)	3.6 2.9	5500	<i>Hine and Mookerjee</i> [1975] <i>Janini and Quaddora</i> [1986]	V X	 3
isopropyl propanoate $\text{C}_2\text{H}_5\text{COOC}_3\text{H}_7$ (isopropyl propionate)	1.7		<i>Hine and Mookerjee</i> [1975]	V	
butyl ethanoate $\text{CH}_3\text{COOC}_4\text{H}_9$ (butyl acetate)	3.0 3.6 3.5 3.5 2.1	6000 7500 3200	<i>Hine and Mookerjee</i> [1975] <i>Kieckbusch and King</i> [1979] <i>Meylan and Howard</i> [1991] <i>Janini and Quaddora</i> [1986] <i>USEPA</i> [1982]	V M X X X	 3 3 3
butyl dodecanoate $\text{C}_{16}\text{H}_{32}\text{O}_2$ (butyl laurate) [106-18-3]	7.2×10^{-1}		<i>Krop et al.</i> [1997]	V	

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
2-methylpropyl methanoate HCOOC ₄ H ₉ (isobutyl formate)	1.7		<i>Hine and Mookerjee</i> [1975]	V	
2-methylpropyl ethanoate CH ₃ COOC ₄ H ₉ (isobutyl acetate) [110-19-0]	2.2		<i>Hine and Mookerjee</i> [1975]	V	
pentyl ethanoate CH ₃ COOC ₅ H ₁₁ (amyl acetate)	2.6 2.8	6500	<i>Hine and Mookerjee</i> [1975] <i>Kieckbusch and King</i> [1979]	V M	
pentyl propanoate C ₂ H ₅ COOC ₅ H ₁₁ (amyl propionate)	1.2		<i>Hine and Mookerjee</i> [1975]	V	
isopentyl methanoate HCOOC ₅ H ₁₁ (isoamyl formate)	1.5		<i>Hine and Mookerjee</i> [1975]	V	
isopentyl ethanoate CH ₃ COOC ₅ H ₁₁ (isoamyl acetate)	1.7 2.4	5000	<i>Hine and Mookerjee</i> [1975] <i>USEPA</i> [1982]	V X	3
hexyl ethanoate CH ₃ COOC ₆ H ₁₃ (hexyl acetate)	1.9		<i>Hine and Mookerjee</i> [1975]	V	
2-ethylhexyl dodecanoate (2-ethylhexyl laurate)	3.1×10^{-1}		<i>Krop et al.</i> [1997]	V	
ethenyl ethanoate CH ₃ COOCHCH ₂ (vinyl acetate)	1.7	2600	<i>USEPA</i> [1982]	X	3
dimethyl phthalate C ₁₀ H ₁₀ O ₄ [131-11-3]	3.0×10^3	5700	<i>USEPA</i> [1982]	X	3
diethyl phthalate C ₁₂ H ₁₄ O ₄ [84-66-2]	1.2×10^3	5600	<i>USEPA</i> [1982]	X	3

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
ethers (ROR) (C, H, and O only)					
dimethyl ether CH ₃ OCH ₃	9.9×10 ⁻¹ 1.0		<i>Hine and Weimar</i> [1965] <i>Hine and Mookerjee</i> [1975]	R V	
ethyl methyl ether C ₂ H ₅ OCH ₃	9.0×10 ⁻¹		<i>Saxena and Hildemann</i> [1996]	E	51
diethyl ether C ₂ H ₅ OC ₂ H ₅	1.1 1.1 8.0×10 ⁻¹ 1.2 7.8×10 ⁻¹ 7.9×10 ⁻¹	5300	<i>Butler and Ramchandani</i> [1935] <i>Hine and Weimar</i> [1965] <i>Signer et al.</i> [1969] <i>Nielsen et al.</i> [1994] <i>Hoff et al.</i> [1993] <i>Lamarche and Droste</i> [1989]	V V M M ? X	13 3
methyl propyl ether CH ₃ OC ₃ H ₇	6.8×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
methyl 2-propyl ether CH ₃ OC ₃ H ₇	1.2		<i>Hine and Mookerjee</i> [1975]	V	
methyl <i>tert</i> -butyl ether CH ₃ OC(CH ₃) ₃	1.7 1.6	7700	<i>Guthrie</i> [1973] <i>Robbins et al.</i> [1993]	V M	
ethyl propyl ether C ₂ H ₅ OC ₃ H ₇	8.7×10 ⁻¹ 8.7×10 ⁻¹		<i>Butler and Ramchandani</i> [1935] <i>Hine and Mookerjee</i> [1975]	V V	
dipropyl ether C ₃ H ₇ OC ₃ H ₇	2.8×10 ⁻¹ 2.9×10 ⁻¹ 1.9×10 ⁻¹ 2.3×10 ⁻¹ 4.5×10 ⁻¹	8900	<i>Butler and Ramchandani</i> [1935] <i>Hine and Mookerjee</i> [1975] <i>Hoff et al.</i> [1993] <i>Hartkopf and Karger</i> [1973] <i>Yaws and Yang</i> [1992]	V V ? M ?	13 39
diisopropyl ether C ₃ H ₇ OC ₃ H ₇	9.9×10 ⁻² 1.0×10 ⁻¹ 4.9×10 ⁻¹ 5.8×10 ⁻¹		<i>Hine and Weimar</i> [1965] <i>Hine and Mookerjee</i> [1975] <i>Nielsen et al.</i> [1994] <i>Yaws and Yang</i> [1992]	V V M ?	39
dibutyl ether C ₄ H ₉ OC ₄ H ₉	1.7×10 ⁻¹		<i>Pierotti et al.</i> [1957]	X	53
methoxybenzene C ₆ H ₅ OCH ₃ (anisole) [100-66-3]	2.4×10 ⁻¹ 2.4×10 ⁻¹		<i>Hine and Weimar</i> [1965] <i>Hine and Mookerjee</i> [1975]	R V	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
miscellaneous, e.g. multiple functional groups (C, H, and O only)					
1,2-epoxypropane C ₃ H ₆ O (propyleneoxide) [75-56-9]	5.3	3500	USEPA [1982]	X	3
2-methoxyethanol C ₃ H ₈ O ₂ [109-86-4]	2.2 × 10 ⁻²	-870	Ashworth et al. [1988]	X	3
dimethoxymethane CH ₃ OCH ₂ OCH ₃	5.8		Pierotti et al. [1957]	X	53
trimethoxymethane HC(OCH ₃) ₃	7.0 × 10 ¹		Guthrie [1973]	V	
1,1-diethoxyethane (C ₂ H ₅ O) ₂ CHCH ₃	1.0 × 10 ¹		Hine and Mookerjee [1975]	V	
1,2-diethoxyethane C ₂ H ₅ OC ₂ H ₄ OC ₂ H ₅	1.6 × 10 ¹		Hine and Mookerjee [1975]	V	
1,1,1-trimethoxyethane CH ₃ C(OCH ₃) ₃	6.5 × 10 ¹		Guthrie [1973]	V	
3-oxapentane-1,5-diol HO(CH ₂) ₂ O(CH ₂) ₂ OH (diethylene glycol) [111-46-6]	2.0 × 10 ⁹		Saxena and Hildemann [1996]	E	51
3,6-dioxaoctane-1,8-diol HO(CH ₂ CH ₂ O) ₃ H (triethylene glycol) [112-27-6]	9.0 × 10 ¹¹		Saxena and Hildemann [1996]	E	51
propanal CH ₃ COCHO (methylglyoxal, pyruvaldehyde)	3.7 × 10 ³ 3.2 × 10 ⁴	7500	Betterton and Hoffmann [1988] Zhou and Mopper [1990]	M M	63
2-hydroxyethanal HOCH ₂ CHO (hydroxyacetaldehyde)	4.1 × 10 ⁴	4600	Betterton and Hoffmann [1988]	M	63
oxoethanoic acid OHCCOOH (glyoxylic acid) [298-12-4]	9.0 × 10 ³		Saxena and Hildemann [1996]	E	51
2-oxopropanoic acid CH ₃ COCOOH (pyruvic acid)	3.1 × 10 ⁵ 3.0 × 10 ⁵ 3.1 × 10 ⁵	5100 5200	Khan et al. [1995] Staudinger and Roberts [1996] Khan et al. [1992]	M ? M	70

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
3-oxopropanoic acid OHCCH ₂ COOH	7.0×10^3		<i>Saxena and Hildemann</i> [1996]	E	51
4-oxobutanoic acid OHC(CH ₂) ₂ COOH	5.0×10^3		<i>Saxena and Hildemann</i> [1996]	E	51
5-oxopentanoic acid OHC(CH ₂) ₃ COOH	4.0×10^3		<i>Saxena and Hildemann</i> [1996]	E	51
oxacyclopentadiene C ₄ H ₄ O (furan, furfuran) [110-00-9]	1.8×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
tetrahydrofurane C ₄ H ₈ O (THF)	1.4×10^1 2.2×10^1	5700	<i>Cabani et al.</i> [1971a] <i>Signer et al.</i> [1969]	M M	
2-methyltetrahydrofurane CH ₃ C ₄ H ₇ O	1.1×10^1	6200	<i>Cabani et al.</i> [1971a]	M	
2,5-dimethyltetrahydrofurane (CH ₃) ₂ C ₄ H ₆ O	5.7	6800	<i>Cabani et al.</i> [1971a]	M	
tetrahydropyran C ₅ H ₁₀ O (THP)	8.0	5900	<i>Cabani et al.</i> [1971a]	M	
1,3-dioxolane C ₃ H ₆ O ₂	4.0×10^1	4800	<i>Cabani et al.</i> [1971a]	M	
1,4-dioxane C ₄ H ₈ O ₂ (dioxane)	2.1×10^2 2.2×10^2 1.4×10^2 2.0×10^2 1.4×10^2	5800	<i>Cabani et al.</i> [1971a] <i>Rohrschneider</i> [1973] <i>Friant and Suffet</i> [1979] <i>Cabani et al.</i> [1971a] <i>Yaws and Yang</i> [1992]	X M M M ?	11 49 39
1,3-dimethoxy-2-hydroxybenzene C ₈ H ₁₀ O ₃ (2,6-dimethoxyphenol) [91-10-1]	4.9×10^3	6700	<i>Sagebiel et al.</i> [1992]	X	3
1-hydroxy-2-methoxybenzene C ₇ H ₈ O ₂ (guaicol) [90-05-1]	9.1×10^2	7500	<i>Sagebiel et al.</i> [1992]	X	3
4-methyl-2-methoxyphenol	7.2×10^2	7400	<i>Sagebiel et al.</i> [1992]	X	3
hydroxybutanedioic acid HOOCCH ₂ CHOHCOOH (malic acid)	2.0×10^{13}		<i>Saxena and Hildemann</i> [1996]	E	51

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
2-hydroxy-1,2,3-propanetricarboxylic acid $\text{C}_6\text{H}_8\text{O}_7$ (citric acid) [77-92-9]	3.0×10^{18}		<i>Saxena and Hildemann</i> [1996]	E	51
2-oxopentanedioic acid $\text{HOOC}(\text{CH}_2)_2\text{COCOOH}$ (α -keto glutaric acid) [328-50-7]	1.0×10^9		<i>Saxena and Hildemann</i> [1996]	E	51
2-hydroxypropanoic acid $\text{CH}_3\text{CHOHCOOH}$ (lactic acid)	7.0×10^7		<i>Saxena and Hildemann</i> [1996]	E	51
2,3-dihydroxybutanedioic acid HOOCCHOHCHOHCOOH (tartaric acid) [87-69-4]	1.0×10^{18}		<i>Saxena and Hildemann</i> [1996]	E	51
2,3-dihydroxypropanal $\text{C}_3\text{H}_6\text{O}_3$ (glyceraldehyde)	2.0×10^{10}		<i>Saxena and Hildemann</i> [1996]	E	51
carbon monoxide CO	7.4×10^{-3} 8.2×10^{-4} 9.5×10^{-4} 9.5×10^{-4} 9.9×10^{-4} 8.7×10^{-4}	1300 1600 1300	<i>Meadows and Spedding</i> [1974] <i>Liss and Slater</i> [1974] <i>Wilhelm et al.</i> [1977] <i>Dean</i> [1992] <i>Lide and Frederikse</i> [1995] <i>Yaws and Yang</i> [1992]	M c L ? L ?	2 39
carbon dioxide CO ₂	3.4×10^{-2} 3.4×10^{-2} 3.4×10^{-2} 3.5×10^{-2} 3.4×10^{-2} 3.1×10^{-2} 3.4×10^{-2} 3.4×10^{-2} 3.4×10^{-2} 3.4×10^{-2} 3.5×10^{-2} 3.4×10^{-2} 3.5×10^{-2} 4.5×10^{-2} 3.2×10^{-2} 3.6×10^{-2}	2400 2400 2400 2400 2400 2400 2400 2400 2400 2400 2300 2600 2400 2400 2400 2200	<i>Morgan and Maass</i> [1931] <i>Sillen and Martell</i> [1964] <i>Wilhelm et al.</i> [1977] <i>Edwards et al.</i> [1978] <i>Durham et al.</i> [1981] <i>Chameides</i> [1984] <i>Hoffmann and Jacob</i> [1984] <i>Jacob</i> [1986] <i>Pandis and Seinfeld</i> [1989] <i>Lelieveld and Crutzen</i> [1991] <i>Carroll et al.</i> [1991] <i>Dean</i> [1992] <i>Lide and Frederikse</i> [1995] <i>Yaws and Yang</i> [1992] <i>Kavanaugh and Trussell</i> [1980] <i>Zheng et al.</i> [1997]	M X L L C T ? C C C L ? L ? X M	1 4 2 39 3

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
compounds with nitrogen: amines (RNH₂) (C, H, O, and N only)					
methylamine CH ₃ NH ₂	3.6×10 ¹ 9.0×10 ¹ 1.4×10 ²	2600	<i>Wilhelm et al.</i> [1977] <i>Christie and Crisp</i> [1967] <i>Bone et al.</i> [1983]	L M ?	12
ethylamine C ₂ H ₅ NH ₂ [75-04-7]	1.0×10 ² 3.5×10 ¹ 8.1×10 ¹	3600	<i>Butler and Ramchandani</i> [1935] <i>Wilhelm et al.</i> [1977] <i>Christie and Crisp</i> [1967]	M L M	
propylamine C ₃ H ₇ NH ₂ [107-10-8]	8.0×10 ¹ 6.7×10 ¹		<i>Butler and Ramchandani</i> [1935] <i>Christie and Crisp</i> [1967]	M M	
butylamine C ₄ H ₉ NH ₂ [109-73-9]	6.6×10 ¹ 5.8×10 ¹		<i>Butler and Ramchandani</i> [1935] <i>Christie and Crisp</i> [1967]	M M	
pentylamine C ₅ H ₁₁ NH ₂	4.1×10 ¹		<i>Christie and Crisp</i> [1967]	M	
hexylamine C ₆ H ₁₃ NH ₂	3.7×10 ¹		<i>Christie and Crisp</i> [1967]	M	
dimethylamine (CH ₃) ₂ NH [124-40-3]	3.1×10 ¹ 5.7×10 ¹	4000	<i>Wilhelm et al.</i> [1977] <i>Christie and Crisp</i> [1967]	L M	
diethylamine (C ₂ H ₅) ₂ NH [109-89-7]	3.9×10 ¹ 1.5×10 ¹ 1.3×10 ² 3.9×10 ¹	10000	<i>Christie and Crisp</i> [1967] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Meylan and Howard</i> [1991]	M ? X X	39 3 3
dipropylamine (C ₃ H ₇) ₂ NH	1.9×10 ¹ see note		<i>Christie and Crisp</i> [1967] see note	M ?	66
dibutylamine (C ₄ H ₉) ₂ NH	1.1×10 ¹		<i>Christie and Crisp</i> [1967]	M	
trimethylamine (CH ₃) ₃ N [75-50-3]	9.6		<i>Christie and Crisp</i> [1967]	M	
triethylamine (C ₂ H ₅) ₃ N	6.7		<i>Christie and Crisp</i> [1967]	M	
ethylenediamine H ₂ NCH ₂ CH ₂ NH ₂	5.9×10 ⁵		<i>Westheimer and Ingraham</i> [1956]	M	
hexamethyleneimine (CH ₂) ₆ NH	1.6×10 ²	8200	<i>Cabani et al.</i> [1971b]	M	
ethanolamine HOC ₂ H ₄ NH ₂ [141-43-5]	6.2×10 ⁶		<i>Bone et al.</i> [1983]	M	8

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
compounds with nitrogen: amino acids (RCHNH₂COOH)					
glutamic acid	1.0×10^{13}		<i>Saxena and Hildemann</i> [1996]	E	51
asparagine	1.0×10^{13}		<i>Saxena and Hildemann</i> [1996]	E	51
serine	4.0×10^{12}		<i>Saxena and Hildemann</i> [1996]	E	51
glutamine	1.0×10^{13}		<i>Saxena and Hildemann</i> [1996]	E	51
glycine	9.0×10^7		<i>Saxena and Hildemann</i> [1996]	E	51
arginine	1.0×10^{17}		<i>Saxena and Hildemann</i> [1996]	E	51
alanine	6.0×10^7		<i>Saxena and Hildemann</i> [1996]	E	51
leucine	2.0×10^7		<i>Saxena and Hildemann</i> [1996]	E	51
compounds with nitrogen: heterocycles (C, H, O, and N only)					
pyrrolidine C ₄ H ₈ NH	4.2×10^2	7600	<i>Cabani et al.</i> [1971b]	M	
N-methyl-pyrrolidine C ₄ H ₈ NCH ₃	3.3×10^1	7600	<i>Cabani et al.</i> [1971b]	M	
piperidine C ₅ H ₁₀ NH	2.2×10^2	7900	<i>Cabani et al.</i> [1971b]	M	
N-methyl-piperidine C ₅ H ₁₀ NCH ₃	2.9×10^1	7900	<i>Cabani et al.</i> [1971b]	M	
pyridine C ₅ H ₅ N [110-86-1]	1.1×10^2 9.0×10^1	5900	<i>Andon et al.</i> [1954] <i>Yaws and Yang</i> [1992]	M ?	39
2-methylpyridine C ₅ H ₄ NCH ₃ (2-picoline, α -picoline) [109-06-8]	3.4×10^1 1.0×10^2	6400	<i>Yaws and Yang</i> [1992] <i>Andon et al.</i> [1954]	? M	39
3-methylpyridine C ₅ H ₄ NCH ₃ (3-picoline, β -picoline) [108-99-6]	5.5×10^1 1.3×10^2	6400	<i>Yaws and Yang</i> [1992] <i>Andon et al.</i> [1954]	? M	39
4-methylpyridine C ₅ H ₄ NCH ₃	1.7×10^2	6600	<i>Andon et al.</i> [1954]	M	
2-ethylpyridine C ₅ H ₄ NC ₂ H ₅	6.1×10^1	6700	<i>Andon et al.</i> [1954]	M	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
3-ethylpyridine <chem>C5H4NC2H5</chem>	9.6×10^1	6500	<i>Andon et al.</i> [1954]	M	
4-ethylpyridine <chem>C5H4NC2H5</chem>	1.2×10^2	6300	<i>Andon et al.</i> [1954]	M	
2,3-dimethylpyridine <chem>C5H3N(CH3)2</chem> [583-61-9]	1.4×10^2	700	<i>Andon et al.</i> [1954]	M	
2,4-dimethylpyridine <chem>C5H3N(CH3)2</chem>	1.5×10^2	7100	<i>Andon et al.</i> [1954]	M	
2,5-dimethylpyridine <chem>C5H3N(CH3)2</chem>	1.2×10^2	7100	<i>Andon et al.</i> [1954]	M	
2,6-dimethylpyridine <chem>C5H3N(CH3)2</chem>	9.5×10^1	7300	<i>Andon et al.</i> [1954]	M	
3,4-dimethylpyridine <chem>C5H3N(CH3)2</chem>	2.7×10^2	6900	<i>Andon et al.</i> [1954]	M	
3,5-dimethylpyridine <chem>C5H3N(CH3)2</chem>	1.4×10^2	6800	<i>Andon et al.</i> [1954]	M	
2-methylpyrazine <chem>C4N2H3CH3</chem>	4.5×10^2		<i>Buttery et al.</i> [1971]	M	
2-ethylpyrazine <chem>C4N2H3(C2H5)</chem>	4.0×10^2		<i>Buttery et al.</i> [1971]	M	
2-isobutylpyrazine <chem>C4N2H3C4H9</chem>	2.0×10^2		<i>Buttery et al.</i> [1971]	M	
2-ethyl-3-methoxypyrazine <chem>C4N2H3(C2H5)OCH3</chem>	6.8×10^1		<i>Buttery et al.</i> [1971]	M	
2-isobutyl-3-methoxypyrazine <chem>C4N2H3(C4H9)OCH3</chem>	2.0×10^1 1.3×10^1		<i>Buttery et al.</i> [1971] <i>Karl and Lindinger</i> [1997]	M M	43
benzo[b]pyridine <chem>C9H7N</chem> (quinoline) [91-22-5]	3.7×10^3	5400	<i>USEPA</i> [1982]	X	3

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
compounds with nitrogen: nitrates (RONO₂) (C, H, O, and N only)					
methyl nitrate CH ₃ ONO ₂	2.0	4700	<i>Kames and Schurath</i> [1992]	M	
ethyl nitrate C ₂ H ₅ ONO ₂	1.6	5400	<i>Kames and Schurath</i> [1992]	M	
1-propyl nitrate C ₃ H ₇ ONO ₂ [627-13-4]	1.1 1.1 7.9×10 ⁻¹	5500	<i>Kames and Schurath</i> [1992] <i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	M V M	
2-propyl nitrate C ₃ H ₇ ONO ₂	7.9×10 ⁻¹ 6.2×10 ⁻¹ 8.3×10 ⁻¹	5400	<i>Kames and Schurath</i> [1992] <i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	M M V	
1-butyl nitrate C ₄ H ₉ ONO ₂ [928-45-0]	1.0 1.0 6.5×10 ⁻¹ 8.6×10 ⁻¹	6000 5800	<i>Luke et al.</i> [1989] <i>Kames and Schurath</i> [1992] <i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	M M M V	
2-butyl nitrate C ₄ H ₉ ONO ₂ (isobutyl nitrate) [543-29-3]	6.5×10 ⁻¹ 6.5×10 ⁻¹ 4.4×10 ⁻¹ 6.5×10 ⁻¹	5600 5400	<i>Luke et al.</i> [1989] <i>Kames and Schurath</i> [1992] <i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	M M M V	
<i>tert</i> -butyl nitrate C ₄ H ₉ ONO ₂	7.0×10 ⁻¹	5200	<i>Kames and Schurath</i> [1992]	M	
1-pentyl nitrate C ₅ H ₁₁ ONO ₂ (amyl nitrate) [1002-16-0]	1.2 4.1×10 ⁻¹ 6.0×10 ⁻¹		<i>Kames and Schurath</i> [1992] <i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	M V M	8
2-pentyl nitrate C ₅ H ₁₁ ONO ₂ [21981-48-6]	3.7×10 ⁻¹ 3.4×10 ⁻¹ 4.9×10 ⁻¹	6300	<i>Kames and Schurath</i> [1992] <i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	M M V	
3-pentyl nitrate C ₅ H ₁₃ ONO ₂	3.7×10 ⁻¹ 4.9×10 ⁻¹		<i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	M V	
3-methyl-1-butanol nitrate C ₅ H ₁₁ ONO ₂ (isoamyl nitrate) [543-87-3]	4.5×10 ⁻¹		<i>Hauff et al.</i> [1998]	M	
1-hexyl nitrate C ₆ H ₁₃ ONO ₂	3.7×10 ⁻¹ 6.7×10 ⁻¹		<i>Hauff et al.</i> [1998] <i>Hauff et al.</i> [1998]	V M	

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
2-nitrooxy ethanol <chem>HOC2H4ONO2</chem>	4.0×10^4 3.9×10^4	8600	<i>Kames and Schurath</i> [1992] <i>Shepson et al.</i> [1996]	M M	8
nitrooxy propanol <chem>C3H7O4N</chem> (1,2 and 2,1)	7.3×10^3 6.7×10^3		<i>Kames and Schurath</i> [1992] <i>Kames and Schurath</i> [1992]	M M	8, 72 8, 72
1-nitrooxy-2-propanol <chem>C3H7O4N</chem>	1.1×10^4	10000	<i>Shepson et al.</i> [1996]	M	
2-nitrooxy-1-propanol <chem>C3H7O4N</chem>	4.5×10^3	8800	<i>Shepson et al.</i> [1996]	M	
2-nitrooxy-3-butanol <chem>C4H9O4N</chem>	1.0×10^4	9500	<i>Shepson et al.</i> [1996]	M	
1-nitrooxy-2-butanol <chem>C4H9O4N</chem>	5.8×10^3	9200	<i>Shepson et al.</i> [1996]	M	
2-nitrooxy-1-butanol <chem>C4H9O4N</chem>	6.0×10^3	9600	<i>Shepson et al.</i> [1996]	M	
nitrooxyacetone <chem>CH3COCH2ONO2</chem>	1.0×10^3		<i>Kames and Schurath</i> [1992]	M	8

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1,2-ethanediol dinitrate $\text{O}_3\text{NCH}_2\text{CH}_2\text{ONO}_2$ (1,2-ethane dinitrate) [628-96-6]	6.4×10^2 7.9×10^1		<i>Kames and Schurath</i> [1992] <i>Fischer and Ballschmiter</i> [1998b]	M M	8 73
1,2-propanediol dinitrate $\text{C}_3\text{H}_6(\text{ONO}_2)_2$ (1,2-propane dinitrate) [6423-43-4]	1.8×10^2 3.2×10^1		<i>Kames and Schurath</i> [1992] <i>Fischer and Ballschmiter</i> [1998b]	M M	8 73
1,2-propanediol dinitrate					
1,3-propanediol dinitrate $\text{C}_3\text{H}_6\text{N}_2\text{O}_6$ [3457-90-7]	1.3×10^2		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,2-butanediol dinitrate	2.1×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,3-butanediol dinitrate	5.8×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,4-butanediol dinitrate	1.6×10^2		<i>Fischer and Ballschmiter</i> [1998b]	M	73
2,3-butanediol dinitrate	1.2×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,2-pentanediol dinitrate	1.3×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,4-pentanediol dinitrate	3.9×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,5-pentanediol dinitrate	1.2×10^2		<i>Fischer and Ballschmiter</i> [1998b]	M	73
c-2,4-pentanediol dinitrate	2.2×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
t-2,4-pentanediol dinitrate	1.5×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,2-hexanediol dinitrate	9.7×10^0		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,5-hexanediol dinitrate	2.8×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,6-hexanediol dinitrate	1.5×10^2		<i>Fischer and Ballschmiter</i> [1998b]	M	73
2,5-hexanediol dinitrate	3.2×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
<i>cis</i> -1,2-cyclohexanediol dinitrate	1.3×10^2		<i>Fischer and Ballschmiter</i> [1998b]	M	73
<i>trans</i> -1,2-cyclohexanediol dinitrate	5.2×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
<i>cis</i> -1,3-cyclohexanediol dinitrate	3.5×10^2		<i>Fischer and Ballschmiter</i> [1998b]	M	73
<i>trans</i> -1,3-cyclohexanediol dinitrate	6.9×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,7-heptanediol dinitrate	1.2×10^2		<i>Fischer and Ballschmiter</i> [1998b]	M	73
<i>trans</i> -1,2-cycloheptanediol dinitrate	8.9×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,2-octanediol dinitrate	5.3×10^0		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,8-octanediol dinitrate	7.9×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,2-decanediol dinitrate	2.0×10^0		<i>Fischer and Ballschmiter</i> [1998b]	M	73
1,10-decanediol dinitrate	4.3×10^1		<i>Fischer and Ballschmiter</i> [1998b]	M	73
peroxyacetyl nitrate CH ₃ COONO ₂ (PAN)	3.6 5.0 2.9 2.8 4.1 see note see note	5900 6500	<i>Gaffney and Senum</i> [1984] <i>Holdren et al.</i> [1984] <i>Pandis and Seinfeld</i> [1989] <i>Kames et al.</i> [1991] <i>Kames and Schurath</i> [1995] <i>Warneck et al.</i> [1996] <i>Schurath et al.</i> [1996]	X M C M M ? ?	48 74 8 75 76
peroxypropionyl nitrate C ₂ H ₅ COONO ₂ (PPN)	2.9 see note see note		<i>Kames and Schurath</i> [1995] <i>Warneck et al.</i> [1996] <i>Schurath et al.</i> [1996]	M ? ?	8 75 76
peroxy- <i>n</i> -butyryl nitrate C ₃ H ₇ COONO ₂ (PnBN)	2.3 see note see note		<i>Kames and Schurath</i> [1995] <i>Warneck et al.</i> [1996] <i>Schurath et al.</i> [1996]	M ? ?	8 75 76
peroxy-2-propenoyl nitrate CH ₂ C(CH ₃)COONO ₂ (peroxymethacryloyl nitrate, MPAN)	1.7 see note see note		<i>Kames and Schurath</i> [1995] <i>Warneck et al.</i> [1996] <i>Schurath et al.</i> [1996]	M ? ?	8 75 76
peroxy-isobutyryl nitrate C ₃ H ₇ COONO ₂ (PiBN)	1.0 see note see note		<i>Kames and Schurath</i> [1995] <i>Warneck et al.</i> [1996] <i>Schurath et al.</i> [1996]	M ? ?	8 75 76

substance	$\frac{k_H^\ominus}{[M/atm]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
compounds with nitrogen: nitriles (RCN) (C, H, O, and N only)					
cyanide radical CN	8.0×10^{-2}	1400	<i>Berdnikov and Bazhin</i> [1970]	T	5
hydrocyanic acid HCN	9.3 1.2×10^1 7.5	5000	<i>Hine and Weimar</i> [1965] <i>Edwards et al.</i> [1978] <i>Gaffney and Senum</i> [1984]	R L X	48
ethane nitrile CH ₃ CN (acetonitrile) [75-05-8]	2.9×10^1 2.9×10^1 5.4×10^1 4.9×10^1 4.8×10^1 5.3×10^1 4.9×10^1	4100 4000 3500 4100	<i>Hine and Weimar</i> [1965] <i>Gaffney and Senum</i> [1984] <i>Hamm et al.</i> [1984] <i>Snider and Dawson</i> [1985] <i>Arijs and Brasseur</i> [1986] <i>Benkelberg et al.</i> [1995] <i>Yaws and Yang</i> [1992]	R X M M L M ?	48 39
propane nitrile C ₂ H ₅ CN (propionitrile) [107-12-0]	2.7×10^1		<i>Butler and Ramchandani</i> [1935]	M	
butane nitrile C ₃ H ₇ CN (butyronitrile)	1.9×10^1		<i>Butler and Ramchandani</i> [1935]	M	
benzenenitrile C ₆ H ₅ CN (benzonitrile) [100-47-0]	1.8		<i>Yaws and Yang</i> [1992]	?	39, 77
ethanedinitrile C ₂ N ₂ (cyanogen) [460-19-5]	1.9×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39, 8
2-propenenitrile C ₃ H ₃ N (acrylonitrile) [107-13-1]	1.1×10^1 7.3	2800	<i>USEPA</i> [1982] <i>Meylan and Howard</i> [1991]	X X	3 3

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
compounds with nitrogen: nitro (RNO₂) (C, H, O, and N only)					
nitromethane CH ₃ NO ₂	3.5×10 ¹ 4.5×10 ¹ 3.6		<i>Gaffney and Senum</i> [1984] <i>Rohrschneider</i> [1973] <i>Yaws and Yang</i> [1992]	X M ?	48 39
nitroethane C ₂ H ₅ NO ₂	2.1×10 ¹ 2.1×10 ¹ 1.4×10 ²		<i>Hine and Mookerjee</i> [1975] <i>Gaffney and Senum</i> [1984] <i>Friant and Suffet</i> [1979]	V X M	 48 49
1-nitropropane C ₃ H ₇ NO ₂	1.2×10 ¹ 1.6×10 ¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	 39, 8
2-nitropropane CH ₃ CH(NO ₂)CH ₃	8.2 1.1×10 ¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	 39, 8
nitrobenzene C ₆ H ₅ NO ₂ [98-95-3]	4.3×10 ¹ 4.1×10 ¹ 4.7×10 ¹	4500	<i>Hine and Mookerjee</i> [1975] <i>Meylan and Howard</i> [1991] <i>USEPA</i> [1982]	V X X	 3 3
2-nitrotoluene C ₆ H ₄ (NO ₂)CH ₃ [88-72-2]	1.7×10 ¹ 7.8	2900	<i>Hine and Mookerjee</i> [1975] <i>USEPA</i> [1982]	V X	 3
3-nitrotoluene C ₆ H ₄ (NO ₂)CH ₃	1.4×10 ¹ 1.4×10 ¹	3200	<i>Hine and Mookerjee</i> [1975] <i>USEPA</i> [1982]	V X	 3
4-nitrotoluene C ₆ H ₄ (NO ₂)CH ₃	1.6×10 ¹	3100	<i>USEPA</i> [1982]	X	3
1-methyl-2,4-dinitrobenzene C ₇ H ₆ N ₂ O ₄ (DNT) [121-14-2]	2.1×10 ¹	2900	<i>USEPA</i> [1982]	X	3

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
2-nitrophenol $\text{HO C}_6\text{H}_4(\text{NO}_2)$ [88-75-5]	7.0×10^1 7.4×10^1 7.9×10^1	4600	<i>USEPA</i> [1982] <i>Schwarzenbach et al.</i> [1988] <i>Tremp et al.</i> [1993]	X V X	3 8 55,8
3-nitrophenol $\text{HO C}_6\text{H}_4(\text{NO}_2)$	5.0×10^5		<i>Gaffney and Senum</i> [1984]	X	48
4-nitrophenol $\text{HO C}_6\text{H}_4(\text{NO}_2)$ [100-02-7]	2.6×10^6 9.9×10^2 3.0×10^4 7.9×10^4	9100 6000	<i>Parsons et al.</i> [1971] <i>USEPA</i> [1982] <i>Schwarzenbach et al.</i> [1988] <i>Tremp et al.</i> [1993]	M X V X	54 3 8 55,8
3-methyl-2-nitrophenol $\text{C}_7\text{H}_7\text{NO}_3$ [4920-77-8]	2.5×10^2		<i>Schwarzenbach et al.</i> [1988]	V	8
4-methyl-2-nitrophenol $\text{C}_7\text{H}_7\text{NO}_3$ [119-33-5]	6.2×10^1		<i>Schwarzenbach et al.</i> [1988]	V	8
5-methyl-2-nitrophenol $\text{C}_7\text{H}_7\text{NO}_3$ [700-38-9]	6.8×10^1		<i>Schwarzenbach et al.</i> [1988]	V	8
4-(1-methylpropyl)-2-nitrophenol $\text{C}_{10}\text{H}_{13}\text{NO}_3$ [3555-18-8]	2.4×10^1		<i>Schwarzenbach et al.</i> [1988]	V	8
4-methoxy-2-nitrophenol $\text{C}_7\text{H}_7\text{NO}_4$ [1568-70-3]	2.3×10^1		<i>Schwarzenbach et al.</i> [1988]	V	8
4-hydroxy-3-nitro-benzaldehyde $\text{C}_7\text{H}_5\text{NO}_4$ [3011-34-5]	9.5×10^2		<i>Schwarzenbach et al.</i> [1988]	V	8
2,4-dinitrophenol $\text{C}_6\text{H}_4\text{N}_2\text{O}_5$ [51-28-5]	3.5×10^3 1.2×10^4		<i>Schwarzenbach et al.</i> [1988] <i>Tremp et al.</i> [1993]	V X	8 55,8
2,5-dinitrophenol $\text{C}_6\text{H}_4\text{N}_2\text{O}_5$ [329-71-5]	1.5×10^3		<i>Schwarzenbach et al.</i> [1988]	V	8
2-methyl-4,6-dinitrophenol $\text{C}_7\text{H}_6\text{N}_2\text{O}_5$ (dinitro-o-cresol,DNOC) [534-52-1]	2.3×10^3 4.6×10^3		<i>Schwarzenbach et al.</i> [1988] <i>Tremp et al.</i> [1993]	V X	8 55,8

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
compounds with fluorine					
fluoromethane CH ₃ F	5.9×10 ⁻² 5.9×10 ⁻² 5.2×10 ⁻² 7.2×10 ⁻²	2200	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L L ?	39, 38
difluoromethane CH ₂ F ₂	8.7×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
trifluoromethane CHF ₃ (R23)	1.1×10 ⁻² 1.3×10 ⁻² 1.3×10 ⁻² 1.4×10 ⁻²	3200 2200	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992] <i>Zheng et al.</i> [1997]	V L ? M	39
tetrafluoromethane CF ₄ (carbontetrafluoride)	2.0×10 ⁻⁴ 2.0×10 ⁻⁴ 2.1×10 ⁻⁴ 1.9×10 ⁻⁴	1500 1800	<i>Hine and Mookerjee</i> [1975] <i>Morrison and Johnstone</i> [1954] <i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992]	V M L ?	39
fluoroethane C ₂ H ₅ F	4.4×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
1,1-difluoroethane C ₂ H ₄ F ₂ (R152a)	4.9×10 ⁻² 3.7×10 ⁻² 5.4×10 ⁻²	2600	<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992] <i>Zheng et al.</i> [1997]	V ? M	39, 78
1,1,1,2-tetrafluoroethane C ₂ H ₂ F ₄ (R134a)	1.8×10 ⁻²	2700	<i>Zheng et al.</i> [1997]	M	
hexafluoroethane C ₂ F ₆	5.9×10 ⁻⁵		<i>Yaws and Yang</i> [1992]	?	39
1-fluoropropane C ₃ H ₇ F	6.2×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39, 79
2-fluoropropane C ₃ H ₇ F	5.9×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39, 38
octafluorocyclobutane C ₄ F ₈	2.5×10 ⁻⁴		<i>Yaws and Yang</i> [1992]	?	39
1,1-difluoroethene C ₂ H ₂ F ₂	2.5×10 ⁻³		<i>Yaws and Yang</i> [1992]	?	39
tetrafluoroethene C ₂ F ₄	1.6×10 ⁻³ 1.6×10 ⁻³	2100	<i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992]	L ?	39
hexafluoropropene C ₃ F ₆	2.9×10 ⁻⁴	2400	<i>Wilhelm et al.</i> [1977]	L	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
carbonyl fluoride COF ₂	2.0×10 ¹ 3.5×10 ¹		<i>Kanakidou et al.</i> [1995] <i>Mirabel et al.</i> [1996]	C M	
formyl fluoride FCHO	3.0		<i>Kanakidou et al.</i> [1995]	E	
2,2,2-trifluoroethanol CF ₃ CH ₂ OH	5.9×10 ¹	5900	<i>Rochester and Symonds</i> [1973]	M	
1,1,1-trifluoro-2-propanol CF ₃ CHOHCH ₃	4.5×10 ¹	6300	<i>Rochester and Symonds</i> [1973]	M	
2,2,3,3-tetrafluoro-1-propanol CHF ₂ CF ₂ CH ₂ OH	1.6×10 ²	6700	<i>Rochester and Symonds</i> [1973]	M	
2,2,3,3,3-pentafluoro-1-propanol CF ₃ CF ₂ CH ₂ OH	4.5×10 ¹	6000	<i>Rochester and Symonds</i> [1973]	M	
1,1,1,3,3,3-hexafluoro-2-propanol CF ₃ CHOHCF ₃	2.4×10 ¹	6700	<i>Rochester and Symonds</i> [1973]	M	
trifluoroacetylfluoride CF ₃ COF	3.0 3.0		<i>Kanakidou et al.</i> [1995] <i>Mirabel et al.</i> [1996]	C M	
1,1,1-trifluoro-2-propanone CF ₃ COCH ₃	1.4×10 ²	8900	<i>Betterton</i> [1991]	M	
fluoroethanoic acid CH ₂ FCOOH (fluoroacetic acid) [144-49-0]	8.1×10 ⁴		<i>Bowden et al.</i> [1998b]	M	
difluoroethanoic acid CHF ₂ COOH (difluoroacetic acid) [381-73-7]	3.0×10 ⁴	6900	<i>Bowden et al.</i> [1998b]	M	
trifluoroethanoic acid CF ₃ COOH (trifluoroacetic acid) [76-05-1]	8.9×10 ³	9300	<i>Bowden et al.</i> [1996]	M	
generic peroxide with fluorine ROOH	3.0×10 ¹		<i>Kanakidou et al.</i> [1995]	E	80

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
fluorobenzene $\text{C}_6\text{H}_5\text{F}$	1.6×10^{-1} 1.2×10^{-1} 1.6×10^{-1} 1.6×10^{-1}	4100	<i>Mackay and Shiu</i> [1981] <i>Hoff et al.</i> [1993] <i>Hartkopf and Karger</i> [1973] <i>Yaws and Yang</i> [1992]	L ? M ?	13 39
1,2-difluorobenzene $\text{C}_6\text{H}_4\text{F}_2$ (o-difluorobenzene)	1.4×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
1,3-difluorobenzene $\text{C}_6\text{H}_4\text{F}_2$ (m-difluorobenzene)	1.3×10^{-2}		<i>Yaws and Yang</i> [1992]	?	39
1,4-difluorobenzene $\text{C}_6\text{H}_4\text{F}_2$ (p-difluorobenzene)	1.3×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
(trifluoromethyl)-benzene $\text{C}_6\text{H}_5\text{CF}_3$ (α,α,α -trifluorotoluene)	6.3×10^{-2} 6.2×10^{-2}		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
5-fluoro-2-nitrophenol $\text{C}_6\text{H}_4\text{FNO}_3$ [446-36-6]	5.9×10^2		<i>Schwarzenbach et al.</i> [1988]	V	8

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
aliphatic compounds with chlorine					
chloromethane CH ₃ Cl (methylchloride)	1.3×10 ⁻¹ 1.0×10 ⁻¹ 1.0×10 ⁻¹ 1.1×10 ⁻¹ 1.2×10 ⁻¹ 9.4×10 ⁻² 1.1×10 ⁻¹ 1.2×10 ⁻¹ 1.2×10 ⁻¹ 2.9×10 ⁻² 1.0×10 ⁻¹	 2800 4200 3000 -630 2900	<i>Pearson and McConnell</i> [1975] <i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Gossett</i> [1987] <i>Moore et al.</i> [1995] <i>Dilling</i> [1977] <i>Dilling</i> [1977] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Kavanaugh and Trussell</i> [1980]	M V L L M M V V ? X X	81,8 8 39 3 3
dichloromethane CH ₂ Cl ₂ [75-09-2]	3.3×10 ⁻¹ 4.4×10 ⁻¹ 3.9×10 ⁻¹ 3.5×10 ⁻¹ 4.7×10 ⁻¹ 4.0×10 ⁻¹ 4.0×10 ⁻¹ 1.2 3.7×10 ⁻¹ 4.1×10 ⁻¹ 4.4×10 ⁻¹ 4.0×10 ⁻¹ 3.1×10 ⁻¹ 3.6×10 ⁻¹ 8.6×10 ⁻¹ 3.1×10 ⁻¹ 3.4×10 ⁻¹ 3.5×10 ⁻¹ 3.8×10 ⁻¹ 3.9×10 ⁻¹ 4.0×10 ⁻¹	 4200 3800 3800 4100 4100 4200 3700 4300 4200 3500 4500 3900	<i>Pearson and McConnell</i> [1975] <i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Lincoff and Gossett</i> [1984] <i>Gossett</i> [1987] <i>Wright et al.</i> [1992b] <i>Dilling</i> [1977] <i>Dilling</i> [1977] <i>Dilling</i> [1977] <i>Hoff et al.</i> [1993] <i>Hartkopf and Karger</i> [1973] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Staudinger and Roberts</i> [1996] <i>Kavanaugh and Trussell</i> [1980] <i>Leighton and Calo</i> [1981] <i>Ashworth et al.</i> [1988] <i>Gossett et al.</i> [1985] <i>Tse et al.</i> [1992] <i>Gossett et al.</i> [1985] <i>Wright et al.</i> [1992a]	M V L M M M V V C M M ? X L X X X X X X X X	81,8 82 39 3 3 3 3 3 3

substance	k_{H}^{\ominus} [M/atm]	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
trichloromethane	3.5×10^{-1}		<i>Pearson and McConnell</i> [1975]	M	81,8
CHCl ₃	2.3×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
(chloroform)	2.7×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
[67-66-3]	2.0×10^{-1}	3900	<i>Hunter-Smith et al.</i> [1983]	M	83
	3.3×10^{-1}		<i>Nicholson et al.</i> [1984]	M	
	2.8×10^{-1}		<i>Nicholson et al.</i> [1984]	C	
	3.2×10^{-1}		<i>Nicholson et al.</i> [1984]	C	
	2.1×10^{-1}		<i>Nicholson et al.</i> [1984]	C	
	2.4×10^{-1}	4200	<i>Lincoff and Gossett</i> [1984]	M	
	2.8×10^{-1}	4600	<i>Gossett</i> [1987]	M	
	4.9×10^{-1}	7300	<i>Tancredi and Yanagisawa</i> [1990]	M	
	2.6×10^{-1}	3900	<i>Wright et al.</i> [1992b]	M	
	2.7×10^{-1}	4100	<i>Dewulf et al.</i> [1995]	M	
	2.3×10^{-1}	3800	<i>Moore et al.</i> [1995]	M	
	2.5×10^{-1}		<i>Dilling</i> [1977]	V	
	9.1×10^{-1}		<i>Dilling</i> [1977]	V	82
	3.1×10^{-1}		<i>Dilling</i> [1977]	C	
	2.5×10^{-1}		<i>Hoff et al.</i> [1993]	M	
	2.9×10^{-1}	4800	<i>Hartkopf and Karger</i> [1973]	M	
	2.4×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
	2.5×10^{-1}	4100	<i>Barr and Newsham</i> [1987]	X	3
	2.5×10^{-1}	4600	<i>Kavanaugh and Trussell</i> [1980]	X	3
	2.6×10^{-1}	4000	<i>Wright et al.</i> [1992a]	X	3
	3.0×10^{-1}	4400	<i>USEPA</i> [1982]	X	3
	1.5×10^{-1}	5600	<i>Ervin et al.</i> [1980]	X	3
	2.3×10^{-1}	4200	<i>Gossett et al.</i> [1985]	X	3
	2.3×10^{-1}	5000	<i>Ashworth et al.</i> [1988]	X	3
	2.4×10^{-1}	2200	<i>Lamarche and Droste</i> [1989]	X	3
	2.5×10^{-1}	4100	<i>Leighton and Calo</i> [1981]	X	3
	2.5×10^{-1}	4300	<i>Gossett et al.</i> [1985]	X	3
	2.5×10^{-1}	4500	<i>Staudinger and Roberts</i> [1996]	L	
	2.6×10^{-1}	4300	<i>Munz and Roberts</i> [1987]	X	3

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
tetrachloromethane CCl ₄ (carbontetrachloride) [56-23-5]	3.8×10 ⁻²		<i>Liss and Slater</i> [1974]	C	
	4.5×10 ⁻²		<i>Pearson and McConnell</i> [1975]	M	81,8
	3.5×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
	5.1×10 ⁻²		<i>Mackay and Shiu</i> [1981]	L	
	4.2×10 ⁻²	3200	<i>Hunter-Smith et al.</i> [1983]	M	
	3.3×10 ⁻²	4400	<i>Gossett</i> [1987]	M	
	3.5×10 ⁻²	4100	<i>Tancredi and Yanagisawa</i> [1990]	M	
	3.0×10 ⁻²	4200	<i>Wright et al.</i> [1992b]	M	
	3.8×10 ⁻²	4100	<i>Dewulf et al.</i> [1995]	M	
	3.4×10 ⁻²	3600	<i>Hansen et al.</i> [1995]	M	
	3.4×10 ⁻²		<i>Dilling</i> [1977]	V	
	4.7×10 ⁻²		<i>Dilling</i> [1977]	C	
	3.6×10 ⁻²		<i>Hoff et al.</i> [1993]	M	
	3.9×10 ⁻²	4900	<i>Hartkopf and Karger</i> [1973]	M	
	3.4×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
	3.1×10 ⁻²	4200	<i>Wright et al.</i> [1992a]	X	3
	3.3×10 ⁻²	1100	<i>USEPA</i> [1982]	X	3
	3.3×10 ⁻²	4700	<i>Kavanaugh and Trussell</i> [1980]	X	3
	3.8×10 ⁻²	3600	<i>Tse et al.</i> [1992]	X	3
	2.8×10 ⁻²	5600	<i>Bissonette et al.</i> [1990]	X	3
	3.2×10 ⁻²	3400	<i>Hansen et al.</i> [1993]	X	3
	3.3×10 ⁻²	4000	<i>Ashworth et al.</i> [1988]	X	3
	3.3×10 ⁻²	4300	<i>Munz and Roberts</i> [1987]	X	3
	3.4×10 ⁻²	4200	<i>Staudinger and Roberts</i> [1996]	L	
	3.6×10 ⁻²	4400	<i>Leighton and Calo</i> [1981]	X	3
chloroethane C ₂ H ₅ Cl [75-00-3]	1.2×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
	5.1×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	8.9×10 ⁻²	3100	<i>Gossett</i> [1987]	M	
	8.9×10 ⁻²		<i>Dilling</i> [1977]	V	
	1.4×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39, 8
	6.9×10 ⁻²	750	<i>USEPA</i> [1982]	X	3
	8.5×10 ⁻²	2900	<i>Staudinger and Roberts</i> [1996]	L	
	8.1×10 ⁻²	2600	<i>Ashworth et al.</i> [1988]	X	3
1,1-dichloroethane CHCl ₂ CH ₃ [75-34-3]	1.7×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
	1.7×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	1.8×10 ⁻¹	4100	<i>Gossett</i> [1987]	M	
	1.7×10 ⁻¹	3600	<i>Wright et al.</i> [1992b]	M	
	2.0×10 ⁻¹	4000	<i>Dewulf et al.</i> [1995]	M	
	1.7×10 ⁻¹		<i>Dilling</i> [1977]	V	
	1.7×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
	1.6×10 ⁻¹	3600	<i>Wright et al.</i> [1992a]	X	3
	1.7×10 ⁻¹	3800	<i>Barr and Newsham</i> [1987]	X	3
	1.8×10 ⁻¹	1700	<i>USEPA</i> [1982]	X	3
	1.8×10 ⁻¹	3300	<i>Tse et al.</i> [1992]	X	3
	1.8×10 ⁻¹	4400	<i>Kavanaugh and Trussell</i> [1980]	X	3
	1.3×10 ⁻¹	4900	<i>Ervin et al.</i> [1980]	X	3
	1.5×10 ⁻¹	3100	<i>Ashworth et al.</i> [1988]	X	3
	1.6×10 ⁻¹	3600	<i>Staudinger and Roberts</i> [1996]	L	
	1.7×10 ⁻¹	2100	<i>Lamarche and Droste</i> [1989]	X	3

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1,2-dichloroethane CH ₂ ClCH ₂ Cl [107-06-2]	1.1		<i>Pearson and McConnell</i> [1975]	M	81,8
	7.6×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
	9.2×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
	8.7×10^{-1}	3900	<i>Wright et al.</i> [1992b]	M	
	9.5×10^{-1}	4300	<i>Dewulf et al.</i> [1995]	M	
	8.2×10^{-1}		<i>Dilling</i> [1977]	V	
	1.0		<i>Dilling</i> [1977]	C	
	8.4×10^{-1}		<i>Hoff et al.</i> [1993]	M	
	8.4×10^{-1}	4100	<i>Hartkopf and Karger</i> [1973]	M	
	8.5×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
	8.3×10^{-1}	3800	<i>Tse et al.</i> [1992]	X	3
	8.6×10^{-1}	3900	<i>Wright et al.</i> [1992a]	X	3
	8.7×10^{-1}	3700	<i>Barr and Newsham</i> [1987]	X	3
	9.1×10^{-1}	2400	<i>USEPA</i> [1982]	X	3
	6.5×10^{-1}	1500	<i>Ashworth et al.</i> [1988]	X	3
	6.5×10^{-1}	4500	<i>Bissonette et al.</i> [1990]	X	3
	7.0×10^{-1}	4700	<i>Lamarche and Droste</i> [1989]	X	3
7.3×10^{-1}	4200	<i>Staudinger and Roberts</i> [1996]	L		
8.5×10^{-1}	3500	<i>Leighton and Calo</i> [1981]	X	3	
1,1,1-trichloroethane CH ₃ CCl ₃ (methylchloroform, MCF) [71-55-6]	2.9×10^{-2}		<i>Pearson and McConnell</i> [1975]	M	81,8
	6.2×10^{-2}		<i>Hine and Mookerjee</i> [1975]	V	
	3.6×10^{-2}		<i>Mackay and Shiu</i> [1981]	L	
	7.7×10^{-2}	3200	<i>Hunter-Smith et al.</i> [1983]	M	
	5.9×10^{-2}	4300	<i>Lincoff and Gossett</i> [1984]	M	
	5.9×10^{-2}	4100	<i>Gossett</i> [1987]	M	
	8.7×10^{-2}		<i>Kolb et al.</i> [1992]	X	45
	6.1×10^{-2}	3500	<i>Wright et al.</i> [1992b]	M	
	5.7×10^{-2}	3200	<i>Robbins et al.</i> [1993]	M	
	7.1×10^{-2}	4700	<i>Kanakidou et al.</i> [1995]	C	
	6.8×10^{-2}	3800	<i>Dewulf et al.</i> [1995]	M	
	6.0×10^{-2}	3100	<i>Hansen et al.</i> [1995]	M	
	3.4×10^{-2}		<i>Dilling</i> [1977]	V	
	4.0×10^{-2}		<i>Dilling</i> [1977]	V	8
	1.1×10^{-1}		<i>Dilling</i> [1977]	V	82
	5.4×10^{-2}		<i>Hoff et al.</i> [1993]	M	
	1.1×10^{-1}	4600	<i>Kavanaugh and Trussell</i> [1980]	X	3
	2.2×10^{-1}	1700	<i>USEPA</i> [1982]	X	3
	5.9×10^{-2}	3400	<i>Wright et al.</i> [1992a]	X	3
	5.9×10^{-2}	4000	<i>Barr and Newsham</i> [1987]	X	3
	6.4×10^{-2}	3700	<i>Tse et al.</i> [1992]	X	3
	2.7×10^{-2}	7000	<i>Ervin et al.</i> [1980]	X	3
	5.1×10^{-2}	4400	<i>Leighton and Calo</i> [1981]	X	3
	5.2×10^{-2}	5200	<i>Bissonette et al.</i> [1990]	X	3
	5.8×10^{-2}	3400	<i>Ashworth et al.</i> [1988]	X	3
	5.9×10^{-2}	3900	<i>Staudinger and Roberts</i> [1996]	L	
	5.9×10^{-2}	4200	<i>Gossett et al.</i> [1985]	X	3
6.0×10^{-2}	3200	<i>Hansen et al.</i> [1993]	X	3	
6.0×10^{-2}	4100	<i>Munz and Roberts</i> [1987]	X	3	
6.0×10^{-2}	4300	<i>Gossett et al.</i> [1985]	X	3	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
1,1,2-trichloroethane CHCl ₂ CH ₂ Cl [79-00-5]	1.1		<i>Hine and Mookerjee</i> [1975]	V	
	8.4×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
	1.2	3900	<i>Wright et al.</i> [1992b]	M	
	1.3	5900	<i>Hansen et al.</i> [1995]	M	
	1.1		<i>Dilling</i> [1977]	V	
	1.0		<i>Yaws and Yang</i> [1992]	?	39
	1.2	2700	<i>USEPA</i> [1982]	X	3
	1.2	3800	<i>Wright et al.</i> [1992a]	X	3
	1.2	4000	<i>Tse et al.</i> [1992]	X	3
	1.2	4300	<i>Barr and Newsham</i> [1987]	X	3
	1.0	4800	<i>Ashworth et al.</i> [1988]	X	3
	1.1	4900	<i>Staudinger and Roberts</i> [1996]	L	
	1.2	3700	<i>Leighton and Calo</i> [1981]	X	3
1.3	6100	<i>Hansen et al.</i> [1993]	X	3	
1,1,1,2-tetrachloroethane CCl ₃ CH ₂ Cl [630-20-6]	2.2		<i>Hine and Mookerjee</i> [1975]	V	
	3.6×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
	4.0×10^{-1}	4800	<i>Wright et al.</i> [1992b]	M	
	3.7×10^{-1}		<i>Dilling</i> [1977]	V	
	3.4×10^{-1}	4500	<i>Wright et al.</i> [1992a]	X	3
4.5×10^{-1}	4600	<i>Tse et al.</i> [1992]	X	3	
1,1,2,2-tetrachloroethane CHCl ₂ CHCl ₂ [79-34-5]	2.1		<i>Mackay and Shiu</i> [1981]	L	
	2.0	5000	<i>Wright et al.</i> [1992b]	M	
	2.1		<i>Dilling</i> [1977]	V	
	3.0		<i>Yaws and Yang</i> [1992]	?	39
	1.8	4200	<i>Barr and Newsham</i> [1987]	X	3
	1.9	4700	<i>Wright et al.</i> [1992a]	X	3
	2.2	2800	<i>Ashworth et al.</i> [1988]	X	3
	2.3	3000	<i>USEPA</i> [1982]	X	3
	2.4	3200	<i>Staudinger and Roberts</i> [1996]	L	
	2.4	4800	<i>Tse et al.</i> [1992]	X	3
2.8	3600	<i>Leighton and Calo</i> [1981]	X	3	
pentachloroethane CHCl ₂ CCl ₃ [76-01-7]	4.1×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
	4.6×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
	4.0×10^{-1}		<i>Dilling</i> [1977]	V	
	5.5×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
hexachloroethane C ₂ Cl ₆ [67-72-1]	4.4×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
	7.8×10^{-2}		<i>Mackay and Shiu</i> [1981]	L	
	8.2×10^{-1}		<i>Dilling</i> [1977]	V	
	4.4×10^{-2}		<i>Yaws and Yang</i> [1992]	?	39
	1.0×10^{-1}	2100	<i>USEPA</i> [1982]	X	3
	2.5×10^{-1}	5600	<i>Staudinger and Roberts</i> [1996]	L	
	1.2×10^{-1}	2600	<i>Ashworth et al.</i> [1988]	X	3
	2.5×10^{-1}	5600	<i>Munz and Roberts</i> [1987]	X	3

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1-chloropropane C_3H_7Cl [540-54-5]	7.4×10^{-2} 9.2×10^{-2} 9.3×10^{-2}		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	V L ?	 39, 8
2-chloropropane C_3H_7Cl [75-29-6]	6.2×10^{-2} 6.9×10^{-2}		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	 39, 8
1,2-dichloropropane $C_3H_6Cl_2$ [78-87-5]	3.4×10^{-1} 3.7×10^{-1} 3.7×10^{-1} 3.4×10^{-1} 3.4×10^{-1} 4.0×10^{-1} 3.0×10^{-1} 3.4×10^{-1} 3.5×10^{-1} 3.8×10^{-1}	3800 2100 3600 3700 3800 4300 4300 4700	<i>Hine and Mookerjee</i> [1975] <i>Wright et al.</i> [1992b] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Wright et al.</i> [1992a] <i>Tse et al.</i> [1992] <i>Bissonette et al.</i> [1990] <i>Staudinger and Roberts</i> [1996] <i>Leighton and Calo</i> [1981] <i>Ashworth et al.</i> [1988]	V M ? X X X X L X X	 39 3 3 3 3 3 3
1,3-dichloropropane $C_3H_6Cl_2$ [142-28-9]	1.0 1.0 1.0	 3900	<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992] <i>Leighton and Calo</i> [1981]	V ? X	 39 3
1,2,3-trichloropropane $C_3H_5Cl_3$ [96-18-4]	4.4 3.1 2.9 2.8 3.4	4000 3500 3700	<i>Tancredi and Yanagisawa</i> [1990] <i>Dilling</i> [1977] <i>Yaws and Yang</i> [1992] <i>Leighton and Calo</i> [1981] <i>Staudinger and Roberts</i> [1996]	M V ? X L	 39 3
1-chloro-2-methylpropane C_4H_9Cl [513-36-0]	8.4×10^{-1} 6.4×10^{-2}		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	 39, 8
1-chlorobutane C_4H_9Cl [109-69-3]	5.1×10^{-2} 5.7×10^{-2} 5.9×10^{-2} 6.0×10^{-2}	 3500	<i>Hine and Mookerjee</i> [1975] <i>Hoff et al.</i> [1993] <i>Yaws and Yang</i> [1992] <i>Leighton and Calo</i> [1981]	V ? ? X	 13 39 3
2-chlorobutane C_4H_9Cl [78-86-4]	5.4×10^{-2} 4.1×10^{-2}	 4500	<i>Yaws and Yang</i> [1992] <i>Leighton and Calo</i> [1981]	? X	 39 3
1,1-dichlorobutane $C_4H_8Cl_2$ [541-33-3]	1.3×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
1,4-dichlorobutane $C_4H_8Cl_2$	2.0	3100	<i>Leighton and Calo</i> [1981]	X	3
1-chloropentane $C_5H_{11}Cl$ [543-59-9]	4.6×10^{-2} 2.0×10^{-2} 4.2×10^{-2}	 4700	<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992] <i>Leighton and Calo</i> [1981]	V ? X	 39 3
2-chloropentane $C_5H_{11}Cl$ [625-29-6]	3.6×10^{-2}		<i>Hine and Mookerjee</i> [1975]	V	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
3-chloropentane $\text{C}_5\text{H}_{11}\text{Cl}$ [616-20-6]	3.8×10^{-2}		<i>Hine and Mookerjee</i> [1975]	V	
1,5-dichloropentane $\text{C}_5\text{H}_{10}\text{Cl}_2$	1.8	1600	<i>Leighton and Calo</i> [1981]	X	3
2-chloro-2-methylbutane $\text{C}_5\text{H}_{11}\text{Cl}$ [594-36-5]	3.1×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
1-chlorohexane $\text{C}_6\text{H}_{13}\text{Cl}$	4.1×10^{-2}	4500	<i>Leighton and Calo</i> [1981]	X	3
1,10-dichlorodecane $\text{C}_{10}\text{H}_{20}\text{Cl}_2$	2.0×10^{-1}		<i>Drouillard et al.</i> [1998]	V	
1,2,9,10-tetrachlorodecane $\text{C}_{10}\text{H}_{18}\text{Cl}_4$	5.7		<i>Drouillard et al.</i> [1998]	M	
pentachlorodecane isomers $\text{C}_{10}\text{H}_{17}\text{Cl}_5$	2.1×10^1 3.9×10^1		<i>Drouillard et al.</i> [1998] <i>Drouillard et al.</i> [1998]	M M	
1,2,10,11-tetrachloroundecane $\text{C}_{11}\text{H}_{20}\text{Cl}_4$	1.6×10^1		<i>Drouillard et al.</i> [1998]	M	
pentachloroundecane isomers $\text{C}_{11}\text{H}_{19}\text{Cl}_5$	6.9×10^1 1.5×10^2		<i>Drouillard et al.</i> [1998] <i>Drouillard et al.</i> [1998]	M M	
1,12-dichlorododecane $\text{C}_{12}\text{H}_{24}\text{Cl}_2$	1.6×10^{-1}		<i>Drouillard et al.</i> [1998]	V	
polychlorinated dodecane isomers $\text{C}_{12}\text{H}_x\text{Cl}_y$	7.4×10^1		<i>Drouillard et al.</i> [1998]	M	

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
chloroethene CH ₂ CHCl (vinyl chloride) [75-01-4]	8.2×10^{-4}		<i>Pearson and McConnell</i> [1975]	M	81,74
	1.8×10^{-2}		<i>Hine and Mookerjee</i> [1975]	V	
	4.6×10^{-2}	3000	<i>Wilhelm et al.</i> [1977]	L	
	3.8×10^{-2}	3300	<i>Gossett</i> [1987]	M	
	9.5×10^{-4}		<i>Dilling</i> [1977]	V	
	4.3×10^{-2}		<i>Dilling</i> [1977]	V	
	4.4×10^{-2}		<i>Yaws and Yang</i> [1992]	?	39
	3.9×10^{-2}	3100	<i>Staudinger and Roberts</i> [1996]	L	
	4.0×10^{-2}	2900	<i>Ashworth et al.</i> [1988]	X	3
1,1-dichloroethene CH ₂ CCl ₂ [75-35-4]	6.5×10^{-3}		<i>Pearson and McConnell</i> [1975]	M	81,8
	7.6×10^{-3}		<i>Mackay and Shiu</i> [1981]	L	
	3.9×10^{-2}	3700	<i>Gossett</i> [1987]	M	
	5.3×10^{-3}		<i>Dilling</i> [1977]	V	
	6.2×10^{-3}		<i>Dilling</i> [1977]	V	8
	4.3×10^{-2}		<i>Yaws and Yang</i> [1992]	?	39
	3.7×10^{-2}	3100	<i>Tse et al.</i> [1992]	X	3
	6.6×10^{-2}	1200	<i>USEPA</i> [1982]	X	3
	1.4×10^{-2}	6600	<i>Ervin et al.</i> [1980]	X	3
	2.7×10^{-2}	4600	<i>Leighton and Calo</i> [1981]	X	3
	3.4×10^{-2}	4000	<i>Staudinger and Roberts</i> [1996]	L	
	3.4×10^{-2}	4500	<i>Bissonette et al.</i> [1990]	X	3
	3.7×10^{-2}	2900	<i>Ashworth et al.</i> [1988]	X	3
(Z)-1,2-dichloroethene CHClCHCl (<i>cis</i> -1,2-dichloroethene) [156-59-2]	3.0×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
	1.3×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
	2.7×10^{-1}	4200	<i>Gossett</i> [1987]	M	
	2.4×10^{-1}	3800	<i>Wright et al.</i> [1992b]	M	
	1.3×10^{-1}		<i>Dilling</i> [1977]	V	
	1.3×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
	2.1×10^{-1}	3100	<i>Ashworth et al.</i> [1988]	X	3
	2.2×10^{-1}	4100	<i>Ervin et al.</i> [1980]	X	3
	2.3×10^{-1}	4000	<i>Wright et al.</i> [1992a]	X	3
	2.4×10^{-1}	3900	<i>Staudinger and Roberts</i> [1996]	L	
	2.5×10^{-1}	4200	<i>Bissonette et al.</i> [1990]	X	3
	2.6×10^{-1}	3400	<i>Tse et al.</i> [1992]	X	3

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
(E)-1,2-dichloroethene CHClCHCl (<i>trans</i> -1,2-dichloroethene) [156-60-5]	1.5×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
	1.5×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
	1.1×10^{-1}	4200	<i>Gossett</i> [1987]	M	
	1.0×10^{-1}	4000	<i>Wright et al.</i> [1992b]	M	
	9.9×10^{-2}	3400	<i>Hansen et al.</i> [1995]	M	
	1.5×10^{-1}		<i>Dilling</i> [1977]	V	
	1.5×10^{-1}		<i>Yaws and Yang</i> [1992]	?	39
	1.0×10^{-1}	3000	<i>Ashworth et al.</i> [1988]	X	3
	1.1×10^{-1}	3400	<i>Tse et al.</i> [1992]	X	3
	1.1×10^{-1}	4300	<i>Wright et al.</i> [1992a]	X	3
	1.9×10^{-1}	1700	<i>USEPA</i> [1982]	X	3
	7.1×10^{-2}	5400	<i>Ervin et al.</i> [1980]	X	3
	8.6×10^{-2}	4800	<i>Bissonette et al.</i> [1990]	X	3
	9.1×10^{-2}	4100	<i>Staudinger and Roberts</i> [1996]	L	
	9.8×10^{-2}	4100	<i>Cooling et al.</i> [1992]	X	3
9.9×10^{-2}	3300	<i>Hansen et al.</i> [1993]	X	3	
trichloroethene C ₂ HCl ₃ (trichloroethylene) [79-01-6]	1.1×10^{-1}		<i>Pearson and McConnell</i> [1975]	M	81,8
	8.5×10^{-2}		<i>Hine and Mookerjee</i> [1975]	V	
	8.2×10^{-2}		<i>Mackay and Shiu</i> [1981]	L	
	9.9×10^{-2}	4900	<i>Lincoff and Gossett</i> [1984]	M	
	1.1×10^{-1}	4800	<i>Gossett</i> [1987]	M	
	1.3×10^{-1}	5200	<i>Tancredi and Yanagisawa</i> [1990]	M	
	1.1×10^{-1}	4200	<i>Wright et al.</i> [1992b]	M	
	9.7×10^{-2}	3500	<i>Robbins et al.</i> [1993]	M	
	1.3×10^{-1}		<i>Nielsen et al.</i> [1994]	M	
	1.2×10^{-1}	3600	<i>Dewulf et al.</i> [1995]	M	
	8.4×10^{-2}		<i>Dilling</i> [1977]	V	
	1.0×10^{-1}		<i>Dilling</i> [1977]	V	8
	2.4×10^{-1}		<i>Dilling</i> [1977]	V	82
	1.1×10^{-1}		<i>Hoff et al.</i> [1993]	M	
	8.6×10^{-2}		<i>Yaws and Yang</i> [1992]	?	39
	1.0×10^{-1}	4100	<i>Wright et al.</i> [1992a]	X	3
	1.1×10^{-1}	4400	<i>Cooling et al.</i> [1992]	X	3
	1.2×10^{-1}	3900	<i>Tse et al.</i> [1992]	X	3
	8.2×10^{-2}	4000	<i>Kavanaugh and Trussell</i> [1980]	X	3
	8.9×10^{-2}	1600	<i>USEPA</i> [1982]	X	3
	1.0×10^{-1}	4600	<i>Staudinger and Roberts</i> [1996]	L	
	1.0×10^{-1}	4700	<i>Leighton and Calo</i> [1981]	X	3
	1.0×10^{-1}	5200	<i>Bissonette et al.</i> [1990]	X	3
	1.1×10^{-1}	4300	<i>Gossett et al.</i> [1985]	X	3
	7.5×10^{-2}	4800	<i>Ervin et al.</i> [1980]	X	3
	9.7×10^{-2}	3700	<i>Ashworth et al.</i> [1988]	X	3
	9.7×10^{-2}	4700	<i>Munz and Roberts</i> [1987]	X	3
9.9×10^{-2}	2100	<i>Lamarque and Droste</i> [1989]	X	3	
9.9×10^{-2}	4900	<i>Gossett et al.</i> [1985]	X	3	

substance	k_H^\ominus [M/atm]	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
tetrachloroethene C ₂ Cl ₄ (tetrachloroethylene) [127-18-4]	5.0×10 ⁻²		<i>Pearson and McConnell</i> [1975]	M	81,8
	3.7×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
	4.4×10 ⁻²		<i>Mackay and Shiu</i> [1981]	L	
	5.7×10 ⁻²	5100	<i>Lincoff and Gossett</i> [1984]	M	
	5.7×10 ⁻²	4900	<i>Gossett</i> [1987]	M	
	6.0×10 ⁻²	5500	<i>Tancredi and Yanagisawa</i> [1990]	M	
	8.2×10 ⁻²		<i>Kolb et al.</i> [1992]	X	45
	5.6×10 ⁻²	3600	<i>Robbins et al.</i> [1993]	M	
	7.0×10 ⁻²	4500	<i>Dewulf et al.</i> [1995]	M	
	3.4×10 ⁻²		<i>Dilling</i> [1977]	V	
	4.0×10 ⁻²		<i>Dilling</i> [1977]	V	8
	1.2×10 ⁻¹		<i>Dilling</i> [1977]	V	82
	8.2×10 ⁻²		<i>Dilling</i> [1977]	C	
	6.4×10 ⁻²		<i>Hoff et al.</i> [1993]	M	
	3.7×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
	3.6×10 ⁻²	1500	<i>USEPA</i> [1982]	X	3
	4.0×10 ⁻²	5000	<i>Kavanaugh and Trussell</i> [1980]	X	3
	5.9×10 ⁻²	4800	<i>Staudinger and Roberts</i> [1996]	L	
	5.5×10 ⁻²	4400	<i>Ashworth et al.</i> [1988]	X	3
	5.5×10 ⁻²	4400	<i>Munz and Roberts</i> [1987]	X	3
5.8×10 ⁻²	5100	<i>Gossett et al.</i> [1985]	X	3	
5.8×10 ⁻²	5200	<i>Ervin et al.</i> [1980]	X	3	
6.2×10 ⁻²	4700	<i>Leighton and Calo</i> [1981]	X	3	
6.3×10 ⁻²	5300	<i>Bissonette et al.</i> [1990]	X	3	
6.6×10 ⁻²	4600	<i>Gossett et al.</i> [1985]	X	3	
3-chloro-1-propene C ₃ H ₅ Cl [107-05-1]	1.1×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
	9.3×10 ⁻²		<i>Dilling</i> [1977]	V	
	1.1×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
1,3-dichloropropene C ₃ H ₄ Cl ₂ [542-75-6]	6.5×10 ⁻¹	4200	<i>Wright et al.</i> [1992b]	M	
	2.8×10 ⁻¹	1500	<i>USEPA</i> [1982]	X	3
	5.2×10 ⁻¹		<i>Meylan and Howard</i> [1991]	X	3
<i>cis</i> -1,3-dichloropropene C ₃ H ₄ Cl ₂ [10061-01-5]	4.2×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	4.3×10 ⁻¹		<i>Dilling</i> [1977]	V	
<i>trans</i> -1,3-dichloropropene C ₃ H ₄ Cl ₂	5.6×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	5.7×10 ⁻¹		<i>Dilling</i> [1977]	V	
2,3-dichloropropene C ₃ H ₄ Cl ₂	2.8×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
	2.7×10 ⁻¹		<i>Dilling</i> [1977]	V	
hexachlorobutadiene CCl ₂ CClCClCCl ₂ [87-68-3]	4.0×10 ⁻²		<i>Pearson and McConnell</i> [1975]	M	81,8
	9.7×10 ⁻²		<i>Meylan and Howard</i> [1991]	X	3
	9.9×10 ⁻²	4700	<i>USEPA</i> [1982]	X	3
trichloroethanal CCl ₃ CHO (trichloroacetaldehyde)	3.4×10 ⁵	3500	<i>Betterton and Hoffmann</i> [1988]	M	63
chloro-2-propanone CH ₂ ClCOCH ₃	5.9×10 ¹	5400	<i>Betterton</i> [1991]	M	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
chloroethanoic acid CH ₂ ClCOOH (chloroacetic acid) [79-11-8]	1.1×10 ⁵	9700	<i>Bowden et al.</i> [1998b]	M	
dichloroethanoic acid CHCl ₂ COOH (dichloroacetic acid) [79-43-6]	1.2×10 ⁵	8000	<i>Bowden et al.</i> [1998b]	M	
trichloroethanoic acid CCl ₃ COOH (trichloroacetic acid) [76-03-9]	7.4×10 ⁴	8700	<i>Bowden et al.</i> [1998a]	M	
trichloroacetylchloride CCl ₃ COCl	2.0		<i>Mirabel et al.</i> [1996]	M	
1-chloro-2,3-epoxypropane	2.8×10 ¹	3700	<i>USEPA</i> [1982]	X	3
2-chloroethylvinylether	3.1	2500	<i>USEPA</i> [1982]	X	3
bis(2-chloroethoxy)methane C ₅ H ₁₀ Cl ₂ O ₂ [111-91-1]	2.6×10 ³	5500	<i>USEPA</i> [1982]	X	3
1,5-dichloro-3-oxapentane C ₄ H ₈ Cl ₂ O (bis(2-chloroethyl)ether) [111-44-4]	4.7×10 ¹	4100	<i>USEPA</i> [1982]	X	3
bis(2-chloroisopropyl)ether C ₆ H ₁₂ Cl ₂ O [108-60-1]	6.6	2800	<i>USEPA</i> [1982]	X	3

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-\text{d} \ln k_{\text{H}}}{\text{d}(1/T)}$ [K]	reference	type	note
aromatic compounds with chlorine					
chlorobenzene C ₆ H ₅ Cl [108-90-7]	2.2×10 ⁻¹ 2.7×10 ⁻¹ 2.7×10 ⁻¹ 2.9×10 ⁻¹ 3.2×10 ⁻¹ 2.6×10 ⁻¹ 2.9×10 ⁻¹ 2.2×10 ⁻¹ 2.5×10 ⁻¹ 3.2×10 ⁻¹ 2.4×10 ⁻¹ 2.6×10 ⁻¹ 2.7×10 ⁻¹ 2.9×10 ⁻¹ 3.0×10 ⁻¹	4600 2100 1900 4700 2700 3800 4200 3500	<i>Hine and Mookerjee</i> [1975] <i>Mackay et al.</i> [1979] <i>Mackay et al.</i> [1979] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Hoff et al.</i> [1993] <i>Hartkopf and Karger</i> [1973] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Cooling et al.</i> [1992] <i>Bissonette et al.</i> [1990] <i>Ashworth et al.</i> [1988] <i>Staudinger and Roberts</i> [1996] <i>Ervin et al.</i> [1980] <i>Leighton and Calo</i> [1981]	V M T L M M ? X X X X L X X	39 3 3 3 3 3 3 3 3 3 3 3 3 3 3
1,2-dichlorobenzene C ₆ H ₄ Cl ₂ (o-dichlorobenzene) [95-50-1]	4.1×10 ⁻¹ 5.3×10 ⁻¹ 5.3×10 ⁻¹ 3.3×10 ⁻¹ 5.3×10 ⁻¹ 5.5×10 ⁻¹ 4.9×10 ⁻¹ 5.4×10 ⁻¹ 6.0×10 ⁻¹	2800 5900 5100 1400 6700	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Staudinger and Roberts</i> [1996] <i>Bissonette et al.</i> [1990] <i>Ashworth et al.</i> [1988] <i>Gossett et al.</i> [1985]	V L M ? X L X X X	39 3 3 3 3 3 3 3 3
1,3-dichlorobenzene C ₆ H ₄ Cl ₂ (m-dichlorobenzene) [541-73-1]	2.1×10 ⁻¹ 2.8×10 ⁻¹ 3.4×10 ⁻¹ 3.0×10 ⁻¹ 3.9×10 ⁻¹ 3.0×10 ⁻¹	2400 2600	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Hoff et al.</i> [1993] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Ashworth et al.</i> [1988]	V L M ? X X	39 3 3 3 3 3
1,4-dichlorobenzene C ₆ H ₄ Cl ₂ (p-dichlorobenzene) [106-46-7]	2.2×10 ⁻¹ 6.3×10 ⁻¹ 4.2×10 ⁻¹ 2.3×10 ⁻¹ 3.1×10 ⁻¹ 3.8×10 ⁻¹ 3.1×10 ⁻¹	2700 2700 2700	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988] <i>USEPA</i> [1982] <i>Ashworth et al.</i> [1988]	V L M ? X X X	39 3 3 3 3 3 3
1,2,3-trichlorobenzene C ₆ H ₃ Cl ₃ [87-61-6]	4.3×10 ⁻¹ 8.0×10 ⁻¹		<i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981]	L M	
1,2,4-trichlorobenzene C ₆ H ₃ Cl ₃ [120-82-1]	2.7×10 ⁻¹ 7.1×10 ⁻¹ 4.6×10 ⁻¹	2500 4000	<i>Mackay and Shiu</i> [1981] <i>USEPA</i> [1982] <i>Ashworth et al.</i> [1988]	L X X	3 3 3
1,3,5-trichlorobenzene C ₆ H ₃ Cl ₃ [108-70-3]	6.3×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1,2,3,4-tetrachlorobenzene C ₆ H ₂ Cl ₄ [634-66-2]	3.9×10^{-1} 1.3	4800	<i>Mackay and Shiu</i> [1981] <i>tenHulscher et al.</i> [1992]	L X	3
1,2,3,5-tetrachlorobenzene C ₆ H ₂ Cl ₄ [634-90-2]	1.7×10^{-1} 6.4×10^{-1}		<i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981]	L M	
1,2,4,5-tetrachlorobenzene C ₆ H ₂ Cl ₄ [95-94-3]	3.9×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	
pentachlorobenzene C ₆ HCl ₅	1.0×10^{-1} 1.4	5200	<i>Mackay and Shiu</i> [1981] <i>tenHulscher et al.</i> [1992]	L X	3
hexachlorobenzene C ₆ Cl ₆	2.0×10^1 2.4×10^{-3} 2.1 5.9×10^{-1}	5800 1600	<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>tenHulscher et al.</i> [1992] <i>USEPA</i> [1982]	L ? X X	39 3 3
α -chlorotoluene C ₆ H ₅ CH ₂ Cl	1.6		<i>Mackay and Shiu</i> [1981]	L	
1-chloro-2-methylbenzene C ₇ H ₇ Cl (o-chlorotoluene) [95-49-8]	1.9 2.8×10^{-1}	3000 3500	<i>USEPA</i> [1982] <i>Leighton and Calo</i> [1981]	X X	3 3
1-chloronaphthalene C ₁₀ H ₇ Cl	2.9×10^{-1} 2.9×10^{-1}		<i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981]	L M	
2-chloronaphthalene C ₁₀ H ₇ Cl	3.2 3.2 1.6 3.1	3800	<i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>USEPA</i> [1982] <i>Meylan and Howard</i> [1991]	L M X X	3 3
hydroxypentachlorobenzene C ₆ HCl ₅ O (pentachlorophenol) [87-86-5]	1.1×10^1 4.0×10^4	1300	<i>USEPA</i> [1982] <i>Meylan and Howard</i> [1991]	X X	3 3
2-hydroxychlorobenzene C ₆ H ₅ ClO (2-chlorophenol) [95-57-8]	1.2×10^2	4600	<i>USEPA</i> [1982]	X	3
2,4-dichlorophenol	1.5×10^2	4900	<i>USEPA</i> [1982]	X	3
4-chloro-2-nitrophenol C ₆ H ₄ ClNO ₃ [89-64-5]	7.9×10^1		<i>Schwarzenbach et al.</i> [1988]	V	8
4-chloro-5-methyl-2-nitrophenol C ₇ H ₆ ClNO ₃ (4-chloro-6-nitro-m-cresol) [7147-89-9]	3.6×10^1		<i>Schwarzenbach et al.</i> [1988]	V	8

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
compounds with chlorine and fluorine					
chlorofluoromethane CH ₂ FCl (R31)	1.5×10 ⁻¹ 1.5×10 ⁻¹ 1.5×10 ⁻¹	2600	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992]	V L ?	39
chlorodifluoromethane CHF ₂ Cl (R22)	3.4×10 ⁻² 3.4×10 ⁻² 2.4×10 ⁻¹ 3.3×10 ⁻² 3.1×10 ⁻² 3.7×10 ⁻²	3400 3400 2700	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Kanakidou et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Kavanaugh and Trussell</i> [1980] <i>Zheng et al.</i> [1997]	V L C ? X M	84 39 3
dichlorofluoromethane CHFC ₂ (R21)	1.9×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
chlorotrifluoromethane CF ₃ Cl (R13)	5.8×10 ⁻⁴ 9.4×10 ⁻⁴ 8.9×10 ⁻⁴	1600	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992]	V L ?	39
dichlorodifluoromethane CF ₂ Cl ₂ (R12)	2.5×10 ⁻³ 2.4×10 ⁻³ 2.1×10 ⁻³ 2.3×10 ⁻³ 2.5×10 ⁻³ 3.1×10 ⁻³ 3.5×10 ⁻⁴	1800 3500 -210	<i>Pearson and McConnell</i> [1975] <i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>Munz and Roberts</i> [1987] <i>USEPA</i> [1982]	M V L L ? X X	81,8 39 3 3
trichlorofluoromethane CFCl ₃ (R11)	8.2×10 ⁻³ 1.2×10 ⁻³ 9.2×10 ⁻³ 1.1×10 ⁻² 8.2×10 ⁻³ 1.0×10 ⁻² 1.7×10 ⁻² 1.0×10 ⁻²	2700 3100 740 3500	<i>Liss and Slater</i> [1974] <i>Pearson and McConnell</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Hunter-Smith et al.</i> [1983] <i>Yaws and Yang</i> [1992] <i>Staudinger and Roberts</i> [1996] <i>USEPA</i> [1982] <i>Ashworth et al.</i> [1988]	C M L M ? L X X	81,8 39 3 3
1,1,2,2-tetrachlorodifluoroethane C ₂ F ₂ Cl ₄ (R112)	1.0×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
1,1,2-trichlorotrifluoroethane C ₂ F ₃ Cl ₃ (R113)	2.0×10 ⁻³ 2.0×10 ⁻³ 3.4×10 ⁻³	3200	<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992] <i>Ashworth et al.</i> [1988]	V ? X	39 3
1,1-dichlorotetrafluoroethane C ₂ F ₄ Cl ₂ (R114)	5.9×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975]	V	
1,2-dichlorotetrafluoroethane C ₂ F ₄ Cl ₂ (R114)	8.2×10 ⁻⁴ 8.3×10 ⁻⁴		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39

substance	$\frac{k_H^\ominus}{[\text{M/atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
chloropentafluoroethane C ₂ F ₅ Cl (R115)	3.2×10 ⁻⁴ 3.4×10 ⁻⁴ 3.8×10 ⁻⁴	2800	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Yaws and Yang</i> [1992]	V L ?	39
dichlorotrifluoroethane C ₂ HF ₃ Cl ₂ (R123)	2.9×10 ⁻²	2600	<i>Kanakidou et al.</i> [1995]	C	
1-chloro-1,2,2,2-tetrafluoroethane C ₂ HF ₄ Cl (R124)	1.1×10 ⁻²	3200	<i>Kanakidou et al.</i> [1995]	C	
2-chloro-1,1,1-trifluoroethane C ₂ H ₂ F ₃ Cl (R133)	3.7×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
1,1-dichloro-1-fluoroethane CH ₃ CFCl ₂ (R141B)	7.9×10 ⁻³	5200	<i>Kanakidou et al.</i> [1995]	C	
1-chloro-1,1-difluoroethane CH ₃ CF ₂ Cl (R142B)	1.4×10 ⁻²	2500	<i>Kanakidou et al.</i> [1995]	C	
chlorodifluoroethanoic acid CF ₂ ClCOOH (chlorodifluoroacetic acid) [76-04-0]	2.5×10 ⁴	10000	<i>Bowden et al.</i> [1998b]	M	
chlorodifluoroethanoic peroxyacid CClF ₂ COOOH	3.0×10 ³		<i>Kanakidou et al.</i> [1995]	E	
dichlorofluoroethanoic peroxyacid CCl ₂ FCOOH	3.0×10 ³		<i>Kanakidou et al.</i> [1995]	E	
carbonic chloride fluoride COFCl	1.0×10 ¹		<i>Kanakidou et al.</i> [1995]	C	
trifluoroacetylchloride CF ₃ COCl	2.5 2.0		<i>Kanakidou et al.</i> [1995] <i>Mirabel et al.</i> [1996]	C M	
generic peroxide with fluorine and/or chlorine ROOH	3.0×10 ¹		<i>Kanakidou et al.</i> [1995]	E	80
chlorodifluoronitroxymethane CClF ₂ OONO ₂	2.9	5900	<i>Kanakidou et al.</i> [1995]	E	85

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
compounds with bromine					
bromomethane CH ₃ Br [74-83-9]	1.6×10 ⁻¹ 1.6×10 ⁻¹ 1.9×10 ⁻¹ 1.5×10 ⁻¹ 4.4×10 ⁻³	3100 360	<i>Hine and Mookerjee</i> [1975] <i>Wilhelm et al.</i> [1977] <i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982]	V L L ? X	8 39 3
dibromomethane CH ₂ Br ₂ [74-95-3]	1.1 3.2 1.1 9.3×10 ⁻¹ 1.1 1.1	3900 4400 3700 4000	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Wright et al.</i> [1992b] <i>Moore et al.</i> [1995] <i>Wright et al.</i> [1992a] <i>Tse et al.</i> [1992]	V L M M X X	3 3
tribromomethane CHBr ₃ [75-25-2]	1.5 1.6 2.3 1.7 2.3 1.4 1.8 1.9 2.0 1.7 1.9	5700 5000 2700 4300 5200 5200 4700	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Nicholson et al.</i> [1984] <i>Nicholson et al.</i> [1984] <i>Wright et al.</i> [1992b] <i>Moore et al.</i> [1995] <i>USEPA</i> [1982] <i>Tse et al.</i> [1992] <i>Wright et al.</i> [1992a] <i>Staudinger and Roberts</i> [1996] <i>Munz and Roberts</i> [1987]	V L M C M M X X X L X	3 3 3
bromoethane C ₂ H ₅ Br [74-96-4]	1.3×10 ⁻¹ 1.3×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
1,2-dibromoethane C ₂ H ₄ Br ₂ [106-93-4]	1.4 1.4 1.1 1.5	1900 3900	<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982] <i>Ashworth et al.</i> [1988]	V ? X X	39 3 3
1-bromopropane C ₃ H ₇ Br [106-94-5]	1.1×10 ⁻¹ 1.4×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39, 8
2-bromopropane C ₃ H ₇ Br [75-26-3]	9.2×10 ⁻² 1.0×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39, 8
1,2-dibromopropane C ₃ H ₆ Br ₂ [78-75-1]	1.1 6.8×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
1,3-dibromopropane C ₃ H ₆ Br ₂ [109-64-8]	1.1		<i>Hine and Mookerjee</i> [1975]	V	

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1-bromobutane C ₄ H ₉ Br [109-65-9]	8.2×10 ⁻² 4.7×10 ⁻² 8.3×10 ⁻²		<i>Hine and Mookerjee</i> [1975] <i>Hoff et al.</i> [1993] <i>Yaws and Yang</i> [1992]	V M ?	39
1-bromo-2-methylpropane C ₄ H ₉ Br [78-77-3]	4.3×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
2-bromo-2-methylpropane C ₄ H ₉ Br	3.1×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39, 86
1-bromo-3-methylbutane C ₅ H ₁₁ Br [107-82-4]	2.9×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
1-bromopentane C ₅ H ₁₁ Br	5.1×10 ⁻²		<i>Yaws and Yang</i> [1992]	?	39
3-bromo-1-propene C ₃ H ₅ Br	1.7×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
bromoethanoic acid CH ₂ BrCOOH (bromoacetic acid) [79-08-3]	1.5×10 ⁵	9300	<i>Bowden et al.</i> [1998b]	M	
dibromoethanoic acid CHBr ₂ COOH (dibromoacetic acid) [631-64-1]	2.3×10 ⁵	8900	<i>Bowden et al.</i> [1998b]	M	
tribromoethanoic acid CBr ₃ COOH (tribromoacetic acid) [75-96-7]	3.0×10 ⁵	9000	<i>Bowden et al.</i> [1998b]	M	
bromobenzene C ₆ H ₅ Br [108-86-1]	4.8×10 ⁻¹ 4.8×10 ⁻¹ 4.1×10 ⁻¹ 5.4×10 ⁻¹ 4.7×10 ⁻¹ 5.4×10 ⁻¹	5300 5400	<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981] <i>Mackay and Shiu</i> [1981] <i>Hansen et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>Hansen et al.</i> [1993]	V L M M ? X	39 3
1,3-dibromobenzene C ₆ H ₄ Br ₂ [108-36-1]	5.1×10 ⁻¹		<i>Mackay and Shiu</i> [1981]	L	
1,4-dibromobenzene C ₆ H ₄ Br ₂ [106-37-6]	2.0 4.9×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Mackay and Shiu</i> [1981]	V L	
1-bromo-4-methylbenzene BrC ₆ H ₄ CH ₃ (p-bromotoluene)	4.3×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	
1-bromo-2-ethylbenzene BrC ₆ H ₄ C ₂ H ₅	3.0×10 ⁻¹		<i>Hine and Mookerjee</i> [1975]	V	

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
1-bromo-2-(2-propyl)-benzene BrC ₆ H ₄ C ₃ H ₇ (o-bromocumene)	1.7×10^{-1}		<i>Hine and Mookerjee</i> [1975]	V	
4-bromophenol HO C ₆ H ₄ Br	7.0×10^3	8200	<i>Parsons et al.</i> [1971]	M	54
bromotrifluoromethane CHF ₃ Br	2.0×10^{-3}		<i>Hine and Mookerjee</i> [1975]	V	
bromodichloromethane CHCl ₂ Br	6.3×10^{-1} 4.3×10^{-1} 4.8×10^{-1} 4.0×10^{-1} 4.6×10^{-1} 5.2×10^{-1} 3.5×10^{-1} 4.0×10^{-1}	4700 1200 3900 5200 5200	<i>Nicholson et al.</i> [1984] <i>Nicholson et al.</i> [1984] <i>Nicholson et al.</i> [1984] <i>Moore et al.</i> [1995] <i>USEPA</i> [1982] <i>Tse et al.</i> [1992] <i>Ervin et al.</i> [1980] <i>Staudinger and Roberts</i> [1996]	M C C M X X X L	3 3 3
dibromochloromethane CHClBr ₂	1.1 1.2 1.1 7.3×10^{-1} 1.2 9.8×10^{-1} 8.6×10^{-1} 8.7×10^{-1} 8.7×10^{-1}	4900 2500 4000 6400 5000 5500	<i>Nicholson et al.</i> [1984] <i>Nicholson et al.</i> [1984] <i>Nicholson et al.</i> [1984] <i>Moore et al.</i> [1995] <i>USEPA</i> [1982] <i>Tse et al.</i> [1992] <i>Ashworth et al.</i> [1988] <i>Ervin et al.</i> [1980] <i>Staudinger and Roberts</i> [1996]	M C C M X X X X L	3 3 3 3
1-chloro-2-bromoethane C ₂ H ₄ BrCl [107-04-0]	1.1		<i>Hine and Mookerjee</i> [1975]	V	
1-bromo-4-chlorobenzene ClC ₆ H ₄ Br	6.9×10^{-1}		<i>Mackay and Shiu</i> [1981]	L	

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M/atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
compounds with iodine					
iodomethane CH ₃ I [74-88-4]	1.7×10 ⁻¹ 1.8×10 ⁻¹ 1.9×10 ⁻¹ 1.4×10 ⁻¹ 3.5×10 ⁻¹	3800 4300	<i>Liss and Slater</i> [1974] <i>Hine and Mookerjee</i> [1975] <i>Hunter-Smith et al.</i> [1983] <i>Moore et al.</i> [1995] <i>Yaws and Yang</i> [1992]	C V M M ?	39
diiodomethane CH ₂ I ₂ [75-11-6]	2.3 2.8	5000	<i>Moore et al.</i> [1995] <i>Yaws and Yang</i> [1992]	M ?	39
triiodomethane CHI ₃ (iodoform) [75-47-8]	3.4×10 ⁻¹		<i>Yaws and Yang</i> [1992]	?	39
iodoethane C ₂ H ₅ I [75-03-6]	1.4×10 ⁻¹ 1.8×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39, 8
1-iodopropane C ₃ H ₇ I [107-08-4]	1.1×10 ⁻¹ 1.2×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39
2-iodopropane C ₃ H ₇ I [75-30-9]	8.9×10 ⁻² 1.1×10 ⁻¹		<i>Hine and Mookerjee</i> [1975] <i>Yaws and Yang</i> [1992]	V ?	39, 8
1-iodobutane C ₄ H ₉ I [542-69-8]	6.3×10 ⁻²		<i>Hine and Mookerjee</i> [1975]	V	
iodobenzene C ₆ H ₅ I [591-50-4]	7.8×10 ⁻¹ 7.5×10 ⁻¹		<i>Mackay and Shiu</i> [1981] <i>Yaws and Yang</i> [1992]	L ?	39
chloriodomethane CH ₂ ClI [593-71-5]	8.9×10 ⁻¹	4300	<i>Moore et al.</i> [1995]	M	

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
compounds with sulfur					
methanethiol CH ₃ SH (methyl mercaptan)	3.3×10 ⁻¹ 3.9×10 ⁻¹ 7.1×10 ⁻¹ 2.0×10 ⁻¹ 2.6×10 ⁻¹	3100 2800 1600	<i>Hine and Weimar</i> [1965] <i>Przyjazny et al.</i> [1983] <i>Russell et al.</i> [1992] <i>De Bruyn et al.</i> [1995] <i>USEPA</i> [1982]	M M E M X	87 3
ethanethiol C ₂ H ₅ SH (ethyl mercaptan) [75-08-1]	3.6×10 ⁻¹ 2.8×10 ⁻¹ 2.2×10 ⁻¹ 2.6×10 ⁻¹ 3.4×10 ⁻¹	3400	<i>Hine and Mookerjee</i> [1975] <i>Przyjazny et al.</i> [1983] <i>Vitenberg et al.</i> [1975] <i>Karl and Lindinger</i> [1997] <i>Yaws and Yang</i> [1992]	V M M M ?	43 39
1-propanethiol C ₃ H ₇ SH	2.5×10 ⁻¹	3600	<i>Przyjazny et al.</i> [1983]	M	
1-butanethiol C ₄ H ₉ SH [109-75-5]	2.2×10 ⁻¹ 1.1×10 ⁻¹	3800	<i>Przyjazny et al.</i> [1983] <i>Yaws and Yang</i> [1992]	M ?	39
thiophenol C ₆ H ₅ SH	3.0 3.0		<i>Hine and Weimar</i> [1965] <i>Hine and Mookerjee</i> [1975]	V V	
thioanisole C ₆ H ₅ SCH ₃	4.1 4.1		<i>Hine and Weimar</i> [1965] <i>Hine and Mookerjee</i> [1975]	V V	
dimethyl sulfide CH ₃ SCH ₃ (DMS)	5.5×10 ⁻¹ 1.6×10 ⁻¹ 6.2×10 ⁻¹ 7.1×10 ⁻¹ 5.6×10 ⁻¹ 4.4×10 ⁻¹ 6.2×10 ⁻¹ 5.6×10 ⁻¹ 4.8×10 ⁻¹ 8.0×10 ⁻² 4.8×10 ⁻¹	3700 3500 3500 3100	<i>Hine and Weimar</i> [1965] <i>Lovelock et al.</i> [1972] <i>Vitenberg et al.</i> [1975] <i>Vitenberg et al.</i> [1975] <i>Przyjazny et al.</i> [1983] <i>Cline and Bates</i> [1983] <i>Gaffney and Senum</i> [1984] <i>Dacey et al.</i> [1984] <i>Aneja and Overton</i> [1990] <i>Russell et al.</i> [1992] <i>De Bruyn et al.</i> [1995]	V M M R M C X M X E M	8 8 88, 83 48 89 87
diethyl sulfide C ₂ H ₅ SC ₂ H ₅	4.6×10 ⁻¹ 5.6×10 ⁻¹	4600	<i>Hine and Mookerjee</i> [1975] <i>Przyjazny et al.</i> [1983]	V M	
dipropyl sulfide C ₃ H ₇ SC ₃ H ₇	3.3×10 ⁻¹	4200	<i>Przyjazny et al.</i> [1983]	M	
di-(2-propyl)-sulfide (C ₃ H ₇) ₂ S	3.0×10 ⁻¹	4700	<i>Przyjazny et al.</i> [1983]	M	
dimethyl disulfide CH ₃ SSCH ₃	8.4×10 ⁻¹ 9.2×10 ⁻¹ 9.6×10 ⁻¹	4000	<i>Vitenberg et al.</i> [1975] <i>Vitenberg et al.</i> [1975] <i>Przyjazny et al.</i> [1983]	M R M	8 8
diethyl disulfide C ₂ H ₅ SSC ₂ H ₅	4.7×10 ⁻¹ 6.5×10 ⁻¹ 5.8×10 ⁻¹	4000	<i>Vitenberg et al.</i> [1975] <i>Przyjazny et al.</i> [1983] <i>Yaws and Yang</i> [1992]	M M ?	8 39, 8

substance	$\frac{k_H^\ominus}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_H}{d(1/T)}$ [K]	reference	type	note
thiophene C ₄ H ₄ S [110-02-1]	4.4×10 ⁻¹ 3.4×10 ⁻¹	3700	<i>Przyjazny et al.</i> [1983] <i>Yaws and Yang</i> [1992]	M ?	39
2-methyl-thiophene CH ₃ C ₄ H ₃ S	4.2×10 ⁻¹	4000	<i>Przyjazny et al.</i> [1983]	M	
dimethylsulfoxide CH ₃ SOCH ₃ (DMSO)	1.4×10 ³ >5.0×10 ⁴		<i>Gmehling et al.</i> [1981] <i>De Bruyn et al.</i> [1994]	X C	11
dimethylsulfone CH ₃ SO ₂ CH ₃ (DMSO ₂)	>5.0×10 ⁴		<i>De Bruyn et al.</i> [1994]	E	
methanesulfonic acid CH ₃ SO ₃ H (MSA)	6.5×10 ¹³ /K _A		<i>Brimblecombe and Clegg</i> [1988]	T	20
carbon oxide sulfide OCS (carbonyl sulfide)	3.3×10 ⁻² 2.1×10 ⁻² 2.1×10 ⁻² 2.2×10 ⁻² 2.1×10 ⁻² 1.5×10 ⁻² 2.2×10 ⁻² 1.9×10 ⁻²	3300 3300 3000 3600 2100	<i>Hempel</i> [1901] <i>Winkler</i> [1906] <i>Winkler</i> [1907] <i>Stock and Kuss</i> [1917] <i>Wilhelm et al.</i> [1977] <i>Hoyt</i> [1982] <i>De Bruyn et al.</i> [1995] <i>Yaws and Yang</i> [1992]	X X X X L X M ?	30, 79 30 90 30, 8 91, 83 39
carbon disulfide CS ₂	5.6×10 ⁻² 4.4×10 ⁻² 5.5×10 ⁻² 5.2×10 ⁻² 7.6×10 ⁻²	4000 4100 2800 1200	<i>Rex</i> [1906] <i>Booth and Jolley</i> [1943] <i>De Bruyn et al.</i> [1995] <i>Yaws and Yang</i> [1992] <i>USEPA</i> [1982]	X X M ? X	30 30 39 3
2,2'-dichlorodiethylsulfide (ClCH ₂ CH ₂) ₂ S (mustard gas)	3.0×10 ¹		<i>Hine and Mookerjee</i> [1975]	V	

substance	k_{H}^{\ominus} [M/atm]	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
polychlorobiphenyls (PCB's), pesticides, etc.					
2,7-dichlorodibenzo[b,e][1,4]dioxin C ₁₂ H ₆ O ₂ Cl ₂ (2,7-DiCDD) [33857-26-0]	1.7×10 ¹ 1.2×10 ¹		<i>Santl et al.</i> [1994] <i>Shiu et al.</i> [1988]	M X	92
1,2,4-trichlorodibenzo[b,e][1,4]dioxin C ₁₂ H ₅ O ₂ Cl ₃ (1,2,4-TriCDD)	2.8×10 ¹ 2.6×10 ¹		<i>Santl et al.</i> [1994] <i>Shiu et al.</i> [1988]	M X	92
1,2,3,4-tetrachlorodibenzo[b,e][1,4]dioxin C ₁₂ H ₄ O ₂ Cl ₄ (1,2,3,4-TCDD) [30746-58-8]	5.1×10 ¹ 2.7×10 ¹		<i>Santl et al.</i> [1994] <i>Shiu et al.</i> [1988]	M X	92
aroclor1221	4.4	6700	<i>Burkhard et al.</i> [1985]	X	3
aroclor1242	2.0 2.4 3.0	10000 5900 7300	<i>Murphy et al.</i> [1987] <i>USEPA</i> [1982] <i>Burkhard et al.</i> [1985]	X X X	3 3 3
aroclor1248	2.3	7500	<i>Burkhard et al.</i> [1985]	X	3
aroclor1254	1.2×10 ⁻¹ 3.0 3.6	4700 9700 8000	<i>USEPA</i> [1982] <i>Murphy et al.</i> [1987] <i>Burkhard et al.</i> [1985]	X X X	3 3 3
aroclor1260	3.1 3.3 8.6×10 ⁻²	8300 9700 4400	<i>Burkhard et al.</i> [1985] <i>Murphy et al.</i> [1987] <i>USEPA</i> [1982]	X X X	3 3 3
aroclor1268	2.5	8700	<i>Burkhard et al.</i> [1985]	X	3
2,2'-PCB C ₁₂ H ₈ Cl ₂ (IUPAC-4) [13029-08-8]	4.5 1.8 2.9		<i>Murphy et al.</i> [1983] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X M	93, 94 93
2,5-PCB C ₁₂ H ₈ Cl ₂ (IUPAC-9) [34883-39-1]	3.0 2.6 2.3	5700	<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988] <i>tenHulscher et al.</i> [1992]	X M X	93 3
3,3'-PCB C ₁₂ H ₈ Cl ₂ (IUPAC-11) [2050-67-1]	7.5 4.2		<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X M	93
3,4'-PCB C ₁₂ H ₈ Cl ₂ (IUPAC-12) [2974-92-7]	1.0×10 ¹ 4.8		<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X M	93

substance	k_{H}^{\ominus} [M/atm]	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
4,4'-PCB C ₁₂ H ₈ Cl ₂ (IUPAC-15) [2050-68-2]	3.3 6.9 9.2 5.1		<i>Murphy et al.</i> [1983] <i>Coates</i> [1984] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X X M	93, 94 93 93
2,3',5-PCB C ₁₂ H ₇ Cl ₃ (IUPAC-26) [38444-81-4]	3.5 3.0		<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X M	93
2,4,6-PCB C ₁₂ H ₇ Cl ₃ (IUPAC-30) [35693-92-6]	2.7 1.5 1.4×10 ²	5000	<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988] <i>USEPA</i> [1982]	X M X	93 3
2,4,4'-PCB C ₁₂ H ₇ Cl ₃	3.6	6000	<i>tenHulscher et al.</i> [1992]	X	3
2,2',3,3'-PCB C ₁₂ H ₆ Cl ₄ (IUPAC-40) [38444-93-8]	8.3 4.9 4.9		<i>Oliver</i> [1985] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X M	93, 8 93
2,2',5,5'-PCB C ₁₂ H ₆ Cl ₄ (IUPAC-52) [35693-99-3]	>1.9 <3.2 3.8 8.3 4.0×10 ¹ 1.9 2.9 4.2	6100	<i>Westcott et al.</i> [1981] <i>Westcott et al.</i> [1981] <i>Murphy et al.</i> [1983] <i>Oliver</i> [1985] <i>Hassett and Milicic</i> [1985] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988] <i>tenHulscher et al.</i> [1992]	X X X X X X M X	93 93 93, 94 93, 8 93 93 3
2,2',6,6'-PCB C ₁₂ H ₆ Cl ₄ (IUPAC-54) [15968-05-5]	6.8 5.4×10 ⁻¹ 1.8		<i>Coates</i> [1984] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X M	93 93
2,2',5,6'-PCB C ₁₂ H ₆ Cl ₄ (IUPAC-53) [41464-41-9]	3.9 2.4		<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X M	93
3,3',4,4'-PCB C ₁₂ H ₆ Cl ₄ (IUPAC-77) [32598-13-3]	2.3×10 ¹ 1.1×10 ¹		<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X M	93
2,2',4,5,5'-PCB C ₁₂ H ₅ Cl ₅ (IUPAC-101) [37680-73-2]	>2.8 <9.1 1.4×10 ¹ 3.1 3.9		<i>Westcott et al.</i> [1981] <i>Westcott et al.</i> [1981] <i>Oliver</i> [1985] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X X X M	93 93 93, 8 93

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
2,2',4,6,6'-PCB C ₁₂ H ₅ Cl ₅ (IUPAC-104) [56558-16-8]	5.5×10 ⁻¹ 1.1		<i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X M	93
2,2',3,3',4,4'-PCB C ₁₂ H ₄ Cl ₆ (IUPAC-128) [38380-07-3]	2.0 1.5×10 ¹ 3.3×10 ¹		<i>Murphy et al.</i> [1983] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X M	93, 94 93
2,2',4,4',5,5'-PCB C ₁₂ H ₄ Cl ₆ (IUPAC-153) [35065-27-1]	2.8 8.1 1.6×10 ¹ 5.7 7.6		<i>Murphy et al.</i> [1983] <i>Coates</i> [1984] <i>Oliver</i> [1985] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X X X M	93, 94 93 93, 8 93
2,2',4,4',6,6'-PCB C ₁₂ H ₄ Cl ₆ (IUPAC-155) [33979-03-2]	8.7 6.5×10 ⁻¹ 1.3		<i>Coates</i> [1984] <i>Burkhard et al.</i> [1985] <i>Dunnivant et al.</i> [1988]	X X M	93 93
hexachlorocyclopentadiene C ₅ Cl ₆ [77-47-4]	3.7×10 ⁻² 6.1×10 ⁻²	1500	<i>Meylan and Howard</i> [1991] <i>USEPA</i> [1982]	X X	3 3
α-1,2,3,4,5,6-hexachlorocyclohexane C ₆ H ₆ Cl ₆	1.3×10 ²	6500	<i>Kucklick et al.</i> [1991]	X	3
γ-1,2,3,4,5,6-hexachlorocyclohexane C ₆ H ₆ Cl ₆ (lindane) [58-89-9]	3.2×10 ² 2.2×10 ³ 2.8×10 ²	5500	<i>Mackay and Shiu</i> [1981] <i>Brimblecombe</i> [1986] <i>Kucklick et al.</i> [1991]	L ? X	38 3
dodecachloropentacyclodecane C ₁₀ Cl ₁₂ (mirex) [2385-85-5]	1.2	11000	<i>Yin and Hassett</i> [1986]	X	3

substance	$\frac{k_{\text{H}}^{\ominus}}{[\text{M}/\text{atm}]}$	$\frac{-d \ln k_{\text{H}}}{d(1/T)}$ [K]	reference	type	note
aldrin C ₁₂ H ₈ Cl ₆ [309-00-2]	3.6×10 ¹ 8.5×10 ¹		<i>Mackay and Shiu</i> [1981] <i>Brimblecombe</i> [1986]	L ?	38
dieldrin C ₁₂ H ₈ OCl ₆ [60-57-1]	9.2×10 ¹ 5.8×10 ³		<i>Mackay and Shiu</i> [1981] <i>Brimblecombe</i> [1986]	L ?	38
1,1,1-trichloro-2,2-bis-(4-chlorophenyl)ethane C ₁₄ H ₉ Cl ₅ (DDT) [50-29-3]	1.9×10 ¹ 2.8×10 ¹		<i>Mackay and Shiu</i> [1981] <i>Brimblecombe</i> [1986]	L ?	38
molinate C ₉ H ₁₇ NOS	1.7×10 ²	7300	<i>Sagebiel et al.</i> [1992]	X	3
parathion C ₁₀ H ₁₄ NO ₅ PS [56-38-2]	8.2×10 ²		<i>Mackay and Shiu</i> [1981]	L	
malathion C ₁₀ H ₁₉ O ₆ PS ₂ [121-75-5]	2.7×10 ³		<i>Mackay and Shiu</i> [1981]	L	
methylchlorpyrifos C ₇ H ₇ NO ₃ Cl ₃ PS [5598-13-0]	3.3×10 ²		<i>Mackay and Shiu</i> [1981]	L	
fenitrothion C ₉ H ₁₂ NO ₅ PS [122-14-5]	2.7×10 ³		<i>Mackay and Shiu</i> [1981]	L	
dicapthon C ₈ H ₉ NO ₅ ClPS [2463-84-5]	4.4×10 ³		<i>Mackay and Shiu</i> [1981]	L	
ronnel C ₈ H ₈ O ₃ Cl ₃ PS [299-84-3]	4.8×10 ¹		<i>Mackay and Shiu</i> [1981]	L	
leptophos C ₁₃ H ₁₀ O ₃ BrCl ₂ P [21609-90-5]	3.8×10 ²		<i>Mackay and Shiu</i> [1981]	L	

9 Notes

- 1) The value is taken from the compilation of solubilities by W. Asman (unpublished).
- 2) Only the tabulated data between $T = 273$ K and $T = 303$ K from *Dean* [1992] was used to derive k_{H} and $-\Delta_{\text{soln}}H/R$. Above $T = 303$ K the tabulated data could not be parameterized by equation (4) very well. The partial pressure of water vapor (needed to convert some Henry's law constants) was calculated using the formula given by *Sander et al.* [1994]. The quantities A and α from *Dean* [1992] were assumed to be identical.
- 3) Value given here as quoted by *Staudinger and Roberts* [1996].
- 4) *Hoffmann and Jacob* [1984] refer to several references in their list of Henry's law constants but they don't assign them to specific species.
- 5) Calculated from correlation between the polarizabilities and solubilities of stable gases. The temperature dependence is an estimate of the upper limit.
- 6) *Jacob* [1986] assumed the temperature dependence to be the same as for water.
- 7) *Schwartz* [1984] gives an upper limit of $k_{\text{H}} = 6.8 \times 10^3$ M/atm. In the abstract a range of 1×10^3 M/atm $< k_{\text{H}} < 3 \times 10^3$ M/atm is given. The mean value of this range (2×10^3 M/atm) has been used by *Lelieveld and Crutzen* [1991], *Pandis and Seinfeld* [1989], and *Jacob* [1986].
- 8) Value at $T = 293$ K.
- 9) This value is a correction of the solubility published by *Lind and Kok* [1986].
- 10) This value was measured at low pH. It is superseded by a later publication of the same group [*Lind and Kok*, 1994].
- 11) Value given here as quoted by *Betterton* [1992].
- 12) *Bone et al.* [1983] gives *Carter et al.* [1968] as the source for the data. However, no data was found in that reference.
- 13) Several references are given in the list of Henry's law constants but not assigned to specific species.
- 14) The parametrization given by *Lide and Frederikse* [1995] (parameters A , B , C) doesn't fit the data in the same paper for this substance. Therefore the parametrization of the solubility data (X_1) was recalculated.
- 15) Value at $T = 295$ K.
- 16) Value obtained by estimating the diffusion coefficient for NO_3 to be $D = 1.0 \times 10^{-5}$ cm²/s.
- 17) The value given by *Seinfeld and Pandis* [1998] is wrong.
- 18) The assumption of irreversible hydrolysis is equivalent to an infinite effective Henry's law constant.
- 19) This value was extrapolated from data at $T = 230$ K and $T = 273$ K.
- 20) For strong acids, the solubility is often expressed as $k_{\text{H}} = ([\text{H}^+] + [\text{A}^-])/p(\text{HA})$. To obtain the physical solubility of HA, the value has to be divided by the acidity constant K_{A} .
- 21) *Brimblecombe and Clegg* [1989] corrects erroneous data from *Brimblecombe and Clegg* [1988].
- 22) *Lelieveld and Crutzen* [1991] assume the temperature dependence to be the same as for $a(\text{H}^+)a(\text{NO}_3^-)/p(\text{HNO}_3)$ in *Schwartz and White* [1981].
- 23) *Möller and Mauersberger* [1992] assumed the solubility to be comparable to HNO_3 .
- 24) This value was extrapolated from data at $T = 215$ K and $T = 263$ K.
- 25) fitting parameter used in numerical modeling.
- 26) *Kruis and May* [1962] claim that Cl_2 does not obey Henry's law. Looking at their interpolation formula, however, it seems that this is only because they did not consider the equilibrium $\text{Cl}_2 + \text{H}_2\text{O} \rightleftharpoons \text{HOCl} + \text{HCl}$.
- 27) *Chameides and Stelson* [1992] refer to *Jacob* [1986] and *Chameides* [1984] but this value cannot be found there.
- 28) Data from Table 1 in preprint of the paper. *J. Geophys. Res.* forgot to print the tables.
- 29) *Fickert* [1998] extracted a value for HOBr from wetted-wall flow tube experiments. However, it was later discovered that under the experimental conditions no evaluation of k_{H} is possible (*J. Crowley*, pers. comm., 1999).
- 30) As quoted by *Kruis and May* [1962].
- 31) *Dubik et al.* [1987] measured the solubility in concentrated salt solutions (natural brines).

- 32) This work, using data from *Wagman et al.* [1982] and the aqueous-phase equilibrium $\text{Cl}_2 + \text{Br}_2 \rightleftharpoons 2 \text{BrCl}$ from *Wang et al.* [1994].
- 33) Calculated by R. Vogt (pers. comm., 1996), using data from *Wagman et al.* [1982] and the aqueous-phase equilibrium $\text{BrCl} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$ from *Wang et al.* [1994].
- 34) Value at $T = 290 \text{ K}$.
- 35) *Thompson and Zafirio* [1983] quote a paper as the source that gives only the solubility but not the Henry's law constant.
- 36) *Gmitro and Vermeulen* [1964] give partial pressures of H_2SO_4 over a concentrated solution (e.g. 10^{-7} mmHg for 70 weight-percent at 298 K). Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for k_{H} .
- 37) Interpolation of the original data at $T < 300 \text{ K}$. According to *Morrison and Johnstone* [1954] the solubility increases at higher temperatures.
- 38) Value at $T = 288 \text{ K}$.
- 39) *Yaws and Yang* [1992] give several references for the Henry's law constants but don't assign them to specific species.
- 40) *Hansen et al.* [1995] found that the solubility of 2-methylhexane increases with temperature.
- 41) Value at $T = 294 \text{ K}$.
- 42) Value given here as quoted by *Wasik and Tsang* [1970].
- 43) *Karl and Lindinger* [1997] also measured solubilities in salt solutions.
- 44) The value given by *Wilhelm et al.* [1977] is wrong.
- 45) Value given here as cited in *Dewulf et al.* [1995].
- 46) This paper supersedes earlier work with more concentrated solutions [*Butler et al.*, 1933].
- 47) Value given here as quoted by *Hine and Weimar* [1965].
- 48) Value given here as quoted by *Gaffney et al.* [1987].
- 49) Value at $T = 303 \text{ K}$.
- 50) *Koga* [1995] found that *tert*-butanol does not obey Henry's law at $c > 3.8 \text{ mM}$.
- 51) Value obtained by *Saxena and Hildemann* [1996] using the group contribution method.
- 52) Value at $T = 307 \text{ K}$.
- 53) Value given here as quoted by *Hine and Mookerjee* [1975].
- 54) It is assumed here that the thermodynamic data in *Parsons et al.* [1971] refers to the units $[\text{mol dm}^{-3}]$ and $[\text{atm}]$ as standard states.
- 55) Value given here as quoted by *Lüttke and Levens* [1997].
- 56) It is assumed here that the thermodynamic data in *Parsons et al.* [1972] refers to the units $[\text{mol dm}^{-3}]$ and $[\text{atm}]$ as standard states.
- 57) *Saxena and Hildemann* [1996] say that this value is unreliable.
- 58) Value given here as quoted by *Mackay et al.* [1995].
- 59) *Jacob* [1986] assumes $k_{\text{H}}(\text{CH}_3\text{OO}) = k_{\text{H}}(\text{CH}_3\text{OOH}) \times k_{\text{H}}(\text{HO}_2)/k_{\text{H}}(\text{H}_2\text{O}_2)$.
- 60) *Lelieveld and Crutzen* [1991] assume $k_{\text{H}}(\text{CH}_3\text{OO}) = k_{\text{H}}(\text{HO}_2)$.
- 61) *Ledbury and Blair* [1925] (and also *Blair and Ledbury* [1925]) measured the solubility of HCHO at very high concentrations around 5 to 15 M. Their value of k_{H} increases with HCHO concentration. *Lelieveld and Crutzen* [1991], *Hough* [1991], and *Pandis and Seinfeld* [1989] all use these solubility data but do not specify how they extrapolated to lower concentrations. Since the concentration range is far away from typical values in atmospheric chemistry the data is not reproduced here.
- 62) *Dong and Dasgupta* [1986] found that the Henry's law constant for HCHO is not a true constant but increases with increasing concentration. They recommend the expression

$$[\text{HCHO}] = 10^{(4538/T - 11.34)} \times p(\text{HCHO})^{(252.2/T + 0.2088)}$$

with $[\text{HCHO}]$ = aqueous-phase concentration in [mol/l], $p(\text{HCHO})$ = partial pressure in [atm], and T = temperature in [K]. At $T = 298.15$ K and a partial pressure of $p(\text{HCHO}) = 10^{-9}$ atm, for example, this equation results in $k_{\text{H}} = 2.5 \times 10^3$ M/atm. It should be noted that this expression does not converge asymptotically to a constant value at infinite dilution.

63) *Betterton and Hoffmann* [1988] list effective values that take into account hydration of the aldehydes:

$$k_{\text{H}} = ([\text{RCHO}] + [\text{RCH}(\text{OH})_2])/p(\text{RCHO})$$

64) The data from Table 1 by *Zhou and Mopper* [1990] was used to redo the regression analysis. The data for acetone in their Table 2 is wrong.

65) Value given here as quoted by *Bone et al.* [1983].

66) The value cited by *Betterton* [1992] is wrong.

67) Value given here as quoted by *Vitenberg et al.* [1975].

68) Value given here as cited in *Saxena and Hildemann* [1996].

69) The value given here was measured at a liquid phase volume mixing ratio of 10^{-6} . *Servant et al.* [1991] found that the Henry's law constant changes at higher concentrations.

70) *Staudinger and Roberts* [1996] give 'Khan & Brimblecombe' as the reference but don't include this paper in their list of references.

71) *Pecsar and Martin* [1966] is quoted as the source. However, there only activity coefficients and no vapor pressures are listed.

72) *Kames and Schurath* [1992] couldn't assign the values to the isomers.

73) The same data was also published in *Fischer and Ballschmiter* [1998a].

74) Value at $T = 283$ K.

75) The value given by *Warneck et al.* [1996] is wrong.

76) The value given by *Schurath et al.* [1996] is wrong.

77) Value at $T = 373$ K.

78) Value at $T = 301$ K.

79) Value at $T = 287$ K.

80) Estimate for R = haloalkylgroup.

81) The same data was also published in *McConnell et al.* [1975].

82) Value at $T = 275$ K.

83) Solubility in sea water.

84) The temperature dependence (after a unit conversion) is given as:

$$k_{\text{H}} = \exp(-8.689 + 205.9/(T - 255.1)) \times 11.7 \text{ M/atm}$$

This can obviously only be valid for $T \gg 255.1$ K.

85) *Kanakidou et al.* [1995] assume $k_{\text{H}}(\text{CClF}_2\text{OONO}_2) = k_{\text{H}}(\text{PAN})$.

86) Value at $T = 291$ K.

87) Calculated molecular structure relationship.

88) *Cline and Bates* [1983] refer to an unpublished manuscript; no details are available.

89) Value given here as quoted by *De Bruyn et al.* [1995].

90) Value given here as quoted by *Loomis* [1928].

91) Value given here as quoted by *Rasmussen et al.* [1982].

92) Value given here as quoted by *Santl et al.* [1994].

93) Value given here as quoted by *Dunnivant et al.* [1988].

94) Value at 'room temperature'.

10 Acknowledgements

Compiling this data set would not have been possible without the help I received. For valuable discussions and for pointing out additional references to me I would like to thank C. Allen, W. Asman, M. Barth, E. Betterton, S. Clegg, N. Couffin, P. J. Crutzen, F. Dentener, D. J. Jacob, H.-W. Jacobi, W. C. Keene, J. Matthijssen, J. Montgomery, R. M. Moore, M. Mozurkewich, F. Müller, O. Pahl, S. Pandis, J. Perlinger, J.-M. Régimbal, S. E. Schwartz, W. Y. Shiu, T. A. Staffelbach, G. Tyndall, C. Verlinde, R. Vogt, and P. Warneck.

References

- Allen, J. M., W. X. Balcavage, B. R. Ramachandran, and A. L. ShROUT. Determination of Henry's Law constants by equilibrium partitioning in a closed system using a new in situ optical absorbance method. *Environ. Toxicol. Chem.*, *17*, 1216–1221, 1998.
- Amels, P., H. Elias, U. Götz, U. Steingens, and K. J. Wannowius. Chapter 3.1: Kinetic investigation of the stability of peroxynitric acid and of its reaction with sulfur(IV) in aqueous solution. In P. Warneck, editor, *Heterogeneous and Liquid-Phase Processes*, pages 77–88. Springer Verlag, Berlin, 1996.
- Andon, R. J. L., J. D. Cox, and E. F. G. Herington. Phase relationships in the pyridine series. Part V. The thermodynamic properties of dilute solutions of pyridine bases in water at 25 ° and 40 °. *J. Chem. Soc.*, pages 3188–3196, 1954.
- Aneja, V. P. and J. H. Overton. The emission rate of dimethyl sulfide at the atmospheric oceanic interface. *Chem. Eng. Comm.*, *98*, 199–209, 1990.
- Arijs, E. and G. Brasseur. Acetonitrile in the stratosphere and implications for positive ion composition. *J. Geophys. Res.*, *91D*, 4003–4016, 1986.
- Ashworth, R. A., G. B. Howe, M. E. Mullins, and T. N. Rogers. Air-water partitioning coefficients of organics in dilute aqueous solutions. *J. Hazard. Mater.*, *18*, 25–36, 1988.
- Barr, R. S. and D. M. T. Newsham. Phase equilibria in very dilute mixtures of water and chlorinated hydrocarbons. I. Experimental results. *Fluid Phase Equil.*, *35*, 189–205, 1987.
- Bartlett, W. B. and D. W. Margerum. The temperature dependence of the Henry's law constant and the dissociation equilibrium constants of bromine chloride. *Eos, Trans. AGU (Abstract Supplement)*, *79/45*, F97, 1998.
- Becker, K. H., J. Kleffmann, R. Kurtenbach, and P. Wiesen. Solubility of nitrous acid (HONO) in sulfuric acid solutions. *J. Phys. Chem.*, *100*, 14984–14990, 1996.
- Becker, K. H., J. Kleffmann, R. M. Negri, and P. Wiesen. Solubility of nitrous acid (HONO) in ammonium sulfate solutions. *J. Chem. Soc. Faraday Trans.*, *94*, 1583–1586, 1998.
- Behnke, W., C. George, V. Scheer, and C. Zetzsch. Production and decay of ClNO₂ from the reaction of gaseous N₂O₅ with NaCl solution: Bulk and aerosol experiments. *J. Geophys. Res.*, *102D*, 3795–3804, 1997.
- Benkelberg, H.-J., S. Hamm, and P. Warneck. Henry's law coefficients for aqueous solutions of acetone, acetaldehyde and acetonitrile, and equilibrium constants for the addition compounds of acetone and acetaldehyde with bisulfite. *J. Atmos. Chem.*, *20*, 17–34, 1995.
- Berdnikov, V. M. and N. M. Bazhin. Oxidation-reduction potentials of certain inorganic radicals in aqueous solutions. *Russ. J. Phys. Chem., Engl. Transl.*, *44*, 395–398, 1970.
- Betterton, E. A. The partitioning of ketones between the gas and aqueous phases. *Atmos. Environ.*, *25A*, 1473–1477, 1991.
- Betterton, E. A. Henry's law constants of soluble and moderately soluble organic gases: Effects on aqueous phase chemistry. *Adv. Environ. Sci. Technol.*, *24*, 1–50, 1992.
- Betterton, E. A. and M. R. Hoffmann. Henry's law constants of some environmentally important aldehydes. *Environ. Sci. Technol.*, *22*, 1415–1418, 1988.
- Bissonette, E. M., J. J. Westrick, and J. M. Morand. Determination of Henry's coefficient for volatile organic compounds in dilute aqueous systems. In *Proceedings of the Annual Conference of the American Water Works Association, Cincinnati, OH, June 17-21*, pages 1913–1922. 1990.
- Blair, E. W. and W. Ledbury. The partial formaldehyde vapour pressures of aqueous solutions of formaldehyde. Part I. *J. Chem. Soc.*, *127*, 26–40, 1925.
- Blatchley, E. R., III, R. W. Johnson, J. E. Alleman, and W. F. McCoy. Effective Henry's law constants for free chlorine and free bromine. *Wat. Res.*, *26*, 99–106, 1992.
- Bohon, R. J. and W. F. Claussen. The solubility of aromatic hydrocarbons in water. *J. Am. Chem. Soc.*, *73*, 1571–1578, 1951.
- Bone, R., P. Cullis, and R. Wolfenden. Solvent effects on equilibria of addition of nucleophiles to acetaldehyde and the hydrophilic character of diols. *J. Am. Chem. Soc.*, *105*, 1339–1343, 1983.
- Booth, N. and L. J. Jolley. ? *J. Chem. Soc. Ind.*, *62*, 87, 1943.
- Bowden, D. J., S. L. Clegg, and P. Brimblecombe. The Henry's law constant of trifluoroacetic acid and its partitioning into liquid water in the atmosphere. *Chemosphere*, *32*, 405–420, 1996.
- Bowden, D. J., S. L. Clegg, and P. Brimblecombe. The Henry's law constant of trichloroacetic acid. *Water Air Soil Pollut.*, *101*, 197–215, 1998a.
- Bowden, D. J., S. L. Clegg, and P. Brimblecombe. The Henry's law constants of the haloacetic acids. *J. Atmos. Chem.*, *29*, 85–107, 1998b.
- Brennan, R. A., N. Nirmalakhandan, and R. E. Speece. Comparison of predictive methods for Henry's law coefficients of organic chemicals. *Wat. Res.*, *32*, 1901–1911, 1998.
- Brian, P. L. T., J. E. Vivian, and A. G. Habib. The effect of the hydrolysis reaction upon the rate of absorption of chlorine into water. *AIChE J.*, *8*, 205–209, 1962.
- Brimblecombe, P. *Air Composition & Chemistry*. Cambridge University Press, Cambridge, 1986.

- Brimblecombe, P. and S. L. Clegg. The solubility and behaviour of acid gases in the marine aerosol. *J. Atmos. Chem.*, *7*, 1–18, 1988.
- Brimblecombe, P. and S. L. Clegg. Erratum. *J. Atmos. Chem.*, *8*, 95, 1989.
- Briner, E. and E. Perrottet. Détermination des solubilités de l'ozone dans l'eau et dans une solution aqueuse de chlorure de sodium; calcul des solubilités de l'ozone atmosphérique dans les eaux. *Helv. Chim. Acta*, *22*, 397–404, 1939.
- Burkhard, L. P., D. E. Armstrong, and A. W. Andren. Henry's law constants for the polychlorinated biphenyls. *Environ. Sci. Technol.*, *19*, 590–596, 1985. (data in supplement).
- Burnett, M. G. Determination of partition coefficients at infinite dilution by the gas chromatographic analysis of the vapor above dilute solutions. *Anal. Chem.*, *35*, 1567–1570, 1963.
- Butler, J. A. V. and C. N. Ramchandani. The solubility of non-electrolytes. Part II. The influence of the polar group on the free energy of hydration of aliphatic compounds. *J. Chem. Soc.*, pages 952–955, 1935.
- Butler, J. A. V., C. N. Ramchandani, and D. W. Thomson. The solubility of non-electrolytes. Part I. The free energy of hydration of some aliphatic alcohols. *J. Chem. Soc.*, pages 280–285, 1935.
- Butler, J. A. V., D. W. Thomson, and W. H. MacLennan. The free energy of the normal aliphatic alcohols in aqueous solution. Part I. The partial vapour pressures of aqueous solutions of methyl, *n*-propyl, and *n*-butyl alcohols. Part II. The solubilities of some normal aliphatic alcohols in water. Part III. The theory of binary solutions, and its application to aqueous-alcoholic solutions. *J. Chem. Soc.*, pages 674–686, 1933.
- Buttery, R. G., J. L. Bomben, D. G. Guadagni, and L. C. Ling. Some considerations of volatilities of organic flavor compounds in foods. *J. Agric. Food Chem.*, *19*, 1045–1048, 1971.
- Buttery, R. G., L. C. Ling, and D. G. Guadagni. Volatilities of aldehydes, ketones, and esters in dilute water solutions. *J. Agric. Food Chem.*, *17*, 385–389, 1969.
- Cabani, S., G. Conti, and L. Lepori. Thermodynamic study on aqueous dilute solutions of organic compounds. Part 2. — Cyclic ethers. *Trans. Faraday Soc.*, *67*, 1943–1950, 1971a.
- Cabani, S., G. Conti, and L. Lepori. Thermodynamic study on aqueous dilute solutions of organic compounds. Part 1. — Cyclic amines. *Trans. Faraday Soc.*, *67*, 1933–1942, 1971b.
- Carpenter, J. H. New measurements of oxygen solubility in pure and natural water. *Limnol. Oceanogr.*, *11*, 264–277, 1966.
- Carroll, J. J. and A. E. Mather. The solubility of hydrogen sulphide in water from 0 to 90 °C and pressures to 1 MPa. *Geochim. Cosmochim. Acta*, *53*, 1163–1170, 1989.
- Carroll, J. J., J. D. Slupsky, and A. E. Mather. The solubility of carbon dioxide in water at low pressure. *J. Phys. Chem. Ref. Data*, *20*, 1201–1209, 1991.
- Carter, G. B., M. C. McIver, and G. J. Miller. Evidence for the formation of a hexahydrotriazine in the condensation of acetaldehyde with methylamine. *J. Chem. Soc. C*, pages 2591–2592, 1968.
- Chameides, W. L. The photochemistry of a remote marine stratiform cloud. *J. Geophys. Res.*, *89D*, 4739–4755, 1984.
- Chameides, W. L. Reply. *J. Geophys. Res.*, *91D*, 14571–14572, 1986.
- Chameides, W. L. and A. W. Stelson. Aqueous phase chemical processes in deliquescent sea-salt aerosols: A mechanism that couples the atmospheric cycles of S and sea salt. *J. Geophys. Res.*, *97D*, 20565–20580, 1992.
- Chen, C. C., H. I. Britt, J. F. Boston, and L. B. Evans. Extension and application of the Pitzer equation for vapor liquid equilibrium of aqueous electrolyte systems with molecular solutes. *AIChE J.*, *25*, 820–831, 1979.
- Christie, A. O. and D. J. Crisp. Activity coefficients on the *n*-primary, secondary and tertiary aliphatic amines in aqueous solution. *J. Appl. Chem.*, *17*, 11–14, 1967.
- Clegg, S. L. and P. Brimblecombe. Solubility of ammonia in pure aqueous and multicomponent solutions. *J. Phys. Chem.*, *93*, 7237–7238, 1989.
- Cline, J. D. and T. S. Bates. Dimethyl sulfide in the equatorial Pacific Ocean: A natural source of sulfur to the atmosphere. *Geophys. Res. Lett.*, *10*, 949–952, 1983.
- Coates, J. T. ?. Ph.D. thesis, Clemson University, Clemson, SC, USA, 1984.
- Cooling, M. R., B. Khalfaoui, and D. M. T. Newsham. Phase equilibria in very dilute mixtures of water and unsaturated chlorinated hydrocarbons and of water and benzene. *Fluid Phase Equil.*, *81*, 217–229, 1992.
- Dacey, J. W. H., S. G. Wakeham, and B. L. Howes. Henry's law constants for dimethylsulfide in freshwater and seawater. *Geophys. Res. Lett.*, *11*, 991–994, 1984.
- Dasgupta, P. G. and S. Dong. Solubility of ammonia in liquid water and generation of trace levels of standard gaseous ammonia. *Atmos. Environ.*, *20*, 565–570, 1986.
- De Bruyn, W. J., J. A. Shorter, P. Davidovits, D. R. Worsnop, M. S. Zahniser, and C. E. Kolb. Uptake of gas-phase sulfur species methanesulfonic acid, dimethylsulfoxide, and dimethyl sulfone by aqueous surfaces. *J. Geophys. Res.*, *99D*, 16927–16932, 1994.
- De Bruyn, W. J., E. Swartz, J. H. Hu, J. A. Shorter, P. Davidovits, D. R. Worsnop, M. S. Zahniser, and C. E. Kolb. Henry's law solubilities and Setchenow coefficients for biogenic reduced sulfur species obtained from gas-liquid uptake measurements. *J. Geophys. Res.*, *100D*, 7245–7251, 1995.
- De Maagd, P. G.-J., D. T. E. M. Ten Hulscher, H. van den Heuvel, A. Opperhuizen, and D. T. H. M. Sijm. Physicochemical properties of polycyclic aromatic hydrocarbons: Aqueous solubilities, *n*-octanol/water partition coefficients, and Henry's law constants. *Environ. Toxicol. Chem.*, *17*, 251–257, 1998.
- Dean, J. A. *Lange's Handbook of Chemistry*. McGraw-Hill, Inc., 1992.
- Dewulf, J., D. Drijvers, and H. van Langenhove. Measurement of Henry's law constant as function of temperature and salinity for the low temperature range. *Atmos. Environ.*, *29*, 323–331, 1995.

- Dilling, W. L. Interphase transfer processes. II. Evaporation rates of chloro methanes, ethanes, ethylenes, propanes, and propylenes from dilute aqueous solutions. Comparisons with theoretical predictions. *Environ. Sci. Technol.*, *11*, 405–409, 1977.
- Disselkamp, R. S., C. D. Howd, E. G. Chapman, W. R. Barchet, and S. D. Colson. BrCl production in NaBr/NaCl/HNO₃/O₃ solutions representative of sea-salt aerosols in the marine boundary layer. *Geophys. Res. Lett.*, 1998. (submitted).
- Dong, S. and P. G. Dasgupta. Solubility of gaseous formaldehyde in liquid water and generation of trace standard gaseous formaldehyde. *Environ. Sci. Technol.*, *20*, 637–640, 1986.
- Drouillard, K. G., G. T. Tomy, D. C. G. Muir, and K. J. Friesen. Volatility of chlorinated *n*-alkanes (C₁₀-C₁₂): Vapor pressures and Henry's law constants. *Environ. Toxicol. Chem.*, *17*, 1252–1260, 1998.
- Dubik, N. A., G. M. Titova, and E. I. Loshakova. Partition coefficients of bromine and bromine chloride between air and natural brines. *Issled. v Obl. Poluch. Magniya, Ioda, Broma i ikh Soed., M.*, pages 53–57, 1987. (in Russian, see also *Chem. Abstr.*, **109**, 213154j).
- Duce, R. A., P. S. Liss, J. T. Merrill, E. L. Atlas, P. Buat-Menard, B. B. Hicks, J. M. Miller, J. M. Prospero, R. Arimoto, T. M. Church, W. Ellis, J. N. Galloway, L. Hansen, T. D. Jickells, A. H. Knap, K. H. Reinhardt, B. Schneider, A. Soudine, J. J. Tokos, S. Tsunogai, R. Wollast, and M. Zhao. The atmospheric input of trace species to the world oceans. *Global Biogeochem. Cycles*, *5*, 193–259, 1991.
- Dunnivant, F. M., J. T. Coates, and A. W. Elzerman. Experimentally determined Henry's law constants for 17 polychlorobiphenyl congeners. *Environ. Sci. Technol.*, *22*, 448–453, 1988.
- Durham, J. L., J. H. Overton, Jr., and V. P. Aneja. Influence of gaseous nitric acid on sulfate production and acidity in rain. *Atmos. Environ.*, *15*, 1059–1068, 1981.
- Economou, I. G., J. L. Heidman, C. Tsonopoulos, and G. M. Wilson. Mutual solubilities of hydrocarbons and water: III. 1-hexene, 1-octene, C₁₀-C₁₂ hydrocarbons. *AIChE J.*, *43*, 535–546, 1997.
- Edwards, T. J., G. Maurer, J. Newman, and J. M. Prausnitz. Vapor-liquid equilibria in multicomponent aqueous solutions of volatile weak electrolytes. *AIChE J.*, *24*, 966–976, 1978.
- Ervin, A. L., M. A. Mangone, and J. E. Singley. Trace organics removal by air stripping. In *Proceedings of the Annual Conference of the American Water Works Association*, pages 507–530. 1980.
- Ettre, L. S., C. Welter, and B. Kolb. Determination of gas-liquid partition coefficients by automatic equilibrium headspace - gas chromatography utilizing the phase ratio variation method. *Chromatographia*, *35*, 73–84, 1993.
- Fendinger, N. J. and D. E. Glotfelty. A laboratory method for the experimental determination of air-water Henry's law constants for several pesticides. *Environ. Sci. Technol.*, *22*, 1289–1293, 1988.
- Fendinger, N. J., D. E. Glotfelty, and H. P. Freeman. Comparison of two experimental techniques for determining air/water Henry's law constants. *Environ. Sci. Technol.*, *23*, 1528–1531, 1989.
- Fickert, S. *Laboruntersuchungen zur Freisetzung photoreaktiver Halogenverbindungen aus Seesalzaerosol*. Ph.D. thesis, Johannes Gutenberg-Universität, Mainz, FRG, 1998.
- Fischer, R. G. and K. Ballschmiter. Determination of vapor pressure, water solubility, gas-water partition coefficient P_{GW} , Henry's law constant, and octanol-water partition coefficient P_{OW} of 26 alkyl dinitrates. *Chemosphere*, *36*, 2891–2901, 1998a.
- Fischer, R. G. and K. Ballschmiter. Prediction of the environmental distribution of alkyl dinitrates – Chromatographic determination of vapor pressure p^0 , water solubility S_{H_2O} , gas-water partition coefficient K_{GW} (Henry's law constant) and octanol-water partition coefficient K_{OW} . *Fresenius J. Anal. Chem.*, *360*, 769–776, 1998b.
- Frenzel, A., V. Scheer, R. Sikorski, C. George, W. Behnke, and C. Zetzsch. Heterogeneous interconversion reactions of BrNO₂, ClNO₂, Br₂, and Cl₂. *J. Phys. Chem. A*, *102*, 1329–1337, 1998.
- Friant, S. L. and I. H. Suffet. Interactive effects of temperature, salt concentration, and pH on head space analysis for isolating volatile trace organics in aqueous environmental samples. *Anal. Chem.*, *51*, 2167–2172, 1979.
- Fried, A., B. E. Henry, J. G. Calvert, and M. Mozurkewich. The reaction probability of N₂O₅ with sulfuric acid aerosols at stratospheric temperatures and compositions. *J. Geophys. Res.*, *99D*, 3517–3532, 1994.
- Gaffney, J. S. and G. I. Senum. ? In L. Newman, editor, *Gas-Liquid Chemistry of Natural Waters*, pages 5–1–5–7. NTIS TIC-4500, UC-11, BNL 51757 Brookhaven National Laboratory, 1984.
- Gaffney, J. S., G. E. Streit, W. D. Spall, and J. H. Hall. Beyond acid rain. *Environ. Sci. Technol.*, *21*, 519–524, 1987.
- Gan, J. and S. R. Yates. Degradation and phase partition of methyl iodide in soil. *J. Agric. Food Chem.*, *44*, 4001–4008, 1996.
- Gmehling, J., P. Rasmussen, and A. Fredenslund. Vapor-liquid equilibria by UNIFAC group contribution. Revision and extension. 2. *Ind. Eng. Chem. Process Des. Dev.*, *21*, 118, 1981.
- Gmitro, J. I. and T. Vermeulen. Vapor-liquid equilibria for aqueous sulfuric acid. *AIChE J.*, *10*, 740–746, 1964.
- Gossett, J. M. Measurement of Henry's law constants for C₁ and C₂ chlorinated hydrocarbons. *Environ. Sci. Technol.*, *21*, 202–208, 1987.
- Gossett, J. M., C. E. Cameron, B. P. Eckstrom, C. Goodman, and A. H. Lincoff. Mass transfer coefficients and Henry's constants for packed-tower air stripping of volatile organics: Measurements and Correlations. Final Report ESL-TR-85-18, Engineering and Services Laboratory, Tyndall Air Force Base, FL, 1985.
- Graedel, T. E. and K. I. Goldberg. Kinetic studies of raindrop chemistry 1. Inorganic and organic processes. *J. Geophys. Res.*, *88C*, 10865–10882, 1983.
- Guthrie, J. P. Hydration of carboxylic acids and esters. Evaluation of the free energy change for addition of water to acetic and formic acids and their methyl esters. *J. Am. Chem. Soc.*, *95*, 6999–7003, 1973.

- Hales, J. M. and D. R. Drewes. Solubility of ammonia in water at low concentrations. *Atmos. Environ.*, *13*, 1133–1147, 1979.
- Hales, J. M. and S. L. Sutter. Solubility of sulfur dioxide in water at low concentrations. *Atmos. Environ.*, *7*, 997–1001, 1973.
- Hamm, S., J. Hahn, G. Helas, and P. Warneck. Acetonitrile in the troposphere: residence time due to rainout and uptake by the ocean. *Geophys. Res. Lett.*, *11*, 1207–1210, 1984.
- Hansen, K. C., Z. Zhou, C. L. Yaws, and T. M. Aminabhavi. Determination of Henry's law constants of organics in dilute aqueous solutions. *J. Chem. Eng. Data*, *38*, 546–550, 1993.
- Hansen, K. C., Z. Zhou, C. L. Yaws, and T. M. Aminabhavi. A laboratory method for the determination of Henry's law constants of volatile organic chemicals. *J. Chem. Educ.*, *72*, 93–96, 1995.
- Hanson, D. R., J. B. Burkholder, C. J. Howard, and A. R. Ravishankara. Measurement of OH and HO₂ radical uptake coefficients on water and sulfuric acid surfaces. *J. Phys. Chem.*, *96*, 4979–4985, 1992.
- Hanson, D. R. and A. R. Ravishankara. The reaction probabilities of ClONO₂ and N₂O₅ on 40 to 75% sulfuric acid solutions. *J. Geophys. Res.*, *96D*, 17 307–17 314, 1991.
- Hartkopf, A. and B. L. Karger. Study of the interfacial properties of water by gas chromatography. *Acc. Chem. Res.*, *6*, 209–216, 1973.
- Hassett, J. P. and E. Milicic. Determination of equilibrium and rate constants for binding of a polychlorinated biphenyl congener by dissolved humic substances. *Environ. Sci. Technol.*, *19*, 638–643, 1985.
- Hauff, K., R. G. Fischer, and K. Ballschmiter. Determination of C₁-C₅ alkyl nitrates in rain, snow, white frost, and tap water by a combined codistillation head-space gas chromatography technique. Determination of Henry's law constants by head-space GC. *Chemosphere*, *37*, 2599–2615, 1998.
- Hempel, W. Ueber Kohlenoxysulfid. *Z. Angew. Chem.*, *14*, 865–868, 1901.
- Heron, G., T. H. Christensen, and C. G. Enfield. Henry's law constant for trichloroethylene between 10 and 95 °C. *Environ. Sci. Technol.*, *32*, 1433–1437, 1998.
- Hill, J. O., I. G. Worsley, and L. G. Hepler. Calorimetric determination of the distribution coefficient and thermodynamic properties of bromine in water and carbon tetrachloride. *J. Phys. Chem.*, *72*, 3695–3697, 1968.
- Hine, J. and P. K. Mookerjee. The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. *J. Org. Chem.*, *40*, 292–298, 1975.
- Hine, J. and R. D. Weimar, Jr. Carbon basicity. *J. Am. Chem. Soc.*, *87*, 3387–3396, 1965.
- Hoff, J. T., D. Mackay, R. Gillham, and W. Y. Shiu. Partitioning of organic chemicals at the air-water interface in environmental systems. *Environ. Sci. Technol.*, *27*, 2174–2180, 1993.
- Hoffmann, M. R. and D. J. Jacob. Kinetics and mechanisms of the catalytic oxidation of dissolved sulfur dioxide in aqueous solution: An application to nighttime fog water chemistry. In J. G. Calvert, editor, *SO₂, NO and NO₂ Oxidation Mechanisms: Atmospheric Considerations*, pages 101–172. Butterworth Publishers, Boston, MA, 1984.
- Holdren, M. W., C. W. Spicer, and J. M. Hales. Peroxyacetyl nitrate solubility and decomposition rate in acidic water. *Atmos. Environ.*, *18*, 1171–1173, 1984.
- Holzwarth, G., R. G. Balmer, and L. Soni. The fate of chlorine and chloramines in cooling towers. *Wat. Res.*, *18*, 1421–1427, 1984.
- Hough, A. M. Development of a two-dimensional global tropospheric model: Model chemistry. *J. Geophys. Res.*, *96D*, 7325–7362, 1991.
- Howe, G. B., M. E. Mullins, and T. N. Rogers. Evaluation and prediction of Henry's law constants and aqueous solubilities for solvents and hydrocarbon fuel components. Vol. 2. Experimental Henry's law data. Tech. Rep. NTIS ADA-202-262/3, Research Triangle Institute for Engineering and Services Lab., Air Force Engineering and Services Center, Research Triangle Park, NC, USA, 1987.
- Hoyt, S. D. *The ocean-air exchange of carbonyl sulfide (OCS) and halocarbons*. Ph.D. thesis, Oregon Graduate Center, 1982.
- Hunter-Smith, R. J., P. W. Balls, and P. S. Liss. Henry's law constants and the air-sea exchange of various low molecular weight halocarbon gases. *Tellus*, *35B*, 170–176, 1983.
- Huthwelker, T., S. L. Clegg, T. Peter, K. Carslaw, B. P. Luo, and P. Brimblecombe. Solubility of HOCl in water and aqueous H₂SO₄ to stratospheric temperatures. *J. Atmos. Chem.*, *21*, 81–95, 1995.
- Hwang, H. and P. G. Dasgupta. Thermodynamics of the hydrogen peroxide-water system. *Environ. Sci. Technol.*, *19*, 255–258, 1985.
- Iraci, L. T., B. M. Baker, G. S. Tyndall, and J. J. Orlando. Measurements of the Henry's law coefficients of 2-methyl-3-butenol, methacrolein, and methylvinyl ketone. *J. Atmos. Chem.*, 1998. (submitted).
- Irrmann, F. ? *Chem.-Ing.-Tech.*, *37*, 789, 1965.
- Jacob, D. J. Chemistry of OH in remote clouds and its role in the production of formic acid and peroxymonosulfate. *J. Geophys. Res.*, *91D*, 9807–9826, 1986.
- Jacob, D. J., E. W. Gottlieb, and M. J. Prather. Chemistry of a polluted cloudy boundary layer. *J. Geophys. Res.*, *94D*, 12 975–13 002, 1989.
- Janini, G. M. and L. A. Quaddora. Determination of activity coefficients of oxygenated hydrocarbons by liquid-liquid chromatography. *J. Liq. Chromatogr.*, *9*, 39–53, 1986.
- Jenkins, J. and M. B. King. Vapor-liquid equilibria for the system bromine/water at low bromine concentrations. *Chem. Eng. Sci.*, *20*, 921–922, 1965.
- Johnson, B. J. *The carbon isotope content and concentration of ambient formic acid and acetic acid*. Ph.D. thesis, University of Arizona, Tucson, AZ, USA, 1990.
- Johnson, B. J., E. A. Betterton, and D. Craig. Henry's law coefficients of formic and acetic acids. *J. Atmos. Chem.*, *24*, 113–119, 1996.

- Kames, J. and U. Schurath. Alkyl nitrates and bifunctional nitrates of atmospheric interest: Henry's law constants and their temperature dependencies. *J. Atmos. Chem.*, *15*, 79–95, 1992.
- Kames, J. and U. Schurath. Henry's law and hydrolysis-rate constants for peroxyacyl nitrates (PANs) using a homogeneous gas-phase source. *J. Atmos. Chem.*, *21*, 151–164, 1995.
- Kames, J., S. Schweighoefer, and U. Schurath. Henry's law constant and hydrolysis of peroxyacetyl nitrate (PAN). *J. Atmos. Chem.*, *12*, 169–180, 1991.
- Kanakidou, M., F. J. Dentener, and P. J. Crutzen. A global three-dimensional study of the fate of HCFCs and HFC – 134a in the troposphere. *J. Geophys. Res.*, *100D*, 18 781–18 801, 1995.
- Karl, T. and W. Lindinger. Henry's law constants (?). 1997. (personal communication).
- Kavanaugh, M. C. and R. R. Trussell. Design of aeration towers to strip volatile contaminants from drinking water. *J. Am. Water Works Assoc.*, *72*, 684–692, 1980.
- Keene, W. C. and J. N. Galloway. Considerations regarding sources for formic and acetic acids in the troposphere. *J. Geophys. Res.*, *91D*, 14 466–14 474, 1986.
- Keene, W. C., B. W. Mosher, D. J. Jacob, J. W. Munger, R. W. Talbot, R. S. Artz, J. R. Maben, B. C. Daube, and J. N. Galloway. Carboxylic acids in a high-elevation forested site in central Virginia. *J. Geophys. Res.*, *100D*, 9345–9357, 1995.
- Kelley, C. M. and H. V. Tartar. On the system: bromine-water. *J. Am. Chem. Soc.*, *78*, 5752–5756, 1956.
- Khan, I., P. Brimblecombe, and S. L. Clegg. The Henry's law constants of pyruvic and methacrylic acids. *Environ. Technol.*, *13*, 587–593, 1992.
- Khan, I., P. Brimblecombe, and S. L. Clegg. Solubilities of pyruvic acid and the lower (C₁-C₆) carboxylic acids. Experimental determination of equilibrium vapour pressures above pure aqueous and salt solutions. *J. Atmos. Chem.*, *22*, 285–302, 1995.
- Kieckbusch, T. G. and C. J. King. An improved method of determining vapor liquid equilibria for dilute organics in aqueous solution. *J. Chromatogr. Sci.*, *17*, 273–276, 1979.
- Koga, Y. Vapor pressures of dilute aqueous *t*-butyl alcohol: How dilute is the Henry's law region? *J. Phys. Chem.*, *99*, 6231–6233, 1995.
- Kolb, B., C. Welter, and C. Bichler. Determination of partition coefficients by automatic equilibrium headspace gas chromatography by vapor phase calibration. *Chromatographia*, *34*, 235–240, 1992.
- Kosak-Channing, L. F. and G. R. Helz. Solubility of ozone in aqueous solutions of 0–0.6 M ionic strength at 5–30 °C. *Environ. Sci. Technol.*, *17*, 145–149, 1983.
- Krop, H. B., M. J. M. van Velzen, J. R. Parsons, and H. A. J. Govers. *n*-Octanol-water partition coefficients, aqueous solubilities and Henry's law constants of fatty acid esters. *Chemosphere*, *34*, 107–119, 1997.
- Kruis, A. and A. May. Lösungsgleichgewichte von Gasen mit Flüssigkeiten. In K. Schäfer and E. Lax, editors, *Landolt-Börnstein II/2b*, pages (1–1)–(1–210). Springer Verlag, Berlin, 1962.
- Kucklick, J. R., D. A. Hinckley, and T. F. Bidleman. Determination of Henry's law constants for hexachlorocyclohexanes in distilled water and artificial seawater as a function of temperature. *Mar. Chem.*, *34*, 197–209, 1991.
- Lamarche, P. and R. L. Droste. Air stripping mass transfer correlations for volatile organics. *J. Am. Water Works Assoc.*, *81*, 78–89, 1989.
- Ledbury, W. and E. W. Blair. The partial formaldehyde vapour pressures of aqueous solutions of formaldehyde. Part II. *J. Chem. Soc.*, *127*, 2832–2839, 1925.
- Lee, Y.-N. and S. E. Schwartz. Reaction kinetics of nitrogen dioxide with liquid water at low partial pressure. *J. Phys. Chem.*, *85*, 840–848, 1981.
- Leighton, D. T. and J. M. Calo. Distribution coefficients of chlorinated hydrocarbons in dilute air-water systems for groundwater contamination applications. *J. Chem. Eng. Data*, *26*, 382–385, 1981.
- Lelieveld, J. and P. J. Crutzen. The role of clouds in tropospheric photochemistry. *J. Atmos. Chem.*, *12*, 229–267, 1991.
- Leuenberger, C., M. P. Ligocki, and J. F. Pankow. Trace organic compounds in rain: 4. Identities, concentrations, and scavenging mechanisms for phenols in urban air and rain. *Environ. Sci. Technol.*, *19*, 1053–1058, 1985.
- Lide, D. R. and H. P. R. Frederikse, editors. *CRC Handbook of Chemistry and Physics, 76th Edition*. CRC Press, Inc., Boca Raton, FL, 1995.
- Lincoff, A. H. and J. M. Gossett. The determination of Henry's law constant for volatile organics by equilibrium partitioning in closed systems. In W. Brutsaert and G. H. Jirka, editors, *Gas transfer at water surfaces*, pages 17–25. D. Reidel Publishing Company, Dordrecht-Holland, 1984.
- Lind, J. A. and G. L. Kok. Henry's law determinations for aqueous solutions of hydrogen peroxide, methylhydroperoxide, and peroxyacetic acid. *J. Geophys. Res.*, *91D*, 7889–7895, 1986.
- Lind, J. A. and G. L. Kok. Correction to “Henry's law determinations for aqueous solutions of hydrogen peroxide, methylhydroperoxide, and peroxyacetic acid” by John A. Lind and Gregory L. Kok. *J. Geophys. Res.*, *99D*, 21 119, 1994.
- Liss, P. S. and P. G. Slater. Flux of gases across the air-sea interface. *Nature*, *247*, 181–184, 1974.
- Loomis, A. G. Solubilities of gases in water. In E. W. Washburn, C. J. West, N. E. Dorsey, F. R. Bichowsky, and A. Klemenc, editors, *International Critical Tables of Numerical Data, Physics, Chemistry and Technology, Vol. III*, pages 255–261. McGraw-Hill, Inc., 1928.
- Lovelock, J. E., R. J. Maggs, and R. A. Rasmussen. Atmospheric dimethyl sulphide and the natural sulphur cycle. *Nature*, pages 452–453, 1972.
- Luke, W. T., R. R. Dickerson, and L. J. Nunnermacker. Direct measurements of the photolysis rate coefficients and Henry's law constants of several alkyl nitrates. *J. Geophys. Res.*, *94D*, 14 905–14 921, 1989.
- Lüttke, J. and K. Levsen. Phase partitioning of phenol and nitrophenols in clouds. *Atmos. Environ.*, *31*, 2649–2655, 1997.

- Maahs, H. G. Sulfur-dioxide/water equilibria between 0 ° and 50 °C. An examination of data at low concentrations. In D. R. Schryer, editor, *Heterogeneous Atmospheric Chemistry, Geophysical Monograph 26*, pages 187–195. Am. Geophys. Union, Washington, D.C., 1982.
- Mackay, D. and W. Y. Shiu. A critical review of Henry's law constants for chemicals of environmental interest. *J. Phys. Chem. Ref. Data*, 10, 1175–1199, 1981.
- Mackay, D., W. Y. Shiu, and K. C. Ma. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*, volume I of *Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs*. Lewis Publishers, Boca Raton, 1992a.
- Mackay, D., W. Y. Shiu, and K. C. Ma. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*, volume II of *Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans*. Lewis Publishers, Boca Raton, 1992b.
- Mackay, D., W. Y. Shiu, and K. C. Ma. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*, volume III of *Volatile Organic Chemicals*. Lewis Publishers, Boca Raton, 1993.
- Mackay, D., W. Y. Shiu, and K. C. Ma. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*, volume IV of *Oxygen, Nitrogen, and Sulfur Containing Compounds*. Lewis Publishers, Boca Raton, 1995.
- Mackay, D., W. Y. Shiu, and R. P. Sutherland. Determination of air-water Henry's law constants for hydrophobic pollutants. *Environ. Sci. Technol.*, 13, 333–337, 1979.
- Marsh, A. R. W. and W. J. McElroy. The dissociation constant and Henry's law constant of HCl in aqueous solution. *Atmos. Environ.*, 19, 1075–1080, 1985.
- Martin, L. R. Kinetic studies of sulfite oxidation in aqueous solution. In J. G. Calvert, editor, *SO₂, NO and NO₂ Oxidation Mechanisms: Atmospheric Considerations*, pages 63–100. Butterworth Publishers, Boston, MA, 1984.
- Martin, L. R. and D. E. Damschen. Aqueous oxidation of sulfur dioxide by hydrogen peroxide at low pH. *Atmos. Environ.*, 15, 1615–1621, 1981.
- McAuliffe, C. GC determination of solutes by multiple phase equilibrium. *Chem. Technol.*, 1, 46–51, 1971.
- McConnell, G., D. M. Ferguson, and C. R. Pearson. Chlorinated hydrocarbons and the environment. *Endeavour*, 34, 13–18, 1975.
- Meadows, R. W. and D. J. Spedding. The solubility of very low concentrations of carbon monoxide in aqueous solution. *Tellus*, 26, 143–149, 1974.
- Meylan, W. M. and P. H. Howard. Bond contribution method for estimating Henry's law constants. *Environ. Toxicol. Chem.*, 10, 1283–1291, 1991.
- Mirabel, P., C. George, L. Magi, and J. L. Ponche. Chapter 6.3: Gas-liquid interactions. In P. Warneck, editor, *Heterogeneous and Liquid-Phase Processes*, pages 175–181. Springer Verlag, Berlin, 1996.
- Möller, D. and G. Mauersberger. Aqueous phase chemical reaction system used in cloud chemistry modelling. In A. Flossmann, T. Cvitaš, D. Möller, and G. Mauersberger, editors, *EURO-TRAC Special Publication: Clouds: Models and Mechanisms*, pages 77–93. 1992.
- Moore, R. M., C. E. Geen, and V. K. Tait. Determination of Henry's law constants for a suite of naturally occurring halogenated methanes in seawater. *Chemosphere*, 30, 1183–1191, 1995.
- Morgan, O. M. and O. Maass. An investigation of the equilibria existing in gas-water systems forming electrolytes. *Can. J. Res.*, 5, 162–199, 1931.
- Morrison, T. J. and N. B. Johnstone. Solubilities of the inert gases in water. *J. Chem. Soc.*, pages 3441–3446, 1954.
- Mozurkewich, M. Comment on "Possible role of NO₃ in the nighttime chemistry of a cloud" by William L. Chameides. *J. Geophys. Res.*, 91D, 14 569–14 570, 1986.
- Mozurkewich, M. Mechanisms for the release of halogens from sea-salt particles by free radical reactions. *J. Geophys. Res.*, 100D, 14 199–14 207, 1995.
- Munz, C. and P. V. Roberts. Air-water phase equilibria of volatile organic solutes. *J. Am. Water Works Assoc.*, 79, 62–69, 1987.
- Murphy, T. J., M. D. Mullin, and J. A. Meyer. Equilibration of polychlorinated biphenyls and toxaphene with air and water. *Environ. Sci. Technol.*, 21, 155–162, 1987.
- Murphy, T. J., J. C. Pokojowczyk, and M. D. Mullin. ? In D. M. et al., editor, *Physical Behavior of PCBs in the Great Lakes, Chapter 3*, pages 49–58. Ann Arbor Science, Ann Arbor, Mich., 1983.
- Nicholson, B. C., B. P. Maguire, and D. B. Bursill. Henry's law constants for the trihalomethanes: Effects of water composition and temperature. *Environ. Sci. Technol.*, 18, 518–521, 1984.
- Nielsen, F., E. Olsen, and A. Fredenslund. Henry's law constants and infinite dilution activity coefficients for volatile organic compounds in water by a validated batch air stripping method. *Environ. Sci. Technol.*, 28, 2133–2138, 1994.
- Nirmalakhandan, N., R. A. Brennan, and R. E. Speece. Predicting Henry's law constant and the effect of temperature on Henry's law constant. *Wat. Res.*, 31, 1471–1481, 1997.
- Oliver, B. ? *Chemosphere*, 14, 1087–1106, 1985.
- O'Sullivan, D. W., M. Lee, B. C. Noone, and B. G. Heikes. Henry's law constant determinations for hydrogen peroxide, methyl hydroperoxide, hydroxymethyl hydroperoxide, ethyl hydroperoxide, and peroxyacetic acid. *J. Phys. Chem.*, 100, 3241–3247, 1996.
- Palmer, D. A., R. W. Ramette, and R. E. Mesmer. The hydrolysis of iodine: Equilibria at high temperatures. *J. Nucl. Mater.*, 130, 280–286, 1985.
- Pandis, S. N. and J. H. Seinfeld. Sensitivity analysis of a chemical mechanism for aqueous-phase atmospheric chemistry. *J. Geophys. Res.*, 94D, 1105–1126, 1989.
- Park, J.-Y. and Y.-N. Lee. Solubility and decomposition kinetics of nitrous acid in aqueous solution. *J. Phys. Chem.*, 92, 6294–6302, 1988.

- Parsons, G. H., C. H. Rochester, A. Rostron, and P. C. Sykes. The thermodynamics of hydration of phenols. *J. Chem. Soc. Perkin Trans. 2*, pages 136–138, 1972.
- Parsons, G. H., C. H. Rochester, and C. E. C. Wood. Effect of 4-substitution on the thermodynamics of hydration of phenol and the phenoxide anion. *J. Chem. Soc. B*, pages 533–536, 1971.
- Pearson, C. R. and G. McConnell. Chlorinated C₁ and C₂ hydrocarbons in the marine environment. *Proc. R. Soc. Lond. B*, 189, 305–332, 1975.
- Pecsar, R. E. and J. J. Martin. Solution thermodynamics from gas-liquid chromatography. *Anal. Chem.*, 38, 1661–1669, 1966.
- Peng, J. and A. Wan. Measurement of Henry's constants of high-volatility organic compounds using a headspace autosampler. *Environ. Sci. Technol.*, 31, 2998–3003, 1997.
- Perry, R. H. *Perry's Chemical Engineers' Handbook, fourth edition*. McGraw-Hill, Inc., 1963.
- Pierotti, G. J., C. H. Deal, and E. L. Derr. ? *Ind. Eng. Chem.*, 51, 95–102, 1957. (data in supplement, document no. 5782, American Documentation Institute, Library of Congress, Washington, D.C.).
- Przyjazny, A., W. Janicki, W. Chrzanowski, and R. Staszewski. Headspace gas chromatographic determination of distribution coefficients of selected organosulphur compounds and their dependence on some parameters. *J. Chromatogr.*, 280, 249–260, 1983.
- Rasmussen, R. A., S. D. Hoyt, and M. A. K. Khalil. Atmospheric carbonyl sulfide (OCS): Techniques for measurement in air and water. *Chemosphere*, 11, 869–875, 1982.
- Régimbal, J.-M. and M. Mozurkewich. Peroxynitric acid decay mechanisms and kinetics at low pH. *J. Phys. Chem. A*, 101, 8822–8829, 1997.
- Rex, A. Über die Löslichkeit der Halogenderivate der Kohlenwasserstoffe in Wasser. *Z. Phys. Chem.*, 55, 355–370, 1906.
- Rice, C. P., S. M. Chernyak, and L. L. McConnell. Henry's law constants for pesticides measured as a function of temperature and salinity. *J. Agric. Food Chem.*, 45, 2291–2298, 1997.
- Robbins, G. A., S. Wang, and J. D. Stuart. Using the headspace method to determine Henry's law constants. *Anal. Chem.*, 65, 3113–3118, 1993.
- Roberts, P. V. and P. G. Dändliker. Mass transfer of volatile organic contaminants from aqueous solutions to the atmosphere during surface aeration. *Environ. Sci. Technol.*, 17, 484–489, 1983.
- Robinson, R. A. and R. H. Stokes. *Electrolyte Solutions, 2nd ed.* Butterworth, London, 1970.
- Rochester, H. and J. R. Symonds. Thermodynamic studies of fluoroalcohols. *J. Chem. Soc. Faraday Trans. 1*, 69, 1577–1585, 1973.
- Rohrschneider, L. Solvent characterization by gas-liquid partition coefficients of selected solutes. *Anal. Chem.*, 45, 1241–1247, 1973.
- Rudich, Y., R. K. Talukdar, A. R. Ravishankara, and R. W. Fox. Reactive uptake of NO₃ on pure water and ionic solutions. *J. Geophys. Res.*, 101D, 21 023–21 031, 1996.
- Russell, C. J., S. L. Dixon, and P. C. Jurs. Computer-assisted study of the relationship between molecular structure and Henry's law constant. *Anal. Chem.*, 64, 1350–1355, 1992.
- Sagebiel, J. C., J. N. Seiber, and J. E. Woodrow. Comparison of headspace and gas-stripping methods for determining the Henry's law constant (*H*) for organic compounds of low to intermediate *H*. *Chemosphere*, 25, 1763–1768, 1992.
- Sander, R. Modeling atmospheric chemistry: Interactions between gas-phase species and liquid cloud/aerosol particles. *Surv. Geophys.*, 1999. (in press).
- Sander, R. and P. J. Crutzen. Model study indicating halogen activation and ozone destruction in polluted air masses transported to the sea. *J. Geophys. Res.*, 101D, 9121–9138, 1996.
- Sander, R., J. Lelieveld, and P. J. Crutzen. Modelling of the nighttime nitrogen and sulfur chemistry in size resolved droplets of an orographic cloud. *J. Atmos. Chem.*, 20, 89–116, 1994.
- Santl, H., R. Brandsch, and L. Gruber. Experimental determination of Henry's law constant (HLC) for some lower chlorinated dibenzodioxins. *Chemosphere*, 29, 2209–2214, 1994.
- Saxena, P. and L. M. Hildemann. Water-soluble organics in atmospheric particles: A critical review of the literature and application of thermodynamics to identify candidate compounds. *J. Atmos. Chem.*, 24, 57–109, 1996.
- Schaffer, D. L. and T. E. Daubert. Gas-liquid chromatographic determination of solution properties of oxygenated compounds in water. *Anal. Chem.*, 41, 1585–1589, 1969.
- Scheer, V., A. Frenzel, W. Behnke, C. Zetzsch, L. Magi, C. George, and P. Mirabel. Uptake of nitrosyl chloride (NOCl) by aqueous solutions. *J. Phys. Chem. A*, 101, 9359–9366, 1997.
- Schurath, U., A. Bongartz, J. Kames, C. Wunderlich, and T. Carstens. Chapter 6.4: Laboratory determination of physico-chemical rate parameters pertinent to mass transfer into cloud and fog droplets. In P. Warneck, editor, *Heterogeneous and Liquid-Phase Processes*, pages 182–189. Springer Verlag, Berlin, 1996.
- Schwartz, S. E. Gas- and aqueous-phase chemistry of HO₂ in liquid water clouds. *J. Geophys. Res.*, 89D, 11 589–11 598, 1984.
- Schwartz, S. E. and W. H. White. Solubility equilibria of the nitrogen oxides and oxyacids in dilute aqueous solution. In J. R. Pfaflin and E. N. Ziegler, editors, *Advances in Environmental Science and Engineering*, volume 4, pages 1–45. Gordon and Breach Science Publishers, NY, 1981.
- Schwarzenbach, R. P., R. Stierli, B. R. Folsom, and J. Zeyer. Compound properties relevant for assessing the environmental partitioning of nitrophenols. *Environ. Sci. Technol.*, 22, 83–92, 1988.
- Seinfeld, J. H. *Atmospheric Chemistry and Physics of Air Pollution*. Wiley-Interscience Publication, NY, 1986.
- Seinfeld, J. H. and S. N. Pandis. *Atmospheric Chemistry and Physics*. John Wiley & Sons, Inc., 1998.
- Servant, J., G. Kouadio, B. Cros, and R. Delmas. Carboxylic monoacids in the air of Mayombe Forest (Congo): Role of the forest as a source or sink. *J. Atmos. Chem.*, 12, 367–380, 1991.

- Shepson, P. B., E. Mackay, and K. Muthuramu. Henry's law constants and removal processes for several atmospheric β -hydroxy alkyl nitrates. *Environ. Sci. Technol.*, *30*, 3618–3623, 1996.
- Shiu, W. Y., W. Doucette, F. A. P. C. Gobas, A. Andren, and D. Mackay. Physical-chemical properties of chlorinated dibenzo-p-dioxins. *Environ. Sci. Technol.*, *22*, 651–658, 1988.
- Shiu, W.-Y., K.-C. Ma, D. Varhanícková, and D. Mackay. Chlorophenols and alkylphenols: A review and correlation of environmentally relevant properties and fate in an evaluative environment. *Chemosphere*, *29*, 1155–1224, 1994.
- Signer, R., H. Arm, and H. Daenicker. Dampfdrücke, Dichten, thermodynamische Mischfunktionen und Brechungsindices der binären Systeme Wasser-Tetrahydrofuran und Wasser-Diäthyläther bei 25 °. *Helv. Chim. Acta*, *52*, 2347–2351, 1969.
- Sillen, L. G. and A. E. Martell. *Stability constants of metal-ion complexes*, volume Spec. Publ. 17. The Chemical Society, London, 1964.
- Smith, R. M. and A. E. Martell. *Critical Stability Constants. Vol. 4: Inorganic Complexes*. Plenum Press, New York, 1976.
- Snider, J. R. and G. A. Dawson. Tropospheric light alcohols, carbonyls, and acetonitrile: Concentrations in the southwestern United States and Henry's law data. *J. Geophys. Res.*, *90D*, 3797–3805, 1985.
- Staffelbach, T. A. and G. L. Kok. Henry's law constants for aqueous solutions of hydrogen peroxide and hydroxymethyl hydroperoxide. *J. Geophys. Res.*, *98D*, 12 713–12 717, 1993.
- Staudinger, J. and P. V. Roberts. A critical review of Henry's law constants for environmental applications. *Crit. Rev. Environ. Sci. Technol.*, *26*, 205–297, 1996.
- Stock, A. and E. Kuss. ? *Ber. Dtsch. Chem. Ges.*, *50*, 159, 1917.
- Suleimenov, O. M. and R. E. Krupp. Solubility of hydrogen sulfide in pure water and in NaCl solutions, from 20 to 320 °C and at saturation pressures. *Geochim. Cosmochim. Acta*, *58*, 2433–2444, 1994.
- Tancrede, M. V. and Y. Yanagisawa. An analytical method to determine Henry's law constant for selected volatile organic compounds at concentrations and temperatures corresponding to tap water use. *J. Air. Waste Manage. Assoc.*, *40*, 1658–1663, 1990.
- tenHulscher, T. E. M., L. E. van der Velde, and W. A. Bruggeman. Temperature dependence of Henry's law constants for selected chlorobenzenes, polychlorinated biphenyls and polycyclic aromatic hydrocarbons. *Environ. Toxicol. Chem.*, *11*, 1595–1603, 1992.
- Thomas, K., A. Volz-Thomas, and D. Kley. *Zur Wechselwirkung von NO₃-Radikalen mit wässrigen Lösungen: Bestimmung des Henry- und des Massenakkommodationskoeffizienten*. Ph.D. thesis, Institut für Chemie und Dynamik der Geosphäre 2, Forschungszentrum Jülich GmbH, FRG, 1993.
- Thomas, K., A. Volz-Thomas, D. Mihelcic, H. G. J. Smit, and D. Kley. On the exchange of NO₃ radicals with aqueous solutions: Solubility and sticking coefficient. *J. Atmos. Chem.*, *29*, 17–43, 1998.
- Thompson, A. M. and O. C. Zafiriou. Air-sea fluxes of transient atmospheric species. *J. Geophys. Res.*, *88C*, 6696–6708, 1983.
- Timmermans, J. *The Physico-Chemical Constants of Binary Systems in Concentrated Solutions, Vol. 4*. Interscience Publisher, Inc., New York, NY, 1960.
- Trempp, J., P. Mattrel, S. Fingler, and W. Giger. Phenols and nitrophenols as tropospheric pollutants - emissions from automobile exhausts and phase-transfer in the atmosphere. *Water Air Soil Pollut.*, *68*, 113–123, 1993.
- Tse, G., H. Orbey, and S. I. Sandler. Infinite dilution activity coefficients and Henry's law coefficients of some priority water pollutants determined by a relative gas chromatographic method. *Environ. Sci. Technol.*, *26*, 2017–2022, 1992.
- USEPA. Air and steam stripping of toxic pollutants. Tech. Rep. EPA-68-03-002, Industrial Environmental Research Laboratory, Cincinnati, OH, USA, 1982.
- Van Krevelen, D. W., P. J. Hoftijzer, and F. J. Huntjens. Composition and vapor pressures of aqueous solutions of ammonia, carbon dioxide and hydrogen sulfide. *Recl. Trav. Chim. Pays-Bas*, *68*, 191, 1949.
- Villalta, P. W., E. R. Lovejoy, and D. R. Hanson. Reaction probability of peroxyacetyl radical on aqueous surfaces. *Geophys. Res. Lett.*, *23*, 1765–1768, 1996.
- Vitenberg, A. G., B. V. Ioffe, and V. N. Borisov. ? *Chromatographia*, *7*, 610, 1974. (see also *Zh. Anal. Khim.*, *29*, 1795 (1974)).
- Vitenberg, A. G., B. V. Ioffe, Z. S. Dimitrova, and I. L. Butaeva. Determination of gas-liquid partition coefficients by means of gas chromatographic analysis. *J. Chromatogr.*, *112*, 319–327, 1975.
- Vogt, R., P. J. Crutzen, and R. Sander. A mechanism for halogen release from sea-salt aerosol in the remote marine boundary layer. *Nature*, *383*, 327–330, 1996.
- Wagman, D. D., W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall. The NBS tables of chemical thermodynamic properties; Selected values for inorganic and C₁ and C₂ organic substances in SI units. *J. Phys. Chem. Ref. Data*, *11*, suppl. 2, 1982.
- Wang, T. X., M. D. Kelley, J. N. Cooper, R. C. Beckwith, and D. W. Margerum. Equilibrium, kinetic, and UV-spectral characteristics of aqueous bromine chloride, bromine, and chlorine species. *Inorg. Chem.*, *33*, 5872–5878, 1994.
- Warneck, P. *Chemistry of the Natural Atmosphere*. Acad., San Diego, CA, 1988.
- Warneck, P., P. Mirabel, G. A. Salmon, R. van Eldik, C. Vinckier, K. J. Wannowius, and C. Zetzsch. Chapter 2: Review of the activities and achievements of the EUROTRAC subproject HALIPP. In P. Warneck, editor, *Heterogeneous and Liquid-Phase Processes*, pages 7–74. Springer Verlag, Berlin, 1996.
- Wasik, S. P. and W. Tsang. Gas chromatographic determination of partition coefficients of some unsaturated hydrocarbons and their deuterated isomers in aqueous silver nitrate solutions. *J. Phys. Chem.*, *74*, 2970–2976, 1970.
- Watts, S. F. and P. Brimblecombe. The Henry's law constant of dimethyl sulphoxide. *Environ. Technol. Lett.*, *8*, 483–486, 1987.

- Weinstein-Lloyd, J. and S. E. Schwartz. Low-intensity radiolysis study of free-radical reactions in cloudwater: H_2O_2 production and destruction. *Environ. Sci. Technol.*, *25*, 791–800, 1991.
- Westcott, J. W., C. G. Simon, and T. F. Bidleman. Determination of polychlorinated biphenyl vapor pressures by a semimicro gas saturation method. *Environ. Sci. Technol.*, *15*, 1375–1378, 1981.
- Westheimer, F. H. and L. L. Ingraham. The entropy of chelation. *J. Phys. Chem.*, *60*, 1668–1670, 1956.
- Wilhelm, E., R. Battino, and R. J. Wilcock. Low-pressure solubility of gases in liquid water. *Chem. Rev.*, *77*, 219–262, 1977.
- Winiwarter, W., H. Puxbaum, S. Fuzzi, M. C. Facchini, G. Orsi, N. Beltz, K.-H. Enderle, and W. Jaeschke. Organic acid gas and liquid-phase measurements in Po valley fall-winter conditions in the presence of fog. *Tellus*, *40B*, 348–357, 1988.
- Winkler, L. W. Löslichkeit des Broms in Wasser. *Chem. Ztg.*, *23*, 687–689, 1899.
- Winkler, L. W. Gesetzmässigkeit bei der Absorption der Gase in Flüssigkeiten. *Z. Phys. Chem.*, *55*, 344–354, 1906.
- Winkler, L. W. ?*Math. Termesz. Ertesitö*, *25*, 86, 1907.
- Wong, P. K. and Y. H. Wang. Determination of the Henry's law constant for dimethyl sulfide in seawater. *Chemosphere*, *35*, 535–544, 1997.
- Wright, D. A., S. I. Sandler, and D. DeVoll. Infinite dilution activity coefficients and solubilities of halogenated hydrocarbons in water at ambient temperatures. *Environ. Sci. Technol.*, *26*, 1828–1831, 1992a.
- Wright, D. A., S. I. Sandler, and D. DeVoll. Infinite dilution activity coefficients and solubilities of halogenated hydrocarbons in water at ambient temperatures. *Environ. Sci. Technol.*, *26*, 1828–1831, 1992b.
- Yaws, C. L. and H.-C. Yang. Henry's law constant for compound in water. In C. L. Yaws, editor, *Thermodynamic and Physical Property Data*, pages 181–206. Gulf Publishing Company, Houston, TX, 1992.
- Yin, C. and J. P. Hassett. Gas-partitioning approach for laboratory and field studies of mirex fugacity in water. *Environ. Sci. Technol.*, *20*, 1213–1217, 1986.
- Yoshizumi, K., K. Aoki, I. Nouchi, T. Okita, T. Kobayashi, S. Kamakura, and M. Tajima. Measurements of the concentration in rainwater and of the Henry's law constant of hydrogen peroxide. *Atmos. Environ.*, *18*, 395–401, 1984.
- Zafiriou, O. C. and M. McFarland. Determination of trace levels of nitric oxide in aqueous solution. *Anal. Chem.*, *52*, 1662–1667, 1980.
- Zheng, D.-Q., T.-M. Guo, and H. Knapp. Experimental and modeling studies on the solubility of CO_2 , CHClF_2 , CHF_3 , $\text{C}_2\text{H}_2\text{F}_4$ and $\text{C}_2\text{H}_4\text{F}_2$ in water and aqueous NaCl solutions under low pressures. *Fluid Phase Equilib.*, *129*, 197–209, 1997.
- Zhou, X. and Y.-N. Lee. Aqueous solubility and reaction kinetics of hydroxymethyl hydroperoxide. *J. Phys. Chem.*, *96*, 265–272, 1992.
- Zhou, X. and K. Mopper. Apparent partition coefficients of 15 carbonyl compounds between air and seawater and between air and freshwater; Implications for air-sea exchange. *Environ. Sci. Technol.*, *24*, 1864–1869, 1990.

Sander, R., 1999, Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry, version 3, 8 Apr 1999
<http://www.mpch-mainz.mpg.de/~sander/res/henry.html>

Errata (collected from the above web site 4 June 2003)

Well, I knew it would happen... A big list like this just couldn't be perfect. I have now added a list of errors that I have made in my compilation.

Errata for version 3 (17 Feb 99)

In note 20, the solubility for strong acids should be defined as:

$$kH = ([H^+] * [A^-]) / p(HA)$$

and NOT

$$kH = ([H^+] + [A^-]) / p(HA)$$

Thanks to J. C. Wheeler for pointing this out to me.

There's a nasty little error in the sign of the temperature dependence in all tables: The values given in the third column are

$$d \ln kH / d (1/T)$$

and NOT

$$- d \ln kH / d (1/T)$$

The solubility decreases with increasing temperature, of course. This is shown correctly in equation (5) on page 3.

Data from Allen et al. (1998) are measured, not estimated.

The reference Gmehling et al. (1981) should be: J. Gmehling and U. Onken and W. Arlt. Vapor-Liquid Equilibrium Data Collection. D. Behrens and R. Eckermann (eds.). Dechema, Frankfurt/Main Vol. 1a (1981)