

Physicochemical Properties of Higher Nonaromatic Hydrocarbons: A Literature Study

Eric M. J. Verbruggen,^{a)} Joop L. M. Hermens, and Johannes Tolls

Research Institute of Toxicology, Utrecht University, P.O. Box 80176, 3508 TD Utrecht, The Netherlands

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Few data are available on the behavior of higher aliphatic hydrocarbons in the environment and especially in relation to hydrophobicity. Sorption to soil and bioconcentration by aquatic organisms are examples of processes that can be estimated from hydrophobicity parameters, such as aqueous solubility and octanol-water partition coefficient. A literature study was carried out on these physicochemical properties of aliphatic hydrocarbons containing ten or more carbon atoms. In general, very few experimental data were found, probably as a consequence of the fact that these parameters are very difficult to determine for these compounds. Reliable data on hydrophobicity parameters, for example, were not found for *n*-alkanes higher than tridecane. © 2001 American Institute of Physics. [S0047-2689(00)00206-3]

Key words: aliphatic hydrocarbons; alkanes; aqueous solubility; Henry's law constant; K_{oa} ; K_{ow} ; molar volume; vapor pressure.

Contents

1. Introduction.....	1435
2. Molar Volume at Boiling Point (V_b).....	1436
3. Molecular Weight (M), Boiling Point (T_b), Melting Point (T_m), and Density (ρ).....	1436
4. Aqueous Solubility (S).....	1436
5. Octanol-Water Partition Coefficient (K_{ow}).....	1442
6. Vapor Pressure (p).....	1443
7. Henry's Law Constant (H) and octanol-air partition coefficient (K_{oa}).....	1443
8. Concluding Remarks.....	1444
9. Acknowledgment.....	1445
10. References.....	1445

List of Tables

1. Data on molecular weight (M), boiling point (T_b), melting point (T_m), and density (ρ) and calculated molar volume at boiling point (V_b) for aliphatic hydrocarbons.....	1437
2. Vapor pressure (p), solubility (S), and $\log K_{ow}$ for aliphatic hydrocarbons.....	1439
3. Selected values for aliphatic hydrocarbons containing ten or more carbon atoms.....	1444
4. Linear regression relationships between molar volume [ml/mole] [estimated by Eq. (1)] and the logarithms of solubility [M], K_{ow} [$m_{water}^3/m_{octanol}^3$], vapor pressure [Pa], Henry's law constant (estimated) [m_{water}^3/m_{air}^3] and K_{oa} (estimated) [$m_{air}^3/m_{octanol}^3$] for liquid aliphatic	

hydrocarbons (at 25 °C).....	1445
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List of Figures

1. Literature data on aqueous solubility or accommodation for linear, branched, and cycloalkanes expressed as a function of the molar volume.....	1441
2. Literature data on aqueous solubility for aliphatic hydrocarbons expressed as a function of molar volume.....	1442
3. Literature data on $\log K_{ow}$ for <i>n</i> -alkanes expressed as a function of the molar volume.....	1443
4. Literature data on $\log K_{ow}$ for aliphatic hydrocarbons expressed as a function of the molar volume.....	1443
5. Literature data on vapor pressure (p) for linear, branched, and cycloalkanes expressed as a function of the molar volume.....	1443
6. Literature data on vapor pressure (p) for aliphatic hydrocarbons expressed as a function of the molar volume.....	1443
7. Estimated Henry's law constant (H) for linear, branched, and cycloalkanes expressed as a function of the molar volume.....	1444
8. Estimated Henry's law constant (H) for aliphatic hydrocarbons expressed as a function of the molar volume.....	1444
9. Estimated octanol-air partition coefficients (K_{oa}) for aliphatic hydrocarbons expressed as a function of the molar volume.....	1444

1. Introduction

Hydrophobicity is an important physicochemical property in environmental chemistry and toxicology. The octanol-water partition coefficient (K_{ow}), aqueous solubility (S) or

^{a)}Present working address: National Institute of Public Health and the Environment (RIVM), P.O. Box 1, 3720 BA Bilthoven, The Netherlands; Tele: +31 30 274 36 57; Fax: +31 30 274 54 77; Electronic mail: eric.verbruggen@rivm.nl

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reversed phase HPLC capacity factors (k') are parameters that are often used to reflect the hydrophobicity. Environmental partition coefficients can be related to one of these parameters and many correlations of bioconcentration factors (BCF)¹⁻⁴ and sediment or soil sorption partition coefficients^{5,6} with hydrophobicity can be found in the literature. Consequently, hydrophobicity is a very important parameter in exposure assessment and fate-modeling.^{7,8} In the absence of biological transformation, differences in lethal aqueous concentrations can be largely explained by differences in bioconcentration factors for compounds with no specific mode of action (narcotic compounds), such as most aliphatic hydrocarbons.^{9,10} Consequently, strong correlations between aqueous effect concentrations and hydrophobicity have been found.^{11,12}

Another important parameter in the environment is the air-water partition coefficient or Henry's law constant (H or HLC). This parameter is approximated by the quotient of two physicochemical properties, vapor pressure and solubility, and may be used to estimate the rate of volatilization from the aqueous phase. Therefore this is also a parameter important in exposure assessment and fate modeling. Another important process is the partitioning of a compound between a hydrophobic phase and air. This process is reflected by the octanol-air partition coefficient (K_{oa}), which can be estimated from the quotient of K_{ow} and H .

A literature study was carried out to investigate the physicochemical properties of nonaromatic hydrocarbons, containing ten or more carbon atoms. Several sources were used, including literature search systems and databases on compound properties, e.g., Shaw^{13,14} and Mackay *et al.*¹⁵ The results of the literature study are presented below. Because of the scarce data on compounds containing ten or more carbon atoms, data on lower hydrocarbons are also considered in order to identify trends. For this purpose, data on parameters are related to molar volume.

2. Molar Volume at Boiling Point (V_b)

Solubilities and partition coefficients are determined by the free energy of the transition from one phase to another. For homologous series of compounds that differ in molecular volume, such as alkanes, this free energy depends on the size of the solute molecules. Therefore partition coefficients and solubilities are often related to the molecular volume.¹⁶

At the boiling point of a compound, the specific interactions between molecules are almost reduced to zero, and the molar volume is a good representative of the molecular volume. Because the molar volume at the boiling point can be derived from other easily accessible parameters, it was used to compare solubilities and partition coefficients of different compounds. The molar volume at the boiling point was calculated using Grain's equation (as given by Nelken¹⁷):

$$V_b = \frac{M \cdot \left(3 - 2 \frac{T}{T_b}\right)^{0.29}}{\rho_L} \quad (1)$$

In this equation, V_b is the molar volume at the boiling point, M is the molecular weight [g/mol], ρ_L is the density of the liquid hydrocarbon [g/ml] at temperature T [K], T_b is the boiling point [K], and 0.29 is a constant, which is specific for hydrocarbons. If one of these values was missing, the value estimated by ASTER was used,¹⁸ calculated according to Schroeder's method, which has an average error of 3.4%.¹⁷ This method calculates the molar volume from the molecular structure by means of fragment constants.¹⁷ Schroeder's method and Grain's equation give similar values for molar volume (average difference 1.7%).

3. Molecular Weight (M), Boiling Point (T_b), Melting Point (T_m) and Density (ρ)

Data on molecular weight, boiling point, melting point, and density were retrieved from databases^{18,19} and are tabulated in Table 1. All values for boiling point, melting point, and density from these data sources originate from experimental data. Some of these parameters were used to calculate the molar volume as described above.

4. Aqueous Solubility (S)

Data on aqueous solubility were found for many hydrocarbons, including straight-chain, branched, unsaturated, and cyclic structures. The number of compounds with more than ten carbon atoms for which solubility data are available is very limited (13, 11 of which are *n*-alkanes). To observe trends in solubility, the lower hydrocarbons are also taken into account in Table 2.

Literature values for *n*-alkane aqueous solubility²⁰⁻³⁰ are presented in Fig. 1, as a function of the molar volume. Up to molar volumes of 310 ml/mol, each increase of 21.5 ml/mol in molar volume in this series represents an increase of one carbon atom. Data are included for all alkanes from C_1 to C_{14} . From C_{16} to C_{28} , data are available for alkanes with an even number of carbon atoms and one more data point is included for C_{36} .

Peake and Hodgson³⁰ used several filter sizes to filter the aqueous phase of shake-flask experiments before analysis. The data of C_{12} , C_{20} , C_{22} , C_{24} , and C_{28} using the smallest filter pore size are included in Fig. 1. Peake and Hodgson^{28,30} conclude that the filter pore size has a large influence on the amount of hydrocarbon in water for hydrocarbons containing more than ten carbon atoms. This reflects a change from true aqueous solubility for the lower alkanes to a colloidal accommodation for the higher alkanes, as is also indicated by several other authors.^{24,27,29}

The accommodated amounts in water of C_{12} and C_{20} at 22 °C from Peake and Hodgson³⁰ are still 3 and 5 times higher than the values at 25 °C reported by Sutton and Calder.²⁹ Sutton and Calder used a filter pore size of 0.45 μm and they allowed the dispersed droplets to rise to the surface for 24 h after filtration. The filter pore size used by Peake and Hodgson was 0.05 μm but colloids were allowed

TABLE 1. Data on molecular weight (M), boiling point (T_b), melting point (T_m), and density (ρ) and calculated molar volume at boiling point (V_b) for aliphatic hydrocarbons.

Compound name	M [g/mol]	T_m [°C]	T_b [°C]	ρ [kg/l]	at °C	V_b^a [ml/mol]	V_b^b [ml/mol]
<i>n-Alkanes</i>							
Methane	16.04	-182.4	-161.5	0.4228	-162	35	38
Ethane	30.07	-182.8	-88.6	0.5446	-89	56	55
Propane	44.10	-189.7	-42.1	0.493	25	77	70
Butane	58.12	-138.2	-0.5	0.573	25	98	96
Pentane	72.15	-129.7	36.0	0.6262	20	119	119
Hexane	86.18	-95.3	68.7	0.6548	25	140	141
Heptane	100.20	-90.6	98.5	0.6837	20	161	162
Octane	114.23	-56.8	125.6	0.6986	25	182	184
Nonane	128.26	-53.5	150.8	0.7176	20	203	205
Decane	142.28	-29.7	174.1	0.7300	20	224	227
Undecane	156.31	-25.6	195.9	0.7402	20	245	248
Dodecane	170.34	-9.6	216.3	0.7487	20	266	270
Tridecane	184.37	-5.3	235.4	0.7564	20	287	291
Tetradecane	198.39	5.8	253.5	0.7628	20	308	313
Pentadecane	212.42	9.9	270.6	0.7685	20	329	334
Hexadecane	226.45	18.1	286.8	0.7733	20	350	356
Heptadecane	240.47	22	302.0	0.7780	20	371	377
Octadecane	254.50	28.2	316.3	0.7768	28	392	399
Nonadecane	268.53	32.1	329.9	0.7855	20	413	420
Eicosane	282.55	36.8	343	0.7886	20	434	441
Docosane	310.61	44.4	368.6	0.7944	20	476	484
Tetracosane	338.66	54	391.3	0.7991	20	518	527
Hexacosane	366.71	56.4	412.2	0.7783	60	560	578
Octacosane	394.77	64.5	431.6	0.8067	20	602	612
Hexatriacontane	506.98	76.5	497 ^c	0.7803	80	770	804
<i>Cycloalkanes</i>							
Cyclopentane	70.13	-93.8	49.3	0.7457	20	98	99
Cyclohexane	84.16	6.6	80.7	0.7785	20	119	118
Methylcyclopentane	84.16	-142.5	71.8	0.7486	20	119	121
Cycloheptane	98.19	-8.0	118.4	0.8098	20	140	136
Methylcyclohexane	98.19	-126.6	100.9	0.7694	20	140	142
Cyclooctane	112.22	14.8	149	0.8349	20	161	154
Propylcyclopentane	112.22	-117.3	131	0.7763	20	161	164
1- <i>trans</i> -4-Dimethylcyclohexane	112.22	-36.9	119.4	0.77	15	161	165
1- <i>cis</i> -2-Dimethylcyclohexane	112.22	-49.9	129.8	0.7963	20	161	160
1,1,3-Trimethylcyclopentane	112.22	-142.4	104.9	0.7439	25	161	167
1,1,3-Trimethylcyclohexane	126.24	-65.7	136.6	0.7749	25	182	185
Adamantane	136.24	268		1.07	25	161	
Decalin	138.25	-43	155.5	0.8965	22	182	177
Pentylcyclopentane	140.27	-83	180	0.7912	20	203	207
1-Methyl-4-isopropyl-cyclohexane	140.27	-87.6	170.7	0.797	25	203	204
<i>Branched alkanes</i>							
Isobutane	58.12	-138.3	-11.7	0.5510	25	98	96
Isopentane	72.15	-159.9	27.8	0.6201	20	119	118
2,2-Dimethylpropane	72.15	-16.6	9.4	0.5852	25	119	119
2-Methylpentane	86.18	-153.7	60.2	0.650	26	140	140
3-Methylpentane	86.18	-162.9	63.2	0.6598	25	140	139
2,2-Dimethylbutane	86.18	-99	49.7	0.6444	25	140	139
2,3-Dimethylbutane	86.18	-128.8	57.9	0.6616	20	140	138
2-Methylhexane	100.20	-118.2	90.0	0.6787	20	161	162
3-Methylhexane	100.20	-119	92	0.6860	20	161	161
2,2-Dimethylpentane	100.20	-123.8	79.2	0.6739	20	161	162
2,3-Dimethylpentane	100.20		89.7	0.6951	20	161	158
2,4-Dimethylpentane	100.20	-119.9	80.4	0.6727	20	161	162
3,3-Dimethylpentane	100.20	-134.9	86.0	0.6936	20	161	158
3-Methylheptane	114.23	-120	116.5	0.7075	16	182	182
2,2,4-Trimethylpentane	114.23	-107.3	99.2	0.6877	25	182	183
2,3,4-Trimethylpentane	114.23	-109.2	113.5	0.7191	20	182	178
4-Methyloctane	128.26	-113.3	142.4	0.716	25	203	204
2,2,5-Trimethylhexane	128.26	-105.7	124.0	0.7072	20	203	205

TABLE 1. Data on molecular weight (M), boiling point (T_b), melting point (T_m), and density (ρ) and calculated molar volume at boiling point (V_b) for aliphatic hydrocarbons—Continued

Compound name	M [g/mol]	T_m [°C]	T_b [°C]	ρ [kg/l]	at °C	V_b^a [ml/mol]	V_b^b [ml/mol]
<i>n-Alkenes</i>							
Ethene	28.05	-169	-103.7	0.5678	-104	49	49
Propene	42.08	-185.2	-47.6	0.505	25	70	62
1-Butene	56.11	-185.3	-6.2	0.588	25	91	88
1-Pentene	70.13	-165.2	29.9	0.6405	20	112	112
(<i>E</i>)-2-Pentene	70.13	-140.2	36.3	0.6431	25	112	111
(<i>Z</i>)-2-Pentene	70.13	-151.4	36.9	0.6556	20	112	110
1-Hexene	84.16	-139.7	63.4	0.6731	20	133	134
1-Heptene	98.19	-119.7	93.6	0.6970	20	154	155
(<i>E</i>)-2-Heptene	98.19	-109.5	98	0.7012	20	154	155
(<i>Z</i>)-2-Heptene	98.19		98.4	0.708	20	154	154
1-Octene	112.22	-101.7	121.2	0.7149	20	175	177
1-Nonene	126.24	-81.3	146.9	0.7253	25	196	199
<i>Cycloalkenes</i>							
Cyclopentene	68.12	-135.1	44.2	0.7720	20	91	92
Cyclohexene	82.15	-103.5	82.9	0.8110	20	112	111
Cycloheptene	96.17	-56	115	0.8228	20	133	131
1-Methylcyclohexene	96.17	-120.4	110.3	0.8102	20	133	133
α -Pinene	136.24	-55	156.2	0.8582	20	175	183
<i>Branched alkenes</i>							
2-Methylpropene	56.11	-140.4	-6.9	0.589	25	91	88
3-Methyl-1-butene	70.13	-168.5	20.1	0.6213	25	112	112
2-Methyl-1-pentene	84.16	-135.7	62.1	0.6799	20	133	132
4-Methyl-1-pentene	84.16	-153.6	53.9	0.6642	20	133	134
<i>Alkadi- and trienes</i>							
1,3-Butadiene	54.09	-108.9	-4.4	0.6149	25	84	82
1,4-Pentadiene	68.12	-148.8	26	0.6608	20	105	104
2-Methyl-1,3-butadiene	68.12	-145.9	34.0	0.679	20	105	103
1,5-Hexadiene	82.15	-140.7	59.4	0.6878	25	126	126
1,6-Heptadiene	96.17		90 ^c			147	
7-Methyl-3-methylene-1,6-octadiene	136.24		167	0.8013	15	203	198
<i>n-Alkynes</i>							
Propyne	40.06	-102.7	-23.2	0.607	25	63	57
1-Butyne	54.09	-125.7	8.0	0.6783	0	84	81
1-Pentyne	68.12	-90	40.1	0.6901	20	105	102
1-Hexyne	82.15	-131.9	71.3	0.7155	20	126	124
1-Heptyne	96.17	-81	99.7	0.7328	20	147	146
1-Octyne	110.20	-79.3	126.3	0.7461	20	168	167
1-Nonyne	124.23	-50	150.8	0.7658	20	189	186
<i>Cycloalkadi- and trienes</i>							
1,4-Cyclohexadiene	80.13	-49.2	85.5	0.8471	20	105	104
1,3,5-Cycloheptatriene	92.14	-79.5	117	0.8875	19	119	117
1,5-Cyclooctadiene	108.18	-56.4	150.8	0.8818	25	147	140
4-Vinylcyclohexene	108.18	-108.9	128	0.8299	20	147	148
γ -Terpinene	136.24		183	0.849	20	189	188
Terpinolene	136.24		186	0.8632	15	189	185
δ -Limonene	136.24	-95	178	0.8402	21	189	189
1,5,9-Cyclododecatriene	162.27	-17	240	0.84	100	224	219
<i>n-Alkadiynes</i>							
1,6-Heptadiyne	92.14	-85	112	0.8164	17	133	127
1,8-Nonadiyne	120.19	-27.3	162	0.8158	20	175	170

^aFrom Ref. 18.^bCalculated by Eq. (1).All data on M , T_m , T_b , and ρ from Ref. 19 except ^c from Ref. 18

TABLE 2. Vapor pressure (p), solubility (S), and $\log K_{ow}$ for aliphatic hydrocarbons

Compound name	S [$\mu\text{g/L}$]	\pm	at $^{\circ}\text{C}$	$\log K_{ow}$	p at 25 $^{\circ}\text{C}$ [Pa]
<i>n-Alkanes</i>					
Methane	24 400 ^{a,b}	1000	25	1.09 ^l	29 300 000 ^e
Ethane	60 400 ^{a,b}	1300	25	1.81 ^l	3 900 000 ^e
Propane	62 400 ^{a,b}	2100	25	2.36 ^l	946 000 ^e
					988 000 ^u
Butane	61 400 ^{a,b}	2600	25	2.89 ^l	238 000 ^e
					243 000 ^u
Pentane	38 500 ^{a,b}	2000	25	3.62 ^d	68 400 ^u
	39 500 ^c	600	25	3.39 ^l	
	40 765 ^d		22		
Hexane	9500 ^{a,b}	1300	25	4.11 ^d	20 100 ^u
	9470 ^c	200	25	3.90 ^l	
	12 324 ^d		22	3.00 ^m	
Heptane	2930 ^{a,b}	200	25	4.66 ^d	6090 ^u
	2240 ^c	40	25		
	3577 ^d		22		
Octane	660 ^{a,b}	60	25	5.18 ^d	1870 ^u
	431 ^c	12	25	4.00 ^m	
	1103 ^d		22		
Nonane	220 ^e	21	25	4.51 ^m	580 ^u
	122 ^c	7	25		
Decane	52 ^e	4.3	25	5.01 ^m	183 ^u
	19.7 ^f				
	16.1 ^g				
Undecane	4.4 ^c	1.8	25		57.2 ^u
Dodecane	8.4 ^f			6.10 ^m	17.6 ^u
	3.5 ^h		25	5.64 ⁿ	
	10 ⁱ		22		
	3.7 ^l		25		
Tridecane	0.33 ^h		25		5.29 ^u
Tetradecane	6.9 ^f			7.20 ^m	1.56 ^u
	2.2 ^j		25		
Hexadecane	6.3 ^f				
	0.9 ^j		25		
Octadecane	6 ^g				0.0258 ^v
	2.1 ^j		25		
Eicosane	1.9 ^j		25		0.0027 ^v
	9.1 ^k		22		
Docosane	6.3 ^k		22		
Tetracosane	3.5 ^k		22		
Hexacosane	1.7 ^j		25		
Octacosane	5.6 ^k		22		
Hexatriacontane	1.7 ^g				
<i>Cycloalkanes</i>					
Cyclopentane	156 000 ^{a,b}	9000	25	3.00 ^l	42 300 ^u
	160 000 ^c	2000	25		
Cyclohexane	55 000 ^{a,b}	2300	25	3.44 ^l	13 000 ^u
	66 500 ^c	800	25		
Methylcyclopentane	42 000 ^{a,b}	1600	25	3.37 ^l	18 400 ^u
	41 800 ^c	1000	25		
Cycloheptane	30 000 ^b	1000	25	4.00 ^l	
Methylcyclohexane	14 000 ^{a,b}	1200	25	3.61 ^l	6170 ^u
	16 000 ^c	200	25		
Cyclooctane	7900 ^b	1800	25		
Propylcyclopentane	2040 ^c	100	25		1650 ^u
1- <i>trans</i> -4-Dimethylcyclohexane	3840 ^c	170	25		
1- <i>cis</i> -2-Dimethylcyclohexane	6000 ^b	800	25		
1,1,3-Trimethylcyclopentane	3730 ^c	170	25		5290 ^u
1,1,3-Trimethylcyclohexane	1770 ^c	50	25		
Adamantane				4.24 ^o	
				5.2 ^p	
Decalin	889 ^c	31	25		147 ^u
Pentylcyclopentane	115 ^c	11	25		159 ^u
1-Methyl-4-isopropyl-cyclohexane				5.56 ^q	

TABLE 2. Vapor pressure (p), solubility (S), and $\log K_{ow}$ for aliphatic hydrocarbons—Continued

Compound name	S [$\mu\text{g/L}$]	\pm	at $^{\circ}\text{C}$	$\log K_{ow}$	p at 25°C [Pa]
<i>Branched alkanes</i>					
Isobutane	48 900 ^{a,b}	2100	25	2.76 ^l	
Isopentane	47 800 ^{a,b}	1600	25		91 700 ^u
	48 000 ^c	1000	25		
2,2-Dimethylpropane	33 200 ^b	1000	25	3.11 ^l	172 000 ^u
2-Methylpentane	13 800 ^{a,b}	900	25		28 300 ^u
	13 000 ^c	200	25		
3-Methylpentane	12 800 ^b	600	25		25 300 ^u
	13 100 ^c	400	25		
2,2-Dimethylbutane	18 400 ^{a,b}	1300	25		42 500 ^u
	21 200 ^c	300	25		
2,3-Dimethylbutane	19 100 ^c	200	25	3.42 ^l	31 300 ^u
2-Methylhexane	2540 ^c	20	25		8790 ^u
3-Methylhexane	2640 ^c	80	25		8210 ^u
2,2-Dimethylpentane	4400 ^c	110	25		14 000 ^u
2,3-Dimethylpentane	5250 ^c	20	25		9200 ^u
2,4-Dimethylpentane	4060 ^{a,b}	290	25		13 100 ^u
	4410 ^c	50	25		
3,3-Dimethylpentane	5940 ^c	30	25		11 000 ^u
3-Methylheptane	792 ^c	28	25		2610 ^u
2,2,4-Trimethylpentane	2440 ^{a,b}	120	25		6570 ^u
	1140 ^c	20	25		
2,3,4-Trimethylpentane	1360 ^c	30	25		3600 ^u
4-Methyloctane	115 ^c	11	25		0.901 ^u
2,2,5-Trimethylhexane	1150 ^b	80	25		2210 ^u
<i>n-Alkenes</i>					
Ethene	131 000 ^b	10 000	25	1.13 ^l	
Propene	200 000 ^b	27 000	25	1.77 ^l	1 140 000 ^u
1-Butene	222 000 ^b	10 000	25	2.40 ^l	296 000 ^u
1-Pentene	148 000 ^b	7000	25		86 500 ^u
2-Pentene	203 000 ^b	8000	25		
1-Hexene	50 000 ^b	1200	25	3.39 ^d	24 800 ^u
	69 684 ^d		22		
1-Heptene	18 165 ^d		22	3.99 ^d	7510 ^u
2-Heptene	15 000 ^b	1400	25		5330 ^u
1-Octene	2700 ^b	200	25	4.57 ^d	2320 ^u
	4096 ^d		22		
1-Nonene	1117 ^d		22	5.15 ^d	712 ^u
<i>Cycloalkenes</i>					
Cyclopentene	535 000 ^b	20 000	25		50 700 ^u
Cyclohexene	213 000 ^b	10 000	25	2.86 ^l	11 800 ^u
Cycloheptene	66 000 ^b	4000	25		
1-Methylcyclohexene	52 000 ^b	2000	25		4080 ^u
α -Pinene				4.83 ^f	
<i>Branched alkenes</i>					
2-Methylpropene	263 000 ^b	23 000	25	2.34 ^l	304 000 ^u
3-Methyl-1-butene	130 000 ^b	14 000	25		120 000 ^u
2-Methyl-1-pentene	78 000 ^b	3200	25		27 500 ^u
4-Methyl-1-pentene	48 000 ^b	2600	25		35 600 ^u
<i>Alkadi- and trienes</i>					
1,3-Butadiene	735 000 ^b	20 000	25	1.99 ^l	280 000 ^u
1,4-Pentadiene	558 000 ^b	27 000	25	2.47 ^l	97 900 ^u
2-Methyl-1,3-butadiene	642 000 ^b	10 000	25		81 300 ^u
1,5-Hexadiene	169 000 ^b	6000	25	2.87 ^l	
1,6-Heptadiene	44 000 ^b	3000	25		
7-Methyl-3-methylene-1,6-octadiene				4.17 ^q	
<i>n-Alkynes</i>					
Propyne	3 640 000 ^b	125 000	25	0.94 ^l	600 000 ^u
1-Butyne	2 870 000 ^b	101 000	25		
1-Pentyne	1 570 000 ^b	33 000	25	2.12 ^d	57 500 ^u
	1 049 048 ^d		22	1.98 ^l	

TABLE 2. Vapor pressure (p), solubility (S), and $\log K_{ow}$ for aliphatic hydrocarbons—Continued

Compound name	S [$\mu\text{g/L}$]	\pm	at $^{\circ}\text{C}$	$\log K_{ow}$	p at 25 $^{\circ}\text{C}$ [Pa]
1-Hexyne	360 000 ^b 687 596 ^d	17 000	25 22	2.73 ^d	18 100 ^u
1-Heptyne	94 000 ^b	3000	25		7000 ^u
1-Octyne	24 000 ^b	800	25		1810 ^u
1-Nonyne	7200 ^b	500	25		835 ^u
<i>Cycloalkadi- and trienes</i>					
1,4-Cyclohexadiene	700 000 ^b	16 000	25	2.30 ^l	
1,3,5-Cycloheptatriene	62 000 ^b	20 000	25	2.63 ^s 3.03 ^s 3.16 ^s 3.94 ^s	
1,5-Cyclooctadiene					
4-Vinylcyclohexene	50 000 ^b	5000	25		
γ -Terpinene				4.5 ^f	
Terpinolene				4.47 ^f	
δ -Limonene				4.57 ^f	
1,5,9-Cyclododecatriene				5.5 ^o 4.12 ^s 5.77 ^s 5.65 ^t	
<i>n-Alkadiynes</i>					
1,6-Heptadiyne	1 650 000 ^b	25 000	25		
1,8-Nonadiyne	125 000 ^b	3000	25		

^aReference 20.^bReference 21.^cReference 22.^dReference 23.^eReference 24.^fReference 25.^gReference 26.^hReference 27.ⁱReference 28.^jReference 29.^kReference 30.^lReference 35.^mReference 33.ⁿReference 34.^oReference 41.^pReference 38.^qReference 39.^rReference 42.^sReference 37.^tReference 36.^uReference 18.^vReference 43.

to rise up for only 4 h. As can be concluded from these experiments, filtration is not sufficient to exclude colloids. Peake and Hodgson²⁸ also showed that the equilibration time, in which the colloids are rising slowly, is very important for the accommodated amount in water. In long term equilibration experiments an extrapolation can be made towards equilibrium. This method was applied by Coates *et al.*²⁷ for dodecane and tridecane. It should be noted that these solubility data were obtained by solvent extraction after filtration.²⁷ Therefore the aqueous concentration might be lowered by volatilization to air. However, these data do not show such an effect, when compared to the data for decane and undecane.²⁴ If these data for dodecane and tridecane are combined with the rest of the data for *n*-alkanes containing fewer than 12 carbon atoms,^{20–26} a linear relationship is obtained between the solubility and the molar volume for the liquid *n*-alkanes, as was suggested by McAuliffe^{20,21} and Coates *et al.*²⁷ This linear relationship is shown in Fig. 1 as a solid line (also see Table 4).

All data on solubility of *n*-alkanes higher than tridecane are either determined by the simple shake-flask method,^{25,29,30} which does not prevent the formation of col-

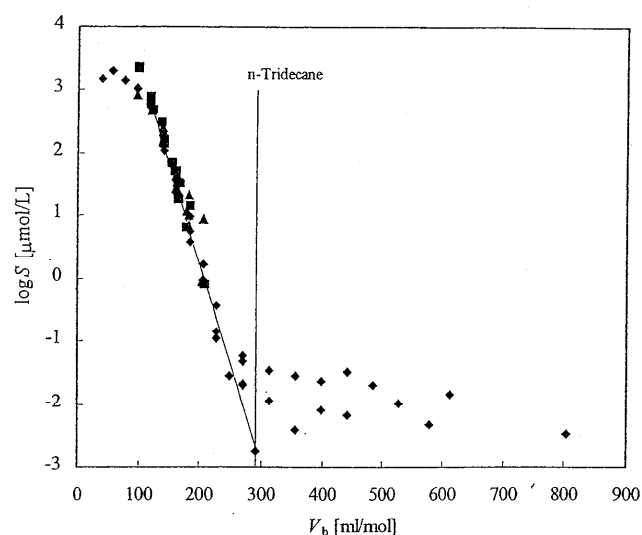


FIG. 1. Literature data on aqueous solubility or accommodation for linear, branched, and cycloalkanes expressed as a function of the molar volume. \blacklozenge : *n*-alkanes, \blacktriangle : branched alkanes, and \blacksquare : cycloalkanes. The drawn line represents linear regression for C_5 to C_{13} *n*-alkanes.

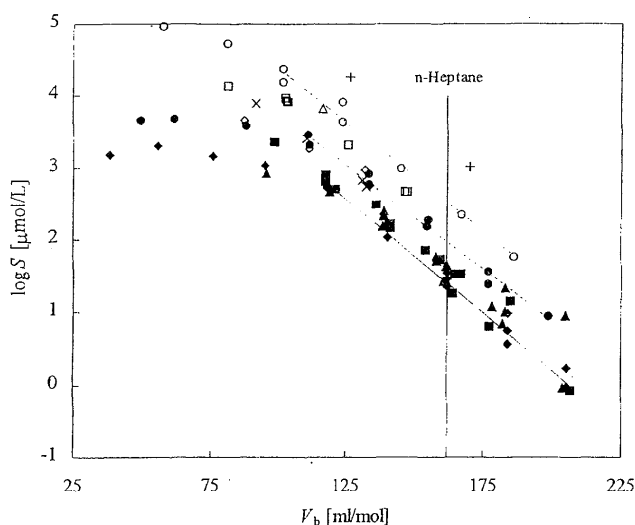


FIG. 2. Literature data on aqueous solubility for aliphatic hydrocarbons expressed as a function of molar volume. \blacklozenge : *n*-alkanes, \blacktriangle : branched alkanes, \blacksquare : cycloalkanes, \bullet : *n*-alkenes, \times : cycloalkenes, \diamond : branched alkenes, \square : alkadienes, \triangle : alkatrienes, \circ : *n*-alkynes, and $+$: *n*-alkadiynes. Lines represent linear regression: — C_5 to C_{13} *n*-alkanes, ---- C_5 to C_9 *n*-alkenes, and - - - C_5 to C_9 *n*-alkynes.

loids, or the method of determination is not reported.²⁶ Further, data were not extrapolated in time towards true aqueous solubility, as was done for dodecane and tridecane by Coates *et al.*²⁷ Therefore all data on the higher alkanes probably do not represent "true" aqueous solubility, but accommodation of colloids. The "generator column" technique, which was applied by Tewari *et al.* for *n*-pentane to *n*-octane,²³ is one of the best methods to determine aqueous solubility and excludes the formation of colloids. Since these data are in good agreement with other data for the lower *n*-alkanes, for example, the data by McAuliffe,^{20,21,24} the data for lower *n*-alkanes are considered to reflect "true" aqueous solubility.

If the deviation from a linear relationship shown in Fig. 1 is real rather than simply an artifact of the methods used, the explanation may be in the molecular conformation. Short unbranched alkanes have a linear global minimum conformation. However, when the chain length of *n*-alkanes increases, this global minimum conformation can change to a more folded one.³¹ The number of carbon atoms, at which this effect takes place, is strongly dependent on the medium (solvent, air, or pure substance). Moreover, different force fields, solvent models, and semiempirical methods yield different results in quantum chemical calculations.³¹ Further, it is not plausible that molecular folding alone can explain the observed deviation from linearity. Other thermodynamic explanations for a deviation from this linear relationship actually deal with colloid formation instead of aqueous solubility.³²

For other nonaromatic hydrocarbons, such as alkenes and alkynes, cyclic compounds and branched compounds, solubility data were found only for compounds containing ten or fewer carbon atoms.^{20–24} These data are presented in Fig. 2.

Data from Coates *et al.*²⁷ were excluded since they were not directly measured, but derived from RP-HPLC. For the solubility of the two cycloalkanes containing ten carbon atoms (decalin and pentylcyclopentane) no experimental details are included in the study report. However, the data in this study²² agree very well with the accurate data for alkanes up to undecane by McAuliffe.^{20,21,24} Moreover, the solubility of these compounds is comparatively high, and colloid formation is probably of minor importance.

Generally, for saturated alkanes, the molar volume correlates very well with the aqueous solubility. However, if double or triple bonds are included in the hydrocarbon molecules, the solubility is higher than for saturated compounds of equal molar volumes, but for both alkenes and alkynes, the molar volume again correlates with solubility (lower and upper dashed lines, respectively, in Fig. 2, see also Table 4). The incorporation of double or triple bonds leads to favorable interactions with water, and thus to an increased solubility. However, for compounds of the same saturation level, the size of the molecule, here expressed as molar volume, seems to be the most important factor for solubility.

5. Octanol-Water Partition Coefficient (K_{ow})

The data for octanol-water partition coefficients are mainly restricted to the linear hydrocarbons, and to some saturated and unsaturated cyclic compounds (Table 2). The only values for linear alkanes, containing more than ten carbon atoms, are data from Hutchinson *et al.*³³ (octane, nonane, decane, dodecane, and tetradecane), and one value for dodecane from Hammers as cited by Geyer *et al.*³⁴

The data by Tewari *et al.*²³ for pentane to octane were determined by a generator column technique, in which both phases (*n*-octanol and water) were analyzed. Consequently, these data can probably be considered as very accurate. These values are consistent with the selected experimental values from ClogP (ClogP star values),³⁵ for methane to hexane (Fig. 3).

The data from Hutchinson *et al.*,³³ starting from octane, show a clear relationship between $\log K_{ow}$ and the molar volume too (Fig. 3). Therefore it is likely that a linear relationship between $\log K_{ow}$ and the molar volume extends to tetradecane. However, the data from Hutchinson *et al.*³³ are systematically lower than extrapolations from the data for lower *n*-alkanes.^{23,35} Therefore these values are probably subject to a systematic error. These values were determined by headspace analysis of an aqueous sample before and after introduction of an amount of octanol, a procedure which reduced the concentration in the gas phase to about half.

Tewari *et al.*²³ also determined $\log K_{ow}$ of some *n*-alkenes and *n*-alkynes (Fig. 4). For these compounds, a linear relationship between $\log K_{ow}$ and molar volume is also observed. Further, the hydrophobicity increases with increasing saturation of the hydrocarbons (the same effect on hydrophobicity was already observed for solubility). Values for $\log K_{ow}$ of other compounds, mostly saturated or unsaturated cyclic

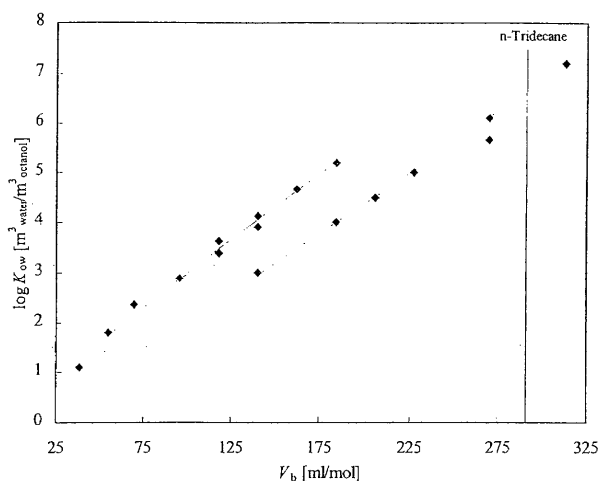


FIG. 3. Literature data on $\log K_{ow}$ for n -alkanes expressed as a function of the molar volume. Lines represent linear regression: — C_1 to C_8 n -alkanes (Refs. 23 and 35) and - - - - C_8 to C_{10} , C_{12} , and C_{14} n -alkanes (Ref. 27).

compounds,³⁶⁻⁴² are similar to those for linear hydrocarbons of the same molar volume and saturation (Fig. 4).

6. Vapor Pressure (p)

A linear relationship exists between vapor pressure^{18,24,43} and molar volume (Fig. 5); for all n -alkanes with 1-14 carbon atoms, data for vapor pressure at 25 °C are included. Further data are for C_{18} and C_{20} , which are extrapolated by the Clapeyron equation from temperatures above the melting point and consequently, represent the vapor pressure of the subcooled liquid at 25 °C.

For cyclic compounds and alkynes the vapor pressure is slightly lower and for branched compounds the vapor pres-

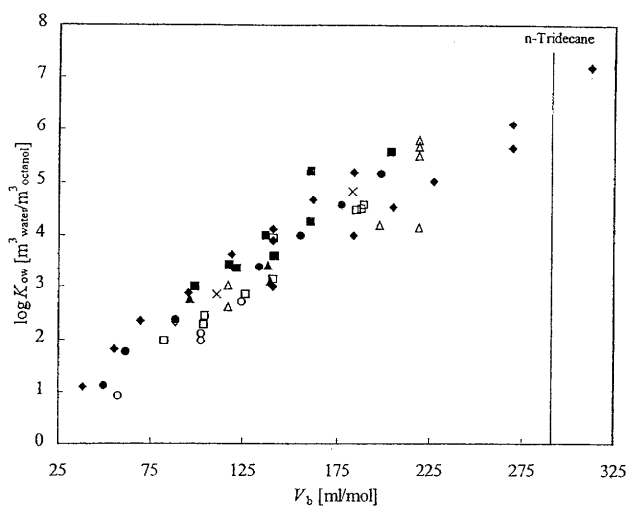


FIG. 4. Literature data on $\log K_{ow}$ for aliphatic hydrocarbons expressed as a function of the molar volume. \blacklozenge : n -alkanes, \blacktriangle : branched alkanes, \blacksquare : cycloalkanes, \bullet : n -alkenes, \times : cycloalkenes, \blacklozenge with \bullet : branched alkenes, \square with \bullet : alkadienes, \triangle with \bullet : alkatrienes, and \circ with \bullet : n -alkynes.

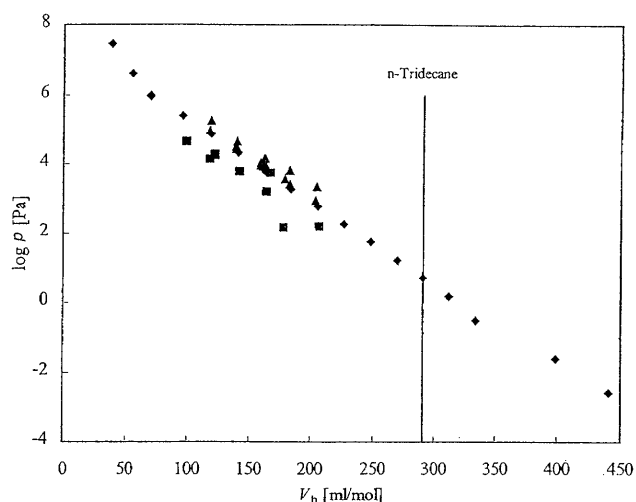


FIG. 5. Literature data on vapor pressure (p) for linear, branched, and cycloalkanes expressed as a function of the molar volume. \blacklozenge : n -alkanes, \blacktriangle : branched alkanes, and \blacksquare : cycloalkanes.

sure is slightly higher in comparison with n -alkanes of the same molar volume (see Figs. 5 and 6 and Table 2).

7. Henry's Law Constant (H) and Octanol-Air Partition Coefficient (K_{oa})

No direct measurements for the Henry's law constant were found. Therefore this parameter is estimated from the quotient of vapor pressure and water solubility. As can be seen from Figs. 7 and 8, for each group of compounds, H tends to increase with increasing molecular size, as was already concluded by Mackay and Shiu.⁴⁴ This effect is also observed for the subset of n -pentane to n -nonane, which have the most reliable solubility data (Table 4). However, for all nonaro-

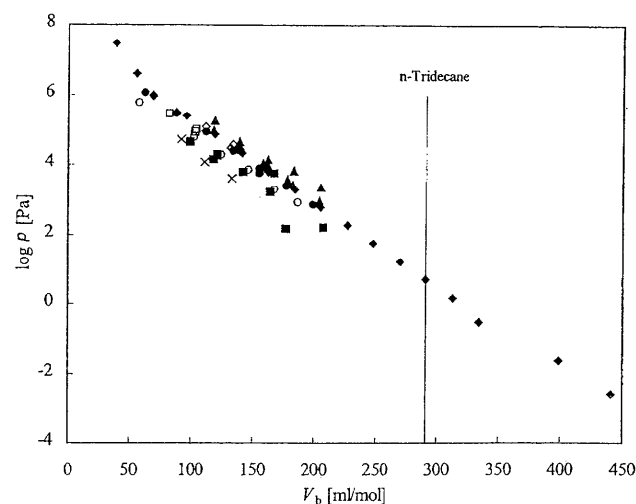


FIG. 6. Literature data on vapor pressure (p) for aliphatic hydrocarbons expressed as a function of the molar volume. \blacklozenge : n -alkanes, \blacktriangle : branched alkanes, \blacksquare : cycloalkanes, \bullet : n -alkenes, \times : cycloalkenes, \blacklozenge with \bullet : branched alkenes, \square with \bullet : alkadienes, and \circ with \bullet : n -alkynes.

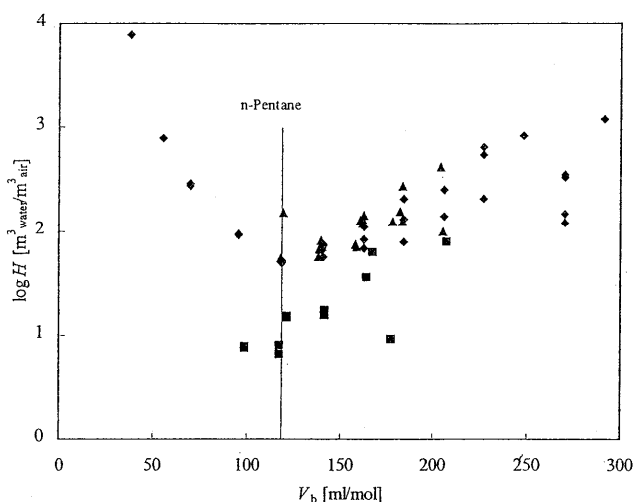


Fig. 7. Estimated Henry's law constant (H) for linear, branched, and cycloalkanes expressed as a function of the molar volume. \blacklozenge : n -alkanes, \blacktriangle : branched alkanes, and \blacksquare : cycloalkanes.

matic hydrocarbons, Henry's law constant is close to ten or higher. These results indicate that volatilization will be an important environmental fate process.

From the quotient of the octanol-water partition coefficient and Henry's law constant the octanol-air partition coefficient can be estimated (Fig. 9). Since the number of reliable data for both K_{ow} and S (and consequently H) is limited, only a few reliable data can be derived. However, from these subsets of reliable K_{ow} and S values, it can be concluded that this parameter also increases with molar volume (Table 4).

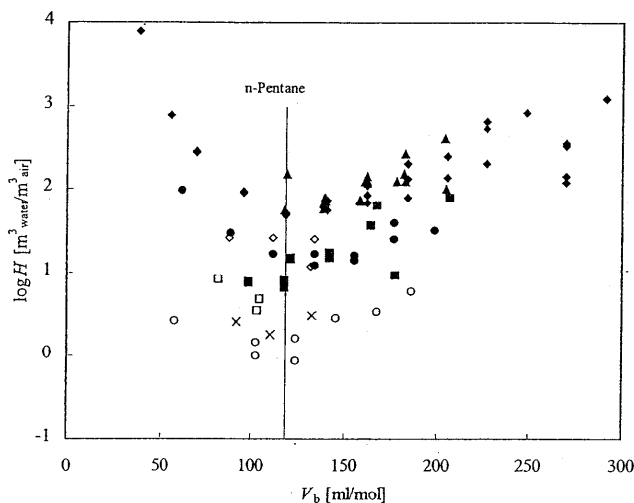


Fig. 8. Estimated Henry's law constant (H) for aliphatic hydrocarbons expressed as a function of the molar volume. \blacklozenge : n -alkanes, \blacktriangle : branched alkanes, \blacksquare : cycloalkanes, \bullet : n -alkenes, \times : cycloalkenes, \diamond : branched alkenes, \square : alkadienes, and \circ : n -alkynes.

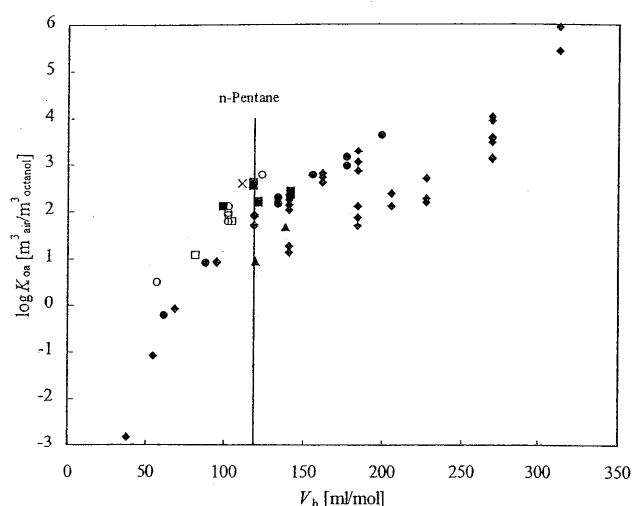


Fig. 9. Estimated octanol-air partition coefficients (K_{ow}) for aliphatic hydrocarbons expressed as a function of the molar volume. \blacklozenge : n -alkanes, \blacktriangle : branched alkanes, \blacksquare : cycloalkanes, \bullet : n -alkenes, \times : cycloalkenes, \square : alkadienes, and \circ : n -alkynes.

8. Concluding Remarks

For both hydrophobicity parameters, solubility and K_{ow} , limited reliable data are available for nonaromatic hydrocarbons, having ten or more carbon atoms. Measurements of these parameters should be carried out by techniques that have been proven to be valid for very hydrophobic chemicals, such as the generator-column²³ and the slow-stirring technique.⁴⁵ Determination of the aqueous concentration must be carried out carefully because of the very low aqueous solubility. Moreover, the high Henry's law constants of these compounds will cause rapid losses from the aqueous phase, if the samples are exposed to air. The "purge and trap" GC method²⁴ may be used to avoid losses during analysis. The method described by Tewari *et al.*,²³ in which the aqueous phase is inserted under a layer of extraction solvent directly after the generator column, also probably avoids volatilization.

In Table 3 the preferred values of the physicochemical parameters are listed for aliphatic hydrocarbons containing

TABLE 3. Selected values for aliphatic hydrocarbons containing ten or more carbon atoms

Compound		S [$\mu\text{g/L}$]	p at 25 °C at °C	p at 25 °C [Pa] ^d	V_b [ml/mol]
n -alkanes	Decane	52 ^a	25	183	227
	Undecane	4.4 ^a	25	57.2	248
	Dodecane	3.5 ^b	23 ± 2	17.6	279
	Tridecane	0.33 ^b	23 ± 2	5.29	291
cycloalkanes	Decalin	889 ^c	25	147	177
	Pentylcyclopentane	115 ^c	25	159	207

^aFrom Ref. 24.

^bFrom Ref. 27.

^cFrom Ref. 22.

^dFrom Ref. 18.

TABLE 4. Linear regression relationships between molar volume [ml/mol] [estimated by Eq. (1)] and the logarithms of solubility [M], K_{ow} [$m^3_{water}/m^3_{octanol}$], vapor pressure [Pa], Henry's law constant (estimated) [m^3_{water}/m^3_{air}], and K_{oa} (estimated) [$m^3_{air}/m^3_{octanol}$] for liquid (at 25 °C) aliphatic hydrocarbons. Replicates were averaged before performing linear regression

Linear regression between log S and V_b	Slope \pm s.e.	Intercept \pm s.e.	r^2 (n)
n -alkanes C_5 to C_{13}	-0.032 ± 0.0010	0.518 ± 0.205	0.9935 (9)
n -alkanes C_5 to C_9	-0.030 ± 0.0003	0.336 ± 0.050	0.9997 (5)
n -alkenes C_5 to C_9	-0.028 ± 0.0010	0.593 ± 0.146	0.9943 (7)
n -alkynes C_5 to C_9	-0.031 ± 0.0011	1.458 ± 0.160	0.9963 (5)
log K_{ow} and V_b			
n -alkanes C_5 to C_8^a	0.026 ± 0.0010	0.399 ± 0.151	0.9971 (4)
n -alkenes C_6 to C_9	0.027 ± 0.0002	-0.212 ± 0.027	0.9999 (4)
log p and V_b			
n -alkanes C_5 to C_{20}	-0.023 ± 0.0003	7.521 ± 0.090	0.9978 (13)
n -alkenes C_5 to C_9	-0.024 ± 0.0011	7.561 ± 0.172	0.9917 (6)
n -alkynes C_5 to C_9	-0.022 ± 0.0007	7.012 ± 0.109	0.9967 (5)
log H (est.) and V_b			
n -alkanes C_5 to C_{13}	0.0078 ± 0.0010	0.729 ± 0.206	0.9030 (9)
n -alkanes C_5 to C_9	0.0064 ± 0.0003	0.924 ± 0.057	0.9914 (5)
n -alkenes C_5 to C_9	0.0043 ± 0.0017	0.628 ± 0.270	0.6092 (6)
n -alkynes C_5 to C_9	0.0084 ± 0.0014	-0.841 ± 0.214	0.9191 (5)
log K_{oa} (est.) and V_b			
n -alkanes C_5 to C_8^a	0.020 ± 0.0012	-0.585 ± 0.191	0.9923 (4)
n -alkenes C_6 to C_9	0.021 ± 0.0017	-0.519 ± 0.284	0.9869 (4)
log S and log K_{ow}			
n -alkanes C_5 to C_8^a	-1.144 ± 0.053	0.723 ± 0.232	0.9957 (4)
n -alkenes C_6 to C_9	-1.108 ± 0.062	0.619 ± 0.268	0.9938 (4)

^aData from Hutchinson *et al.*³³ not included.

ten or more carbon atoms. As can be seen from this table, the number of reliable data for these larger hydrocarbons is very limited. The lack of reliable data on these parameters probably reflects the problems encountered in the experimental determination. No data are included for log K_{ow} because all values for compounds containing ten or more carbon atoms were determined by either the shake-flask method or by RP-HPLC or the method was not clearly stated or the data were likely to be erroneous.

In Table 4 the linear regression relationships are presented for only the data that were considered to be reliable. The physicochemical properties of related aliphatic hydrocarbons with no or suspect data can be estimated from the molar volume at the boiling point by these relationships. Also the consistency of both hydrophobicity parameters (K_{ow} and S) can be examined by the relationship between these parameters.

9. Acknowledgment

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