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Development of an automatic estimation system for both the partition coefficient and aqueous solubility

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SUMMARY

A computer program has been developed for estimating both the partition coefficient between 1-octanol and water phases and the aqueous solubility from the structural formula. This system is an extended version of a previously described program entitled CHEMICALC for the automatic estimation of the partition coefficient. The aqueous solubility is estimated via two pathways. The first is based on the linear relationship between logarithms of the aqueous solubilities of 497 compounds and their estimated 1-octanol/water partition coefficients. In the second, combined handling of two available group contribution methods of Irmann [Chem. Ing. Tech., 37 (1965) 789] and Wakita et al. [Chem. Pharm. Bull., 34 (1986) 4663] is adopted according to compound type. Some revisions and extensions of the methods for estimating the aqueous solubility have been made in both pathways, and the accuracy of the estimated aqueous solubilities for 497 compounds is discussed.

INTRODUCTION

The partition coefficient and aqueous solubility have been widely used in the study of structure-activity relationships, primarily with pharmaceuticals. In most cases, absorption of an administered drug in the gastrointestinal tract and wall depends on passive transport. The combined effect of the partition coefficient and aqueous solubility on absorption is one of the most important factors in drug metabolism. According to available data, drugs having logarithms of 1-octanol/water partition coefficients ($\log P$) greater than or equal to 2 and aqueous solubilities greater than 10 mg/l are supposed to be well absorbed [1].

Extensive quantitative structure-activity relationship studies usually require such properties for a large set of compounds, and there is an ever-increasing need for automatic estimation.

In a previous paper, we proposed a convenient method for estimating $\log P$ based on the group-contribution method and developed a program entitled CHEMICALC for automatic estimation

of $\log P$ [2]. We have developed an extended program entitled CHEMICALC2 which is capable of predicting both $\log P$ and the aqueous solubility from the structure of a molecule. This paper describes our efforts to develop CHEMICALC2 and discusses the accuracy of the calculated values of aqueous solubilities.

ESTIMATION METHOD

There are many ways for estimating aqueous solubility [3]. From a practical viewpoint, the following two basically different approaches are adopted in this system for reliably estimating the aqueous solubility.

Pathway 1 – Estimation from $\log P$

Various regression equations were reported that correlate the aqueous solubility with the 1-octanol/water partition coefficient, but existing equations have some limited applicability and do not always give good estimations [3]. Furthermore, many of the reported correlations have been used primarily to test a theory; few have actually been presented as predictive means. Therefore, we have re-examined a relationship between the aqueous solubility and the 1-octanol/water partition coefficient. The relationship is assumed to be described by the following equation:

$$\log 1/S = a \log P + b(T_m - 25) + c \quad (1)$$

where S is the molar solubility of the compound in water, T_m is the melting point in °C, and a , b and c are constants to be determined. The second term on the right side of Eq. 1 is a correction factor for solids. If the compound is liquid at 25°C, then 25°C is used instead of the melting point. To determine a , b and c , the experimental $\log 1/S$ values taken from the literature [4-6] of 497 compounds were used, including 348 liquids (70 aliphatic hydrocarbons, 23 aromatic hydrocarbons, 81 halogenated hydrocarbons, 22 ethers and oxygen-containing ring compounds, 71 alcohols, 1 phenol, 5 aldehydes, 17 ketones, 30 esters, 8 nitro compounds, 2 nitriles, 1 amine, 2 thiols, 3 sulfides, and 12 multifunctional compounds) and 149 solids (34 aromatic hydrocarbons, 60 halogenated hydrocarbons, 9 oxygen-containing compounds, 9 nitrogen-containing compounds, 3 sulfur-containing compounds, and 34 multifunctional compounds). The $\log P$ values of all compounds were estimated by using CHEMICALC.

The following excellent correlation was obtained by regression analysis:

$$\begin{aligned} \log 1/S &= 1.050 \log P + 0.00956(T_m - 25) - 0.515 \\ &(n = 497, r = 0.976, s = 0.505) \\ &(\text{regression range: } -1.05 \leq \log P \leq 8.85) \end{aligned} \quad (2)$$

Equation 2 covers a wide range of $\log 1/S$ values from -1.96 to 10.49 and chemical classes. It is highly significant that the coefficient of $(T_m - 25)$ in Eq. 2 is close to the theoretical values of 0.0095 [4] and 0.01 [5]. Figure 1 shows the relationship between the observed $\log 1/S$ value and the estimated value based on Eq. 2 for 497 compounds in the data set. The average absolute error of all compounds was $0.39 \log S$ units.

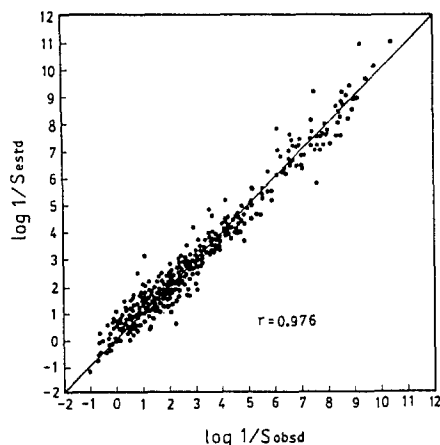


Fig. 1. Observed $\log 1/S$ values plotted against values estimated based on Eq. 2.

Pathway 2 – Group contribution methods

Generally, structure is the most useful basis for estimating molecular properties. The simplest and most general method based on structure is the group contribution method (GCM). For estimating aqueous solubility, only two group contribution methods have a degree of general applicability.

A group contribution method proposed by Irmann [4] is shown in the following equation:

$$\log 1/S = a + \sum n_i b_i + \sum n_j c_j + 0.0095(T_m - 25) \quad (3)$$

where S is in g/gH₂O, a is the contribution of the compound type, b_i is the contribution of the i th atom type which occurs n_i times, c_j is the contribution of the j th structural element which occurs n_j times, and T_m is the melting point of the solid in °C.

Another group contribution method, developed by Wakita et al. [6], can be described by the following equation:

$$\log 1/S = \sum n_i f s_i \quad (4)$$

where S is in mol/l, $f s_i$ is the fragment constant (contribution) for the i th fragment which occurs n_i times in a molecule.

The two methods differ in the descriptors used and their applicability. The applicability of the Irmann method is restricted to hydrocarbons and halogenated hydrocarbons. In contrast, the method of Wakita et al. is applicable to compounds having diverse functionalities. This method, however, is not complete for organic solids [8], because it employs melting points treating as a fragment constant in estimating the heat of fusion for organic solids. The melting point coefficient is 0.0037 for aliphatic solids and 0.0143 for aromatic solids. These values are inconsistent with each other and smaller or larger than the theoretical range of 0.0095-0.01 [4,7].

As the accuracy of these two group contribution methods has not been analyzed elsewhere, we compared them for 173 organic liquids containing 93 hydrocarbons and 80 halogenated hydro-

carbons. In order to compare the relative accuracy of the methods, the absolute and bias error with respect to the experimental data were calculated for each compound for which these methods were applicable. A summary of the overall error statistics for the methods by compound class is presented in Table 1. It can be seen that Irmann's estimated $\log 1/S$ values are closer to the experimental ones than those calculated by the method of Wakita et al. for aromatic and halogenated hydrocarbons. On the other hand, the method of Wakita et al. showed somewhat better results for aliphatic hydrocarbons. It is interesting to note that these two methods showed a trend in bias (i.e., tendency to continually overestimate or underestimate $\log 1/S$). As can be seen from Table 1, the method of Wakita et al. showed negative bias except for aromatic halogenated hydrocarbons, while Irmann's method showed weak positive bias except for cycloaliphatic hydrocarbons.

Based on this evaluation, our system employs both methods according to the classes of the compounds as described below, but some revisions and extensions of the methodology have been made as follows: First, for applying the method of Wakita et al. to calculate organic solids, the same correction factor, $0.0095(T_m - 25)$, as used in Irmann's method is employed in this system. The modified version of Eq. 4 is as follows:

$$\log 1/S = \sum n_i f s_i + 0.0095(T_m - 25) \quad (4')$$

Second, since both methods are insufficient to cover all of the structures which require their aqueous solubilities, pure atomic increments were determined as complements. Their increments were obtained with Eq. 5 based on the same data set used for Eq. 2:

$$\log 1/S = \sum n_i a_i + 0.0095(T_m - 25) \quad (5)$$

($n = 497, r = 0.881, s = 0.802$)

TABLE I
COMPARISON OF THE GROUP CONTRIBUTION METHODS OF IRMANN AND WAKITA ET AL.

Chemical class	Number of compounds	Data range	Irmann		Wakita et al.	
			Ave. error ^a	Bias ^b	Ave. error	Bias
<i>Hydrocarbons</i>						
Saturated aliphatic	17	C2–C9	0.19	0.14	0.13	−0.09
Unsaturated aliphatic	38	C2–C10	0.22	0.20	0.21	−0.14
Cycloaliphatic	15	C3–C8	0.19	−0.18	0.15	−0.10
Aromatic	23	C6–C13	0.10	0.03	0.29	−0.11
<i>Halogenated hydrocarbons</i>						
Aliphatic	56	C1–C5	0.15 ^c	0.08	0.30	−0.14
Aromatic	24	C6–C12	0.11 ^d	0.02	0.20	0.03
Total	173	C1–C13	0.16	0.07	0.23	−0.10

^a Ave. error = $\Sigma |\log 1/S(\text{obsd}) - \log 1/S(\text{estd})|$ / number of compounds. S is in mol/l in both methods.

^b Bias = $\Sigma (\log 1/S(\text{obsd}) - \log 1/S(\text{estd}))$ / number of compounds.

^c Number of compounds which could be calculated is 53.

^d Number of compounds which could be calculated is 23.

In this equation, S is in mol/l, n_i is the number of atoms of type i , and a_i is the contribution of the corresponding atom type. The average absolute error of all compounds was 0.61 log S units.

The determined a_i values are given in Table 2. It is reasonable for the contribution values for carbon, hydrogen and halogens to be positive and for oxygen, nitrogen and sulfur to be negative. However, it should be noted that the relative magnitude of these values is not so rigid, and these contributions cannot be used for purposes of estimating the distribution of lipophilicity on molecular structures, because these contributions are mean values for various atom types in the organic structure and some contribution values are influenced by a small data set.

Although the group contribution method is to be preferred when the required group contributions have been determined, this zero-th order additivity scheme presently covers all possible organic compounds containing C, H, N, O, S, or halogens.

ALGORITHMS

A general schematic for the program organization and processing order is shown in Fig. 2. The steps are as follows:

(1) Input of the molecule of interest is accelerated by the method described in the previous paper [2]. After the molecule has been entered, the structural information is stored in a connection table. For the compound that is a solid at 25 °C, the user is requested to input the melting point (although this is not absolutely necessary, as the solubility of the supercooled liquid is given for the solid whose melting point is not available).

(2) The structural features are perceived from the stored connection table. Carbon and nitrogen atoms are classified in terms of their environment. The carbon atoms are categorized as follows: single-bonded, double-bonded, triple-bonded, aromatic, and aromatic fused carbon. Similarly, nitrogen atoms are categorized into single-bonded, double-bonded, and aromatic nitrogen. General atomic groups, CH₃, CH₂, CH, =CH, OH, NH₂, NO₂, SH, -C=O, and such, are identified. The 'basic groups' (usually consisting of a general atomic group and its neighboring atoms) defined by us [2] are identified in the subsequent sections.

(3) The octanol-water partition coefficient value (log P) is calculated using the computer program CHEMICALC.

TABLE 2
ATOMIC CONTRIBUTIONS TO THE NEGATIVE LOGARITHM OF THE AQUEOUS SOLUBILITY IN MOL/L

Atom type	Contribution	No. of compounds	Frequency of use
C	0.31	497	3717
H	0.03	484	5040
O	-0.59	216	336
N	-0.21	53	64
S	-0.30	10	10
F	0.16	19	48
Cl	0.55	98	298
Br	0.65	31	53
I	1.00	15	22

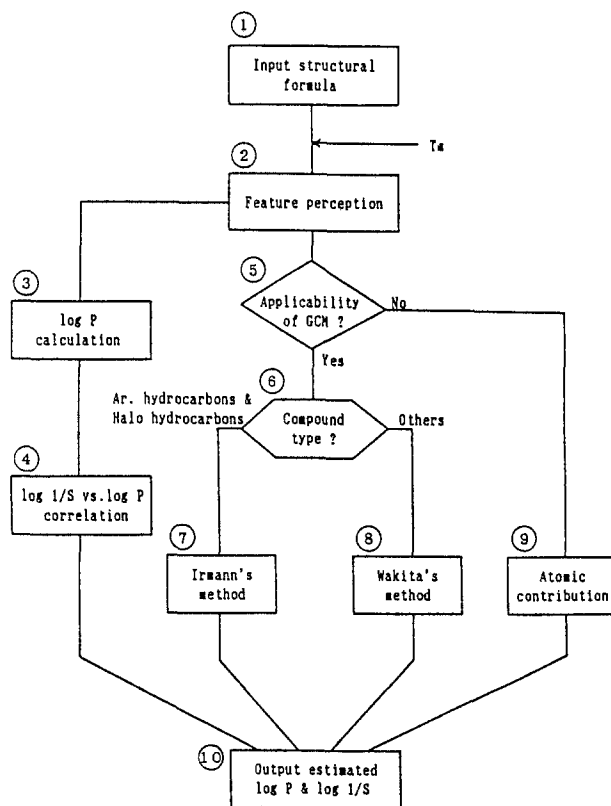


Fig. 2. Schematic flow diagram of CHEMICALC2 program.

(4) The aqueous solubility is calculated by substituting the $\log P$ value from step 3 in Eq. 2. In this step, the program checks extrapolation. If the input value of $\log P$ is outside the range of original $\log P$ values, the message with the estimated $\log P$ value is output.

(5) The applicability of the two group contribution methods of Irmann and Wakita et al. is checked. If the program detects the presence of any unavailable group values for both methods, the groups are output and the program goes to step 9.

(6) The chemical type of the compound is perceived. If the compound belongs to aromatic hydrocarbons or halogenated hydrocarbons, the program goes to step 7. If the compound belongs to one of the other types, the program goes to step 8.

(7) The $\log 1/S$ value is calculated by summing all structural contributions based on Eq. 3.

(8) The $\log 1/S$ value is calculated based on Eq. 4'.

(9) The approximate aqueous solubility value is calculated by summing up the pure atomic increments from Table 2 based on Eq. 5.

(10) The estimated $\log P$ value and the two sets of estimated aqueous solubility values in mol/l via two pathways are output.

This program has been written entirely in Fortran-77 under the MS-DOS operating system on a NEC-9800 series microcomputer. Software conversion to other machines can be readily accomplished.

TABLE 3
EVALUATION RESULTS AND COMPARISON WITH EXISTING METHODS FOR ESTIMATING THE AQUEOUS SOLUBILITY

Chemical class	Number of compounds	Data range	Average absolute error ^a in estimated Log 1/S [S: mol/l] by method of:						
			GCM	Eq.2	Kenaga ^b	Chiou ^c	Briggs ^d	Mackay ^e	Hansch ^f
<i>Liquids</i>									
Aliphatic hydrocarbons	70	C2-C10	0.18	0.32	0.63	0.35	0.27	0.30	0.27
Aromatic hydrocarbons	23	C6-C13	0.10	0.18	0.89	0.60	0.28	0.17	0.53
Halogenated hydrocarbons	81	C1-C12	0.15	0.32	1.14	0.54	0.47	0.34	0.49
Ethers and O-containing ring compd.	22	C4-C8	0.35	0.50	1.41	0.36	0.82	0.63	0.48
Alcohols and phenols	72	C4-C12	0.12	0.51	1.61	0.54	0.91	0.66	0.66
Aldehydes and ketones	22	C4-C10	0.10	0.21	1.12	0.48	0.46	0.30	0.26
Esters	30	C3-C12	0.22	0.23	1.00	0.62	0.24	0.13	0.41
N-containing compounds	11	C1-C7	0.13	0.39	0.77	0.91	0.21	0.25	0.58
S-containing compounds	5	C2-C7	0.18	0.07	1.06	0.27	0.45	0.21	0.22
Multifunctional compounds	12	C4-C14	0.65	0.49	0.97	0.67	0.29	0.41	0.50
<i>Solids</i>									
Aromatic hydrocarbons	34	C10-C24	0.35	0.42	0.78	0.48	0.37	0.38	0.60
Halogenated hydrocarbons	60	C1-C19	0.38	0.47	0.69	1.02	0.46	0.45	0.74
O-containing compounds	9	C5-C18	0.72	0.71	1.17	1.59	0.83	0.69	1.29
N-containing compounds	9	C2-C8	0.44	0.49	0.51	1.14	0.48	0.38	0.95
S-containing compounds	3	C7	0.09	0.24	0.29	1.77	0.27	0.13	0.24
Multifunctional compounds	34	C6-C19	0.45	0.50	0.55	1.22	0.51	0.52	1.01
Total	497	C1-C24	0.25 ^g	0.39	0.98	0.65	0.49	0.40	0.56

^a Average absolute error = $\Sigma |\log 1/S(\text{obsd}) - \log 1/S(\text{estd})| / \text{number of compounds}$.

^b $\log S = -0.922 \log P + 4.184 [S:\text{mg/l}]$ [Ref.9].

^c $\log S = -1.49 \log P + 7.46 [S:\mu\text{mol/l}]$ [Ref.10].

^d $\log S = -\log P - 0.01 - (0.01 T_m - 0.25) [S:\text{mol/l}, T_m:^\circ\text{C}]$ [Ref.11].

^e $\ln S = 7.494 - \ln P + 6.79 (1 - T_m/T) [S:\text{mol/m}^3, T_m:\text{K}, T = 298\text{K}]$ [Ref.12].

^f $\log 1/S = 1.339 \log P - 0.978 [S:\text{mol/l}]$ [Ref.13].

^g Number of compounds calculated by the methods of Eq.3, Eq.4, and Eq.5 are 261, 235, and 1, respectively.

ESTIMATION RESULTS

Since evaluation of calculated $\log P$ values using CHEMICALC was discussed in our previous paper [2], the evaluation of estimated values of aqueous solubilities is presented here. Results of the evaluations for 497 compounds (using regression Eq. 2) are summarized in Table 3. Average absolute errors are shown for individual families of compounds. For estimation pathway 1, comparison with five existing equations [9-13] is also shown in Table 3. The actual compounds and their values of $\log 1/S$ and $\log P$ are relegated to Appendix Table A1.

The proposed estimation pathway 1, based on Eq. 2, produced more accurate results in comparison with the available correlations for most compound classes. The regression equation reported by Mackay et al. [12] gave comparable estimation results with Eq. 2. Except for some compound classes, the results using the group contribution methods were as good or better than the correlations between $\log 1/S$ and $\log P$. However, the average absolute errors for multifunctional compounds by estimation pathway 2 were more than twice as large as those for monofunctional compounds.

Since the present group contribution methods employed are not optimal for all compounds, estimation pathway 1 will be useful for covering such drawbacks. For example, Table 4 lists those compounds showing large errors, greater than 1.0 $\log S$ units, based on the group contribution methods. The method based on Eq. 2 produced more accurate results than the group contribution methods except for a few compounds. In summary, the errors for the adopted two estimation pathways are usually small enough for practical purposes. These results confirmed the usefulness of this system.

TABLE 4
LIST OF COMPOUNDS SHOWING ERRORS GREATER THAN 1.0 LOG S UNITS USING THE GROUP CONTRIBUTION METHODS

Compound	Absolute error ^a using:	
	GCM ^{b, c}	Eq. 2
Ethyl malonate	1.40	0.56
Divinyl ether	1.93	0.03
Cyclopropyl vinyl ether	1.53	0.40
1,1-Diethoxyethane	1.55	0.04
1,2-Diethoxyethane	1.27	0.40
3-Chlorobiphenyl	1.06	0.66
2-Nitroaniline	1.28	0.53
2-Nitrophenol	1.42	0
Coronene	2.09*	1.64
3,3'-Dichlorobenzidine	1.83	0.57
2,4-Dimethylphenol	1.78	1.35
3,3',4,4'-Tetrachlorobiphenyl	1.67*	1.56
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	1.47*	0.10
Decachlorobiphenyl	2.12*	0.51
Thymol	1.64	2.16
<i>o</i> -Toluidine	1.83	1.70
<i>o</i> -Nitroacetanilide	1.21	0.51

^a Absolute error = $|\log 1/S(\text{obsd}) - \log 1/S(\text{estd})|$.

^b GCM = group contribution method.

^c The values denoted by an asterisk were calculated based on Eq. 3. Others were calculated based on Eq. 4'.

CONCLUSION

A computer program, CHEMICALC2 (the extended version of its predecessor CHEMICALC), for estimating both the 1-octanol/water partition coefficient and the aqueous solubility from structural formula has been implemented and tested. Comparison of experimental values of aqueous solubilities and those estimated by this program show good agreement. This system will be useful not only for quantitative structure-activity studies with a large set of compounds but also for preliminary selection of experimental conditions to measure the partition coefficient and/or aqueous solubility.

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APPENDIX

The list of the experimental and estimated log 1/S values for 497 compounds is shown in Table A1.

TABLE A.I
LIST OF THE ORGANIC COMPOUNDS USED FOR THE ANALYSIS

Compound	Empirical formula	log 1/S [S:mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
A. Organic liquids						
Aliphatic hydrocarbons						
1. Acetylene	C ₂ H ₂	-0.29	0.05	-0.38	0.00	0.49
2. Ethane	C ₂ H ₆	1.37	1.46	1.23	1.09	1.53
3. Propyne	C ₃ H ₄	0.41	0.66	0.30	0.76	1.21
4. Propene	C ₃ H ₆	1.28	1.50	1.27	1.24	1.67
5. Cyclopropane	C ₃ H ₆	1.07	1.83	1.62	1.18	1.61
6. Propane	C ₃ H ₈	1.90	2.07	1.89	1.65	2.06
7. Butadiyne	C ₄ H ₂	0.44	-0.14	-0.65	0.42	0.89
8. 1-Butene-3-yne	C ₄ H ₄	1.09	0.70	0.32	0.91	1.36
9. 1-Butyne	C ₄ H ₆	0.88	1.27	0.93	0.99	1.44
10. 1,3-Butadiene	C ₄ H ₆	1.48	1.54	1.28	1.40	1.82
11. 1-Butene	C ₄ H ₈	1.90	2.11	1.90	1.67	2.08
12. cis-2-Butene	C ₄ H ₈	1.93	2.11	1.90	1.99	2.39
13. trans-2-Butene	C ₄ H ₈	2.04	2.11	1.90	1.99	2.39
14. 2-Methylpropene	C ₄ H ₈	1.99	2.01	1.80	1.85	2.25
15. Butane	C ₄ H ₁₀	2.51	2.68	2.51	2.22	2.60
16. Isobutane	C ₄ H ₁₀	2.46	2.58	2.41	2.14	2.53
17. 1-Pentyne	C ₅ H ₈	1.64	1.88	1.53	1.56	1.98
18. 1,4-Pentadiene	C ₅ H ₈	2.08	2.15	1.88	1.56	1.98
19. Cyclopentene	C ₅ H ₈	2.10	2.08	2.23	1.82	2.22
20. 2-Methyl-1,3-butadiene	C ₅ H ₈	2.03	2.05	1.78	2.19	2.58
21. 1-Pentene	C ₅ H ₁₀	2.67	2.72	2.50	2.24	2.62
22. 2-Pentene	C ₅ H ₁₀	2.54	2.72	2.50	2.43	2.80
23. Cyclopentane	C ₅ H ₁₀	2.65	2.65	2.85	2.64	2.68
24. 2-Methyl-1-butene	C ₅ H ₁₀	2.73	2.62	2.40	2.28	2.66
25. 2-Methyl-2-butene	C ₅ H ₁₀	2.56	2.62	2.40	2.60	2.97
26. n-Pentane	C ₅ H ₁₂	3.27	3.29	3.11	3.04	3.14
27. Neopentane	C ₅ H ₁₂	3.12	3.09	2.91	2.62	2.99
28. 2-Methylbutane	C ₅ H ₁₂	3.18	3.19	3.01	2.70	3.06
29. 1,4-Cyclohexadiene	C ₆ H ₈	2.06	2.12	2.20	1.64	2.05
30. 1-Hexyne	C ₆ H ₁₀	2.36	2.49	2.11	2.12	2.51
31. 3-Hexyne	C ₆ H ₁₀	1.99	2.49	2.11	1.99	2.39

TABLE A.I (continued)

Compound	Empirical formula	log 1/S [\$\cdot\$mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Est. T_m [°C]
32. 1,5-Hexadiene	C ₆ H ₁₀	2.69	2.76	2.46	2.24	2.63
33. Cyclohexene	C ₆ H ₁₀	2.58	2.69	2.81	2.37	2.75
34. 2,3-Dimethyl-1,3-butadiene	C ₆ H ₁₀	2.40	2.56	2.26	3.00	3.35
35. 1-Hexene	C ₆ H ₁₂	3.23	3.33	3.08	2.79	3.15
36. Cyclohexane	C ₆ H ₁₂	3.18	3.26	3.43	3.10	3.21
37. Methylcyclopentane	C ₆ H ₁₂	3.30	3.16	3.33	2.78	3.14
38. 2-Methyl-1-pentene	C ₆ H ₁₂	3.03	3.23	2.98	2.83	3.19
39. 4-Methyl-1-pentene	C ₆ H ₁₂	3.24	3.23	2.98	2.72	3.08
40. <i>n</i> -Hexane	C ₆ H ₁₄	3.96	3.90	3.69	3.34	3.67
41. 2-Methylpentane	C ₆ H ₁₄	3.79	3.80	3.59	3.27	3.60
42. 3-Methylpentane	C ₆ H ₁₄	3.83	3.80	3.59	3.27	3.60
43. 2,2-Dimethylbutane	C ₆ H ₁₄	3.67	3.70	3.49	3.50	3.53
44. Cycloheptatriene	C ₇ H ₈	2.17	2.16	2.16	2.38	2.76
45. 1,6-Heptadiene	C ₇ H ₁₀	1.75	1.69	1.11	1.47	1.89
46. 1-Heptyne	C ₇ H ₁₂	3.01	3.10	2.68	2.68	3.05
47. 2-Heptyne	C ₇ H ₁₂	2.64	3.10	2.68	2.88	3.23
48. 2-Methyl-3-hexyne	C ₇ H ₁₂	2.59	3.00	2.58	2.80	3.16
49. 1,6-Heptadiene	C ₇ H ₁₂	3.34	3.37	3.03	2.81	3.17
50. Cycloheptene	C ₇ H ₁₂	3.16	3.30	3.38	2.94	3.29
51. 1-Methylcyclohexene	C ₇ H ₁₂	3.27	3.20	3.28	2.98	3.33
52. 2-Heptene	C ₇ H ₁₄	3.82	3.94	3.64	3.54	3.87
53. Cycloheptane	C ₇ H ₁₄	3.51	3.87	3.99	3.42	3.75
54. Methylcyclohexane	C ₇ H ₁₄	3.85	3.77	3.89	3.34	3.67
55. <i>n</i> -Heptane	C ₇ H ₁₆	4.53	4.51	4.25	3.91	4.21
56. 2,2-Dimethylpentane	C ₇ H ₁₆	3.67	4.31	4.05	3.75	4.06
57. 2,4-Dimethylpentane	C ₇ H ₁₆	4.39	4.31	4.05	3.75	4.06
58. 4-Vinylcyclohexene	C ₈ H ₁₂	3.34	3.24	3.23	3.01	3.36
59. 1-Octyne	C ₈ H ₁₄	3.66	3.71	3.24	3.25	3.59
60. 2,2-Dimethyl-3-hexyne	C ₈ H ₁₄	3.03	3.51	3.04	3.30	3.63
61. 1-Octene	C ₈ H ₁₆	4.62	4.55	4.20	3.93	4.23
62. Cyclooctane	C ₈ H ₁₆	4.15	4.48	4.55	3.99	4.29
63. 1,2-Dimethylcyclohexane	C ₈ H ₁₆	4.27	4.28	4.35	3.83	4.14
64. <i>n</i> -Octane	C ₈ H ₁₈	5.24	5.12	4.81	4.46	4.74
65. 2,2,4-Trimethylpentane	C ₈ H ₁₈	4.67	4.82	4.51	4.24	4.53

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S:mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
66. 1,8-Nonadiyne	C ₉ H ₁₂	2.98	2.91	2.23	2.59	2.96
67. 1-Nonyne	C ₉ H ₁₆	4.24	4.32	3.79	3.81	4.12
68. 2,2,5-Trimethyl-3-hexyne	C ₉ H ₁₆	3.51	4.02	3.49	4.09	4.39
69. 2,2,5-Trimethylhexane	C ₉ H ₂₀	5.05	5.43	5.06	4.80	5.06
70. 2,2,5,5-Tetramethyl-3-hexyne	C ₁₀ H ₁₈	3.69	4.53	3.94	4.59	4.86
<i>Aromatic hydrocarbons</i>						
71. Benzene	C ₆ H ₆	1.64	1.80	1.64	1.79	2.20
72. Toluene	C ₇ H ₈	2.29	2.41	2.21	2.24	2.62
73. Styrene	C ₈ H ₈	2.81	2.45	2.17	2.55	2.92
74. Ethylbenzene	C ₈ H ₁₀	2.88	3.02	2.78	2.78	3.14
75. 1,2-Dimethylbenzene	C ₈ H ₁₀	2.78	3.02	2.78	2.68	3.04
76. 1,3-Dimethylbenzene	C ₈ H ₁₀	2.73	3.02	2.78	2.67	3.04
77. 1,4-Dimethylbenzene	C ₈ H ₁₀	2.73	3.02	2.78	2.67	3.04
78. Indan	C ₉ H ₁₀	3.03	2.99	3.07	2.72	3.09
79. <i>n</i> -Propylbenzene	C ₉ H ₁₂	3.30	3.63	3.33	3.33	3.67
80. Isopropylbenzene	C ₉ H ₁₂	3.38	3.53	3.23	3.44	3.77
81. 1,2,4-Trimethylbenzene	C ₉ H ₁₂	3.32	3.63	3.33	3.11	3.46
82. 1,3,5-Trimethylbenzene	C ₉ H ₁₂	3.09	3.63	3.33	3.11	3.46
83. <i>n</i> -Butylbenzene	C ₁₀ H ₁₄	3.94	4.24	3.88	3.90	4.21
84. <i>s</i> -Butylbenzene	C ₁₀ H ₁₄	3.67	4.14	3.78	4.00	4.30
85. <i>t</i> -Butylbenzene	C ₁₀ H ₁₄	3.60	4.04	3.68	3.94	4.24
86. <i>p</i> -Cymene	C ₁₀ H ₁₄	3.76	4.14	3.78	3.88	4.19
87. 1-Methylnaphthalene	C ₁₁ H ₁₀	3.70	3.37	3.65	3.50	3.82
88. <i>t</i> -Amylbenzene	C ₁₁ H ₁₆	4.15	4.65	4.22	4.32	4.60
89. 1-Ethynaphthalene	C ₁₂ H ₁₂	4.16	3.98	4.19	4.03	4.33
90. 2-Ethynaphthalene	C ₁₂ H ₁₂	4.29	3.98	4.19	4.03	4.33
91. 1,3-Dimethylnaphthalene	C ₁₂ H ₁₂	4.29	3.98	4.19	3.93	4.23
92. 1,4-Dimethylnaphthalene	C ₁₂ H ₁₂	4.14	3.98	4.19	3.93	4.23
93. 1,4,5-Trimethylnaphthalene	C ₁₃ H ₁₄	4.92	4.59	4.73	4.33	4.65
<i>Halogenated hydrocarbons</i>						
94. Tetrachloromethane	CCl ₄	2.28	2.29	1.99	1.76	2.17
95. Bromoform	CHBr ₃	1.90	2.18	1.76	2.34	2.72

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S:mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
96. Chloroform	CHCl ₃	0.92	1.67	1.08	1.31	1.74
97. Dibromomethane	CH ₂ Br ₂	1.18	1.38	1.33	1.54	1.96
98. Bromochloromethane	CH ₂ BrCl	1.16	1.21	1.08	1.20	1.64
99. Dichloromethane	CH ₂ Cl ₂	0.63	1.04	0.78	0.86	1.31
100. Diiodomethane	CH ₂ I ₂	2.34	2.08	2.18	2.57	2.94
101. Iodomethane	CH ₃ I	1.00	1.13	1.50	1.26	1.69
102. Tetrachloroethylene	C ₂ Cl ₄	2.53	3.15	—	2.07	2.46
103. Chloropentafluoroethane	C ₂ ClF ₅	2.79	2.65	2.31	1.85	2.25
104. 1,1-Dichlorotetrafluoroethane	C ₂ Cl ₂ F ₄	2.93	2.70	2.45	2.45	2.82
105. 1,2-Dichlorotetrafluoroethane	C ₂ Cl ₂ F ₄	2.74	2.70	2.45	1.68	2.09
106. Tetrafluoroethylene	C ₂ F ₄	1.60	(1.26 atom)	—	1.09	1.53
107. 1,1,2,2-Tetrachlorodifluoroethane	C ₂ F ₂ Cl ₄	3.19	2.80	2.72	2.37	2.75
108. 1,1,2-Trichlorotrifluoroethane	C ₂ F ₃ Cl ₃	3.04	2.75	2.59	2.03	2.42
109. Trichloroethylene	C ₂ HCl ₃	1.95	2.30	1.82	1.62	2.03
110. Pentachloroethane	C ₂ HCl ₅	2.61	2.27	2.11	2.00	2.40
111. 2-Bromo-2-chloro-1,1,1-trifluoroethane	C ₂ HBrClF ₃	1.70	2.29	1.53	2.43	2.80
112. 1,1,2,2-Tetrabromoethane	C ₂ H ₂ Br ₄	2.73	2.32	2.37	3.52	3.84
113. <i>cis</i> -1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	1.10	1.45	1.24	1.17	1.60
114. <i>trans</i> -1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	1.19	1.45	1.24	1.17	1.60
115. 1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	1.76	1.64	1.57	1.64	2.05
116. 2-Bromo-2-chloro-1,1,1-trifluoroethane	C ₂ HBrClF ₃	1.70	2.29	1.53	2.43	2.80
117. 2-Chloro-1,1,1-trifluoroethane	C ₂ H ₂ ClF ₃	1.15	1.79	1.04	1.47	1.89
118. 1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	2.01	2.18	1.83	1.73	2.14
119. 1,1,2-Trichloroethane	C ₂ H ₃ Cl ₃	1.46	1.31	1.33	1.28	1.71

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
120. 1-Chloro-1,1-difluoro-ethane	C ₂ H ₃ ClF ₂	1.20	2.08	1.11	1.39	1.81
121. 1,2-Dibromoethane	C ₂ H ₄ Br ₂	1.64	1.32	1.56	1.20	1.63
122. 1,1-Dichloroethane	C ₂ H ₄ Cl ₂	1.29	1.55	1.25	1.36	1.79
123. 1,2-Dichloroethane	C ₂ H ₄ Cl ₂	1.04	0.98	1.05	1.04	1.48
124. 1-Chloro-2-bromo-ethane	C ₂ H ₄ BrCl	1.32	1.15	1.33	1.06	1.50
125. 1-Chloro-2-fluoro-ethane	C ₂ H ₄ ClF	0.51	0.93	0.47	0.20	0.68
126. 1,1-Difluoroethane	C ₂ H ₄ F ₂	0.57	1.45	0.48	0.30	0.78
127. Bromoethane	C ₂ H ₅ Br	1.06	1.39	1.26	1.14	1.58
128. 3-Chloropropene	C ₃ H ₅ Cl	1.28	1.26	—	1.15	1.59
129. Iodoethane	C ₂ H ₅ I	1.60	1.74	1.74	1.46	1.88
130. 1,2-Dibromopropane	C ₃ H ₆ Br ₂	2.14	1.83	2.00	2.32	2.70
131. 1,3-Dibromopropane	C ₃ H ₆ Br ₂	2.08	1.93	2.10	1.76	2.17
132. 1,2-Dichloropropane	C ₃ H ₆ Cl ₂	1.61	1.49	1.50	1.33	1.76
133. 1,3-Dichloropropane	C ₃ H ₆ Cl ₂	1.61	1.59	1.60	1.87	2.27
134. 1-Bromopropane	C ₃ H ₇ Br	1.73	2.00	1.81	1.70	2.11
135. 2-Bromopropane	C ₃ H ₇ Br	1.63	1.90	1.71	2.27	2.65
136. 1-Chloropropane	C ₃ H ₇ Cl	1.53	1.83	1.50	1.56	1.98
137. 2-Chloropropane	C ₃ H ₇ Cl	1.36	1.73	1.40	1.48	1.90
138. 1-Iodopropane	C ₃ H ₇ I	2.29	2.35	2.28	2.02	2.41
139. 2-Iodopropane	C ₃ H ₇ I	2.09	2.25	2.18	2.78	3.14
140. Hexachlorobutadiene	C ₄ Cl ₆	4.91	4.16	—	3.66	3.98
141. 1,1-Dichlorobutane	C ₄ H ₈ Cl ₂	2.40	2.77	2.35	2.86	3.22
142. 1-Bromobutane	C ₄ H ₉ Br	2.37	2.61	2.36	2.27	2.65
143. 2-Methyl-1-bromo-propane	C ₄ H ₉ Br	2.43	2.51	2.26	2.19	2.58
144. 1-Chlorobutane	C ₄ H ₉ Cl	2.14	2.44	2.07	2.13	2.52
145. 2-Methyl-1-chloro-propane	C ₄ H ₉ Cl	2.00	2.34	1.97	2.06	2.45
146. 1-Iodobutane	C ₄ H ₉ I	2.96	2.96	2.81	2.68	2.95
147. 3-Methyl-1-bromo-butane	C ₅ H ₁₁ Br	2.89	3.12	2.80	2.75	3.11
148. 1-Chloropentane	C ₅ H ₁₁ Cl	2.73	3.05	2.63	2.70	3.06
149. 2-Chloropentane	C ₅ H ₁₁ Cl	2.63	2.95	2.53	2.60	2.97

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
150. 3-Chloropentane	C ₅ H ₁₁ Cl	2.63	2.95	2.53	2.60	2.97
151. 1,2,4-Trichlorobenzene	C ₆ H ₃ Cl ₃	3.72	4.02	3.66	3.72	4.03
152. 1,2-Dibromobenzene	C ₆ H ₄ Br ₂	3.50	3.34	3.46	3.31	3.64
153. 1,3-Dibromobenzene	C ₆ H ₄ Br ₂	3.38	3.34	3.46	3.70	4.02
154. 2-Bromochlorobenzene	C ₆ H ₄ BrCl	3.19	3.31	3.25	3.31	3.64
155. 3-Bromochlorobenzene	C ₆ H ₄ BrCl	3.21	3.31	3.25	3.43	3.76
156. 1,2-Dichlorobenzene	C ₆ H ₄ Cl ₂	3.01	3.28	3.02	3.03	3.38
157. 1,3-Dichlorobenzene	C ₆ H ₄ Cl ₂	3.08	3.28	3.02	3.16	3.50
158. 2-Chloriodobenzene	C ₆ H ₄ ClI	3.54	3.53	3.68	3.67	3.99
159. 3-Chloriodobenzene	C ₆ H ₄ ClI	3.55	3.53	3.68	3.83	4.14
160. 1,2-Difluorobenzene	C ₆ H ₄ F ₂	2.00	1.98	1.94	2.32	2.70
161. 1,3-Difluorobenzene	C ₆ H ₄ F ₂	2.00	1.98	1.94	2.32	2.70
162. 1,4-Difluorobenzene	C ₆ H ₄ F ₂	1.97	1.98	1.94	2.32	2.70
163. Bromobenzene	C ₆ H ₅ Br	2.55	2.57	2.62	2.75	3.11
164. Chlorobenzene	C ₆ H ₅ Cl	2.36	2.54	2.35	2.48	2.85
165. Fluorobenzene	C ₆ H ₅ F	1.79	1.89	1.80	2.06	2.45
166. Iodobenzene	C ₆ H ₅ I	2.77	2.79	3.06	3.16	3.50
167. 2-Chlorophenol	C ₆ H ₅ ClO	1.05	0.92	—	2.06	2.45
168. α -Chlorotoluene	C ₆ H ₇ Cl	2.43	2.17	2.30	2.31	2.69
169. α,α,α -Trifluorotoluene	C ₇ H ₅ F ₃	2.51	2.98	2.68	2.86	3.21
170. 1-Bromo-2-ethyl-benzene	C ₈ H ₉ Br	3.67	3.79	3.69	3.54	4.05
171. 1-Bromo-2-propyl-benzene	C ₉ H ₁₁ Br	4.19	4.30	4.12	4.39	4.67
172. 2,4-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂	5.20	4.84	5.20	5.19	5.43
173. 2,5-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂	5.59	4.84	5.20	5.19	5.43
174. 3-Chlorobiphenyl	C ₁₂ H ₉ Cl	5.16	4.10	4.58	4.50	4.78
<i>Ethers and oxygen-containing ring compounds</i>						
175. Divinyl ether	C ₄ H ₆ O	0.96	-0.97	—	0.99	1.43
176. Tetrahydrofuran	C ₄ H ₈ O	-0.62	-0.47	—	0.16	0.64
177. Diethyl ether	C ₄ H ₁₀ O	0.06	0.17	—	0.64	1.10
178. Methyl <i>n</i> -propyl ether	C ₄ H ₁₀ O	0.37	0.17	—	0.69	1.15
179. Methyl isopropyl ether	C ₄ H ₁₀ O	0.03	0.07	—	0.49	0.96
180. Cyclopropyl vinyl ether	C ₅ H ₈ O	1.10	-0.53	—	0.70	1.16
181. Cyclopropyl ethyl ether	C ₅ H ₁₀ O	0.64	0.04	—	0.52	0.99

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
182. Pentamethylenoxide	C ₅ H ₁₀ O	-0.05	0.14	-	0.72	1.18
183. α -Methyltetramethylenoxide	C ₆ H ₁₂ O	-0.31	0.04	-	0.52	0.99
184. β -Methyltetramethylenoxide	C ₆ H ₁₂ O	-0.09	0.04	-	0.64	1.10
185. Methyl <i>n</i> -butyl ether	C ₆ H ₁₂ O	0.99	0.78	-	1.25	1.68
186. Methyl isobutyl ether	C ₆ H ₁₂ O	0.90	0.68	-	1.18	1.61
187. Methyl <i>s</i> -butyl ether	C ₆ H ₁₂ O	0.73	0.68	-	1.05	1.49
188. Methyl <i>t</i> -butyl ether	C ₆ H ₁₂ O	0.21	0.58	-	0.89	1.34
189. Ethyl <i>n</i> -propyl ether	C ₆ H ₁₂ O	0.67	0.78	-	1.20	1.63
190. Ethyl isopropyl ether	C ₆ H ₁₂ O	0.55	0.68	-	0.99	1.44
191. Diallyl ether	C ₆ H ₁₀ O	0.02	0.25	-	1.12	1.56
192. <i>n</i> -Propyl ether	C ₆ H ₁₄ O	1.32	1.39	-	1.76	2.17
193. Propyl isopropyl ether	C ₆ H ₁₄ O	1.34	1.29	-	1.56	1.98
194. Diisopropyl ether	C ₆ H ₁₄ O	1.70	1.19	-	1.36	1.79
195. Anisole	C ₇ H ₈ O	2.88	2.49	-	1.60	2.01
196. <i>n</i> -Butyl ether	C ₈ H ₁₈ O	2.77	2.61	-	2.89	3.24
<i>Alcohols and phenols</i>						
197. 1-Butanol	C ₄ H ₁₀ O	-0.03	-0.09	-	0.41	0.88
198. 2-Butanol	C ₄ H ₁₀ O	-0.29	-0.36	-	0.21	0.69
199. 2-Methyl-1-propanol	C ₄ H ₁₀ O	-0.10	-0.19	-	0.33	0.81
200. 1-Penten-3-ol	C ₅ H ₁₀ O	-0.02	-0.32	-	0.37	0.84
201. 3-Penten-2-ol	C ₅ H ₁₀ O	-0.06	-0.32	-	0.56	1.02
202. 4-Penten-1-ol	C ₅ H ₁₀ O	0.15	-0.05	-	0.43	0.90
203. 1-Pentanol	C ₅ H ₁₂ O	0.59	0.52	-	0.98	1.42
204. 2-Pentanol	C ₅ H ₁₂ O	0.28	0.25	-	0.78	1.23
205. 3-Pentanol	C ₅ H ₁₂ O	0.21	0.25	-	0.78	1.23
206. 2-Methyl-1-butanol	C ₆ H ₁₂ O	0.46	0.42	-	0.89	1.34
207. 2-Methyl-2-butanol	C ₆ H ₁₂ O	-0.15	-0.20	-	0.61	1.07
208. 3-Methyl-1-butanol	C ₆ H ₁₂ O	0.51	0.42	-	0.89	1.34
209. 3-Methyl-2-butanol	C ₆ H ₁₂ O	0.18	0.15	-	0.69	1.15
210. Cyclohexanol	C ₆ H ₁₂ O	0.42	0.22	-	0.86	1.31
211. 1-Hexen-3-ol	C ₆ H ₁₂ O	0.59	0.29	-	0.92	1.37
212. 2-Hexen-4-ol	C ₆ H ₁₂ O	0.40	0.29	-	1.12	1.56
213. 2-Methyl-4-penten-3-ol	C ₆ H ₁₂ O	0.50	0.19	-	0.85	1.30

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
214. 2-Methyl-1-pentanol	C ₆ H ₁₄ O	1.11	1.03	-	1.46	1.88
215. 4-Methyl-1-pentanol	C ₆ H ₁₄ O	1.14	1.03	-	1.46	1.88
216. 2-Ethyl-1-butanol	C ₆ H ₁₄ O	1.17	1.03	-	1.46	1.88
217. 2,2-Dimethyl-1-butanol	C ₆ H ₁₄ O	1.04	0.93	-	1.38	1.81
218. 1-Hexanol	C ₆ H ₁₄ O	1.21	1.13	-	1.53	1.95
219. 2-Hexanol	C ₆ H ₁₄ O	0.87	0.86	-	1.33	1.76
220. 3-Hexanol	C ₆ H ₁₄ O	0.80	0.86	-	1.33	1.76
221. 2-Methyl-2-pentanol	C ₆ H ₁₄ O	0.49	0.41	-	1.17	1.60
222. 2-Methyl-3-pentanol	C ₆ H ₁₄ O	0.70	0.76	-	1.26	1.69
223. 3-Methyl-2-pentanol	C ₆ H ₁₄ O	0.71	0.76	-	1.26	1.69
224. 3-Methyl-3-pentanol	C ₆ H ₁₄ O	0.36	0.41	-	1.17	1.60
225. 4-Methyl-2-pentanol	C ₆ H ₁₄ O	0.79	0.76	-	1.26	1.69
226. 2,3-Dimethyl-2-butanol	C ₆ H ₁₄ O	0.37	0.31	-	1.09	1.53
227. 2,3-Dimethyl-1-butanol	C ₆ H ₁₄ O	0.37	0.93	-	1.38	1.80
228. 3,3-Dimethyl-1-butanol	C ₆ H ₁₄ O	1.13	0.93	-	1.38	1.81
229. 3,3-Dimethyl-2-butanol	C ₆ H ₁₄ O	0.61	0.66	-	1.19	1.62
230. <i>m</i> -Cresol	C ₇ H ₈ O	0.66	0.79	-	1.39	1.81
231. Benzyl alcohol	C ₇ H ₈ O	0.45	0.45	-	0.46	0.93
232. 1-Heptanol	C ₇ H ₁₆ O	1.81	1.74	-	2.09	2.49
233. 2-Methyl-2-hexanol	C ₇ H ₁₆ O	1.07	1.02	-	1.73	2.14
234. 3-Methyl-3-hexanol	C ₇ H ₁₆ O	0.98	1.02	-	1.73	2.14
235. 3-Ethyl-3-pentanol	C ₇ H ₁₆ O	0.83	1.02	-	1.73	2.14
236. 2,2-Dimethyl-3-pentanol	C ₇ H ₁₆ O	1.15	1.27	-	1.74	2.15
237. 2,3-Dimethyl-2-pentanol	C ₇ H ₁₆ O	0.87	0.92	-	1.66	2.07
238. 2,3-Dimethyl-3-pentanol	C ₇ H ₁₆ O	0.84	0.92	-	1.66	2.07
239. 2,4-Dimethyl-2-pentanol	C ₇ H ₁₆ O	0.93	0.92	-	1.66	2.07
240. 2,4-Dimethyl-3-pentanol	C ₇ H ₁₆ O	1.22	1.27	-	1.74	2.15
241. 2-Heptanol	C ₇ H ₁₆ O	1.55	1.47	-	1.90	2.30
242. 3-Heptanol	C ₇ H ₁₆ O	1.44	1.47	-	1.90	2.30
243. 4-Heptanol	C ₇ H ₁₆ O	1.40	1.47	-	1.90	2.30
244. 2-Methyl-3-hexanol	C ₇ H ₁₆ O	1.32	1.37	-	1.82	2.22

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Est. T_m [°C]
245. 5-Methyl-2-hexanol	C ₇ H ₁₆ O	1.38	1.37	-	1.82	2.22
246. 2,2-Dimethyl-1-pentanol	C ₇ H ₁₆ O	1.52	1.54	-	1.94	2.34
247. 2,4-Dimethyl-1-pentanol	C ₇ H ₁₆ O	1.60	1.54	-	1.94	2.34
248. 4,4-Dimethyl-1-pentanol	C ₇ H ₁₆ O	1.55	1.54	-	1.94	2.34
249. 2,3,3-Trimethyl-2-butanol	C ₇ H ₁₆ O	0.71	0.82	-	1.59	2.00
250. 1-Octanol	C ₈ H ₁₈ O	2.35	2.35	-	2.66	3.02
251. 2-Octanol	C ₈ H ₁₈ O	2.09	2.08	-	2.46	2.83
252. 2-Ethyl-1-hexanol	C ₈ H ₁₈ O	2.11	2.25	-	2.58	2.95
253. 2-Methyl-2-heptanol	C ₈ H ₁₈ O	1.72	1.63	-	2.29	2.67
254. 3-Methyl-3-heptanol	C ₈ H ₁₈ O	1.60	1.63	-	2.29	2.67
255. 2,2,3-Trimethyl-3-pentanol	C ₈ H ₁₈ O	1.27	1.43	-	2.14	2.53
256. 1-Nonanol	C ₉ H ₂₀ O	3.01	2.96	-	3.22	3.56
257. 2-Nonanol	C ₉ H ₂₀ O	2.74	2.69	-	3.02	3.37
258. 3-Nonanol	C ₉ H ₂₀ O	2.66	2.69	-	3.02	3.37
259. 4-Nonanol	C ₉ H ₂₀ O	2.59	2.69	-	3.02	3.37
260. 5-Nonanol	C ₉ H ₂₀ O	2.49	2.69	-	3.02	3.37
261. 7-Methyl-1-octanol	C ₉ H ₂₀ O	2.49	2.86	-	3.15	3.49
262. 2,2-Diethyl-1-pentanol	C ₉ H ₂₀ O	2.42	2.76	-	3.08	3.42
263. 2,6-Dimethyl-4-heptanol	C ₉ H ₂₀ O	2.51	2.49	-	2.87	3.22
264. 3,5-Dimethyl-4-heptanol	C ₉ H ₂₀ O	2.51	2.49	-	2.87	3.22
265. α -Terpineol	C ₁₀ H ₁₈ O	1.89	1.44	-	2.41	2.79
266. 1-Decanol	C ₁₀ H ₂₂ O	3.63	3.57	-	3.79	4.10
267. 2-Undecanol	C ₁₁ H ₂₄ O	2.94	3.91	-	4.15	4.44
268. 1-Dodecanol	C ₁₂ H ₂₆ O	4.80	4.79	-	4.91	5.17
<i>Aldehydes and ketones</i>						
269. Propionaldehyde	C ₃ H ₆ O	-0.52	-0.48	-	-0.15	0.35
270. 2-Butanone	C ₄ H ₈ O	-0.68	-0.36	-	-0.22	0.28
271. Butyraldehyde	C ₄ H ₈ O	0.29	0.13	-	0.42	0.89

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Est. T_m [°C]
272. Isobutyraldehyde	C ₄ H ₈ O	-0.10	0.03	-	-0.14	0.36
273. 2-Pentanone	C ₅ H ₁₀ O	0.17	0.25	-	0.35	0.82
274. 3-Pentanone	C ₅ H ₁₀ O	0.23	0.25	-	0.29	0.77
275. 3-Methyl-2-butanone	C ₅ H ₁₀ O	0.12	0.15	-	-0.20	0.30
276. 2-Hexanone	C ₆ H ₁₂ O	0.78	0.86	-	0.91	1.36
277. 3-Hexanone	C ₆ H ₁₂ O	0.83	0.86	-	0.85	1.30
278. 3-Methyl-2-pentanone	C ₆ H ₁₂ O	0.67	0.76	-	0.36	0.83
279. 4-Methyl-2-pentanone	C ₆ H ₁₂ O	0.71	0.76	-	0.83	1.28
280. 4-Methyl-3-pentanone	C ₆ H ₁₂ O	0.81	0.76	-	0.30	0.78
281. 3,3-Dimethyl-2-butanone	C ₆ H ₁₂ O	0.71	0.66	-	0.79	1.25
282. Benzaldehyde	C ₇ H ₆ O	1.21	1.21	-	1.23	1.66
283. Heptaldehyde	C ₇ H ₁₄ O	1.96	1.96	-	2.11	2.50
284. 2-Heptanone	C ₇ H ₁₄ O	1.42	1.47	-	1.47	1.89
285. 4-Heptanone	C ₇ H ₁₄ O	1.44	1.47	-	1.42	1.84
286. 2,4-Dimethyl-3-pentanone	C ₇ H ₁₄ O	1.30	1.27	-	0.31	0.79
287. Acetophenone	C ₈ H ₈ O	1.34	1.34	-	1.31	1.74
288. 5-Nonanone	C ₉ H ₁₈ O	2.58	2.69	-	2.54	2.91
289. Carvone	C ₁₀ H ₁₄ O	2.06	1.22	-	2.13	2.52
290. Menthone	C ₁₀ H ₁₈ O	2.35	2.36	-	1.92	2.32
<i>Esters</i>						
291. Ethyl formate	C ₃ H ₆ O ₂	-0.08	-0.44	-	-0.38	0.13
292. Methyl acetate	C ₃ H ₆ O ₂	-0.52	-0.44	-	-0.56	-0.04
293. Ethyl acetate	C ₄ H ₈ O ₂	0.04	0.17	-	-0.04	0.45
294. <i>n</i> -Propyl formate	C ₄ H ₈ O ₂	0.49	0.17	-	0.18	0.66
295. Isopropyl formate	C ₄ H ₈ O ₂	0.63	0.07	-	-0.02	0.47
296. Methyl propionate	C ₄ H ₈ O ₂	0.09	0.17	-	-0.04	0.45
297. Isobutyl formate	C ₅ H ₁₀ O ₂	1.00	0.68	-	0.66	1.12
298. Ethyl propionate	C ₅ H ₁₀ O ₂	0.64	0.78	-	0.46	0.93
299. Methyl butyrate	C ₅ H ₁₀ O ₂	0.78	0.78	-	0.51	0.98
300. <i>n</i> -Propyl acetate	C ₅ H ₁₀ O ₂	0.73	0.78	-	0.52	0.99
301. Isopropyl acetate	C ₅ H ₁₀ O ₂	0.52	0.68	-	0.33	0.80
302. Isoamyl formate	C ₆ H ₁₂ O ₂	1.52	1.29	-	1.23	1.66
303. <i>n</i> -Butyl acetate	C ₆ H ₁₂ O ₂	1.37	1.39	-	1.08	1.52
304. Isobutyl acetate	C ₆ H ₁₂ O ₂	1.24	1.29	-	1.08	1.45

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S:mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
305. <i>n</i> -Propyl propionate	C ₈ H ₁₆ O ₂	1.34	1.39	—	1.02	1.47
306. Isopropyl propionate	C ₈ H ₁₆ O ₂	1.29	1.29	—	0.83	1.28
307. Ethyl butyrate	C ₈ H ₁₆ O ₂	1.28	1.39	—	1.03	1.47
308. Amyl acetate	C ₇ H ₁₄ O ₂	1.86	2.00	—	1.65	2.06
309. Isoamyl acetate	C ₇ H ₁₄ O ₂	1.91	1.90	—	1.56	1.98
310. <i>n</i> -Propyl butyrate	C ₉ H ₁₈ O ₂	1.91	2.00	—	1.60	2.01
311. Ethyl valerate	C ₇ H ₁₄ O ₂	1.77	2.00	—	1.60	2.01
312. Methyl benzoate	C ₈ H ₈ O ₂	1.53	1.60	—	1.66	2.07
313. Hexyl acetate	C ₈ H ₁₆ O ₂	2.05	2.61	—	2.20	2.59
314. Amyl propionate	C ₈ H ₁₆ O ₂	2.25	2.61	—	2.15	2.54
315. Ethyl hexanoate	C ₈ H ₁₆ O ₂	2.36	2.61	—	2.15	2.54
316. Ethyl benzoate	C ₉ H ₁₀ O ₂	2.28	2.21	—	2.17	2.56
317. Ethyl heptanoate	C ₉ H ₁₈ O ₂	2.74	3.22	—	2.72	3.08
318. Ethyl octanoate	C ₁₀ H ₂₀ O ₂	3.39	3.83	—	3.28	3.61
319. Ethyl nonanoate	C ₁₁ H ₂₂ O ₂	3.80	4.44	—	3.84	4.15
320. Ethyl decanoate	C ₁₂ H ₂₄ O ₂	4.10	5.05	—	4.41	4.69

N-containing compounds

321. Nitromethane	CH ₃ NO ₂	-0.19	-0.37	—	-1.32	-0.77
322. Nitroethane	C ₂ H ₅ NO ₂	0.24	0.24	—	-0.11	0.38
323. Propionitrile	C ₃ H ₅ N	-0.28	0.05	—	-0.32	0.19
324. Acrylonitrile	C ₃ H ₃ N	-0.18	-0.52	—	-0.52	0.00
325. 1-Nitropropane	C ₃ H ₇ NO ₂	0.81	0.85	—	0.45	0.92
326. 2-Nitropropane	C ₃ H ₇ NO ₂	0.73	0.75	—	0.20	0.68
327. 1-Nitrobutane	C ₄ H ₉ NO ₂	1.35	1.46	—	1.01	1.45
328. Nitrobenzene	C ₆ H ₅ NO ₂	1.78	1.64	—	1.51	1.93
329. Aniline	C ₆ H ₇ N	0.41	0.41	—	0.44	0.91
330. 2-Nitrotoluene	C ₇ H ₇ NO ₂	2.32	2.25	—	1.95	2.35
331. 3-Nitrotoluene	C ₇ H ₇ NO ₂	2.44	2.25	—	1.95	2.35

S-containing compounds

332. Ethanethiol	C ₂ H ₆ S	0.60	0.60	—	0.76	1.21
333. Dimethyl sulfide	C ₂ H ₆ S	0.45	0.77	—	0.39	0.86
334. Diethyl sulfide	C ₄ H ₁₀ S	1.45	1.99	—	1.53	1.95
335. Thiophenol	C ₆ H ₆ S	2.12	2.12	—	2.16	2.55
336. Thioanisole	C ₇ H ₈ S	2.39	2.39	—	2.36	2.74

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S:mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
<i>Multifunctional compounds</i>						
337. (ClCH ₂ CH ₂) ₂ S	C ₄ H ₈ Cl ₂ S	2.37	1.51	—	1.36	1.79
338. 1,1-Diethoxyethane	C ₆ H ₁₄ O ₂	0.33	-1.22	—	0.37	0.84
339. 1,2-Diethoxyethane	C ₆ H ₁₄ O ₂	0.15	-1.12	—	0.55	1.01
340. 2-Nitroanisole	C ₇ H ₇ NO ₃	1.95	2.33	—	2.09	2.48
341. Ethyl malonate	C ₇ H ₁₂ O ₄	0.89	-0.51	—	0.33	0.81
342. Ethyl succinate	C ₈ H ₁₄ O ₄	0.96	0.10	—	0.48	0.95
343. Ethyl glutamate	C ₉ H ₁₆ O ₄	1.33	0.71	—	0.40	0.87
344. Ethyl adipate	C ₁₀ H ₁₈ O ₄	1.68	1.32	—	0.97	1.41
345. Ethyl pimelate	C ₁₁ H ₂₀ O ₄	2.04	1.93	—	1.53	1.95
346. Ethyl suberate	C ₁₂ H ₂₂ O ₄	2.53	2.54	—	2.09	2.48
347. Ethyl azelate	C ₁₃ H ₂₄ O ₄	2.99	3.15	—	2.66	3.02
348. Ethyl sebacate	C ₁₄ H ₂₆ O ₄	3.51	3.76	—	3.21	3.55

B. Organic solids

<i>Aromatic hydrocarbons</i>						
349. Naphthalene	C ₁₀ H ₈	3.57	3.28	3.63	3.58	3.40
350. 2-Methylnaphthalene	C ₁₁ H ₁₀	3.75	3.46	3.74	3.58	3.82
351. Biphenyl	C ₁₂ H ₁₀	4.31	3.78	4.36	4.25	4.14
352. Acenaphthene	C ₁₂ H ₁₀	4.59	4.01	4.60	4.08	3.74
353. 1,5-Dimethylnaphthalene	C ₁₂ H ₁₂	4.68	4.51	4.73	4.46	4.23
354. 2,3-Dimethylnaphthalene	C ₁₂ H ₁₂	4.72	4.71	4.93	4.66	4.23
355. 2,6-Dimethylnaphthalene	C ₁₂ H ₁₂	4.89	4.77	4.98	4.72	4.23
356. Fluorene	C ₁₃ H ₁₀	4.92	4.19	5.09	4.60	4.04
357. Phenanthrene	C ₁₄ H ₁₀	5.15	4.44	5.22	5.03	4.59
358. Anthracene	C ₁₄ H ₁₀	6.38	5.53	6.32	6.13	4.59
359. 2-Methylantracene	C ₁₅ H ₁₂	6.69	6.03	6.73	6.46	5.01
360. 9-Methylantracene	C ₁₅ H ₁₂	5.87	4.86	5.57	5.41	5.13
361. Pyrene	C ₁₆ H ₁₀	6.18	5.32	6.30	6.04	5.05

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]				log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Eq. 2	Eq. 2
362. Fluoranthene	C ₁₆ H ₁₀	5.90	4.46	5.83	5.46	4.94	107
363. 9,10-Dimethylanthracene	C ₁₈ H ₁₄	6.57	6.43	7.06	6.93	5.66	182
364. 1,2-Benzofluorene	C ₁₇ H ₁₂	6.68	6.42	7.12	6.54	5.24	187
365. 2,3-Benzofluorene	C ₁₇ H ₁₂	7.27	6.04	7.33	6.75	5.24	209
366. Chrysene	C ₁₈ H ₁₂	8.06	6.87	8.05	7.76	5.78	256
367. Triphenylene	C ₁₈ H ₁₂	6.73	6.29	7.47	7.18	5.78	195
368. Naphthalene	C ₁₀ H ₈	8.69	7.83	9.01	8.73	5.78	357
369. 1,2-Benzanthracene	C ₁₈ H ₁₂	7.21	5.93	7.11	6.81	5.78	157
370. Perylene	C ₂₀ H ₁₂	8.80	7.43	9.30	9.02	6.24	277
371. 3,4-Benzopyrene	C ₂₀ H ₁₂	7.82	6.47	7.83	7.47	6.24	175
372. Benzo[<i>a</i>]pyrene	C ₂₀ H ₁₂	7.72	6.47	7.84	7.48	6.24	176
373. Benzo[<i>b</i>]fluoranthene	C ₂₀ H ₁₂	8.23	6.40	7.76	7.40	6.24	168
374. Benzo[<i>j</i>]fluoranthene	C ₂₀ H ₁₂	8.00	6.38	7.99	7.60	6.24	166
375. Benzo[<i>k</i>]fluoranthene	C ₂₀ H ₁₂	8.50	7.20	8.56	8.21	6.24	252
376. 9,10-Dimethyl-1,2-benzanthracene	C ₂₀ H ₁₆	6.63	6.81	7.82	7.60	6.85	121
377. 3-Methylcholanthrene	C ₂₁ H ₁₆	7.97	7.33	8.64	7.96	6.67	179
378. Benzo[<i>g,h,i</i>]perylene	C ₂₂ H ₁₂	9.02	7.32	8.86	8.45	6.70	227
379. Indeno[1,2,3- <i>cd</i>]pyrene	C ₂₂ H ₁₂	9.16	7.78	9.33	8.92	6.70	276
380. Dibenz[<i>a,h</i>]anthracene	C ₂₂ H ₁₄	8.74	7.96	9.51	9.14	6.98	269
381. Dibenz[<i>a,i</i>]anthracene	C ₂₂ H ₁₄	7.51	8.04	9.60	9.23	6.98	278
382. Coronene	C ₂₄ H ₁₂	9.33	9.70	11.42	10.97	7.16	440
<i>Halogenated hydrocarbons</i>							
383. Tetrabromomethane	CBr ₄	3.14	3.57	3.40	3.73	3.47	88
384. Triiodomethane	CHI ₃	3.55	4.18	3.90	4.83	4.18	125
385. Hexachloroethane	C ₂ Cl ₆	3.67	4.44	4.51	3.91	2.74	187
386. 1,2-Diiodoethylene	C ₂ H ₂ I ₂	3.22	3.24	3.05	3.34	3.23	73
387. Hexachlorobenzene	C ₆ Cl ₆	7.76	8.16	7.42	5.75	4.13	227
388. Pentachlorobenzene	C ₆ HCl ₅	5.65	6.04	5.44	4.59	4.34	82
389. 1,2,3,4-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	4.70	4.96	4.48	3.91	4.02	46
390. 1,2,3,5-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	4.79	5.00	4.52	4.29	4.35	50

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]				log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Eq. 2	Eq. 2
391. 1,2,4,5-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	5.56	5.83	5.36	5.35	4.56	138
392. 1,2,4,5-Tetrabromobenzene	C ₆ H ₂ Br ₄	6.98	6.37	6.52	6.32	5.08	182
393. 1,2,4-Tribromobenzene	C ₆ H ₃ Br ₃	4.50	4.29	4.44	4.44	4.55	44
394. 1,3,5-Tribromobenzene	C ₆ H ₃ Br ₃	5.60	5.02	5.17	5.58	4.93	121
395. 1,2,3-Trichlorobenzene	C ₆ H ₃ Cl ₃	3.76	4.27	3.91	3.61	3.90	51
396. 1,3,5-Trichlorobenzene	C ₆ H ₃ Cl ₃	4.44	4.38	4.02	4.19	4.14	63
397. 1,4-Dibromobenzene	C ₆ H ₄ Br ₂	4.07	3.93	4.05	4.30	4.02	87
398. 4-Bromochlorobenzene	C ₆ H ₄ BrCl	3.63	3.70	3.64	3.82	3.76	66
399. 4-Chloriodobenzene	C ₆ H ₄ ClI	4.03	3.80	3.94	4.10	4.14	53
400. 1,4-Dichlorobenzene	C ₆ H ₄ Cl ₂	3.28	3.56	3.29	3.44	3.50	54
401. 1,2-Diiodobenzene	C ₆ H ₄ I ₂	4.24	3.80	4.29	4.53	4.79	27
402. 1,3-Diiodobenzene	C ₆ H ₄ I ₂	4.57	3.92	4.41	4.65	4.79	40
403. 1,4-Diiodobenzene	C ₆ H ₄ I ₂	5.25	4.79	5.28	5.53	4.79	131
404. 4-Bromotoluene	C ₇ H ₇ Br	3.19	3.19	3.16	3.19	3.53	26
405. 2-Bromo-1-isopropylbenzene	C ₉ H ₁₁ Br	4.19	5.07	4.89	5.17	4.68	106
406. Decachlorobiphenyl	C ₁₂ Cl ₁₀	10.49	13.42	12.61	11.00	8.42	305
407. 2,2',3,3',4,4',5,5',6'-Nonachlorobiphenyl	C ₁₂ HCl ₉	9.62	11.74	11.09	9.72	8.10	206
408. 2,2',3,3',4,4',5,5'-Octachlorobiphenyl	C ₁₂ H ₂ Cl ₈	9.16	10.55	10.06	8.94	7.78	159
409. 2,2',3,3',5,5',6,6'-Octachlorobiphenyl	C ₁₂ H ₂ Cl ₈	9.83	10.58	10.08	10.09	8.85	162
410. 2,2',3,4',5,5',6-Heptachlorobiphenyl	C ₁₂ H ₃ Cl ₇	8.89	9.72	9.37	9.41	8.32	149
411. 2,2',3,3',4,4'-Hexachlorobiphenyl	C ₁₂ H ₄ Cl ₆	8.91	8.99	8.79	8.17	7.13	150
412. 2,2',3,3',4,5-Hexachlorobiphenyl	C ₁₂ H ₄ Cl ₆	8.63	8.37	8.18	7.54	7.13	85
413. 2,2',3,3',5,6-Hexachlorobiphenyl	C ₁₂ H ₄ Cl ₆	8.60	8.51	8.32	8.26	7.67	100
414. 2,2',4,4',5,5'-Hexachlorobiphenyl	C ₁₂ H ₄ Cl ₆	8.54	8.35	8.35	8.41	7.79	103

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S:mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
415. 2,2',4,4',6,6'-Hexachlorobiphenyl	C ₁₂ H ₄ Cl ₆	8.60	8.45	8.45	8.76	8.02 114
416. 2,2',3,4,5-Pentachlorobiphenyl	C ₁₂ H ₅ Cl ₅	7.52	7.77	7.73	7.13	6.60 100
417. 2,2',3,4,5'-Pentachlorobiphenyl	C ₁₂ H ₅ Cl ₅	7.86	7.89	7.84	7.59	6.93 112
418. 2,2',3,4,6-Pentachlorobiphenyl	C ₁₂ H ₅ Cl ₅	7.43	7.77	7.73	7.48	6.93 100
419. 2,2',4,5,5'-Pentachlorobiphenyl	C ₁₂ H ₅ Cl ₅	7.50	7.55	7.51	7.61	7.26 77
420. 2,3,4,5,6-Pentachlorobiphenyl	C ₁₂ H ₅ Cl ₅	7.68	8.00	7.95	7.03	6.28 124
421. 2,2',3,3'-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	6.93	7.23	7.33	7.21	6.49 121
422. 2,2',3,5'-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	6.23	6.91	7.00	7.01	6.61 87
423. 2,2',4,4'-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	6.63	6.47	6.57	6.69	6.72 41
424. 2,2',5,5'-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	7.96	6.91	7.00	7.13	6.72 87
425. 2,3',4,4'-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	6.70	7.30	7.39	7.41	6.61 128
426. 2,3,4,5-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	7.18	6.96	7.05	6.38	5.96 92
427. 2,3',4',5-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	6.85	7.07	7.17	7.18	6.61 104
428. 3,3',4,4'-Tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄	6.22	7.79	7.89	9.78	6.49 180
429. 2,2',5-Trichlorobiphenyl	C ₁₂ H ₇ Cl ₃	6.16	5.76	5.99	6.05	6.08 44
430. 2',3,4-Trichlorobiphenyl	C ₁₂ H ₇ Cl ₃	6.52	5.91	6.14	6.08	5.96 60
431. 2,4,4'-Trichlorobiphenyl	C ₁₂ H ₇ Cl ₃	6.48	5.88	6.11	6.17	6.08 57
432. 2,4,5'-Trichlorobiphenyl	C ₁₂ H ₇ Cl ₃	6.45	6.08	6.31	6.25	5.96 78
433. 3,4,4'-Trichlorobiphenyl	C ₁₂ H ₇ Cl ₃	7.23	6.18	6.41	6.35	5.96 88
434. 2,2'-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂	5.17	5.18	5.54	5.53	5.43 61
435. 2,4'-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂	5.54	5.01	5.37	5.36	5.43 43
436. 4,4'-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂	6.56	6.02	6.38	6.37	5.43 149

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S:mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Estd. T_m [°C]
437. 2-Chlorobiphenyl	C ₁₂ H ₉ Cl	4.50	4.19	4.66	4.59	4.78 34
438. 4-Chlorobiphenyl	C ₁₂ H ₉ Cl	5.21	4.60	5.08	5.01	4.78 78
439. DDT	C ₁₄ H ₉ Cl ₅	8.47	7.47	7.64	7.54	6.92 108
440. 6-Fluoro-7-methylbenz[<i>a</i>]-anthracene	C ₁₉ H ₁₃ F	7.72	6.19	7.29	7.20	6.57 110
441. 5-Fluoro-7-methylbenz[<i>a</i>]-anthracene	C ₁₉ H ₁₃ F	7.72	6.49	7.59	7.50	6.57 142
442. 9-Chloro-7-methylbenz[<i>a</i>]-anthracene	C ₁₉ H ₁₃ Cl	7.44	7.29	8.26	8.07	6.97 158
<i>O-containing compounds</i>						
443. 2,2-Dimethyl-1-propanol	C ₆ H ₁₂ O	0.39	0.58	-	1.08	1.27 52
444. 2,4-Dimethylphenol	C ₈ H ₁₀ O	3.19	1.41	-	1.84	2.23 26
445. Thymol	C ₁₀ H ₁₄ O	1.10	2.75	-	3.26	3.38 49
446. Menthol	C ₁₀ H ₂₀ O	2.57	2.53	-	3.04	3.23 43
447. Diphenyl ether	C ₁₂ H ₁₀ O	3.97	3.47	-	3.60	3.89 28
448. 1-Tetradecanol	C ₁₄ H ₃₀ O	5.84	6.13	-	6.16	6.24 38
449. 1-Pentadecanol	C ₁₅ H ₃₂ O	6.35	6.81	-	6.79	6.78 45
450. 1-Hexadecanol	C ₁₆ H ₃₄ O	7.00	7.45	-	7.38	7.31 48
451. 1-Octadecanol	C ₁₈ H ₃₈ O	8.40	8.76	-	8.60	8.38 58
<i>N-containing compounds</i>						
452. Methyl carbamate	C ₂ H ₅ NO ₂	-0.96	-0.90	-	-1.36	-1.05 52
453. Ethyl carbamate	C ₃ H ₇ NO ₂	-0.73	-0.33	-	-0.88	-0.56 48
454. Propyl carbamate	C ₄ H ₉ NO ₂	0.13	0.39	-	-0.21	-0.03 60
455. Isobutyl carbamate	C ₅ H ₁₁ NO ₂	0.77	0.97	-	0.35	0.44 67
456. Isoamyl carbamate	C ₆ H ₁₃ NO ₂	1.44	1.41	-	0.73	0.97 49
457. Benzamide	C ₇ H ₇ NO	1.32	0.82	-	1.63	0.64 130
458. 4-Nitrotoluene	C ₇ H ₇ NO ₂	2.49	2.51	-	2.21	2.35 52
459. <i>o</i> -Toluidine	C ₇ H ₉ N	0.85	2.68	-	2.55	1.33 200
460. Acetanilide	C ₈ H ₉ NO	1.41	0.50	-	1.49	1.11 113
<i>S-containing compounds</i>						
461. <i>o</i> -Toluenesulfonamide	C ₇ H ₉ NO ₂ S	2.02	1.33	-	1.59	0.93 143
462. <i>m</i> -Toluenesulfonamide	C ₇ H ₉ NO ₂ S	1.34	1.00	-	1.25	0.93 108
463. <i>p</i> -Toluenesulfonamide	C ₇ H ₉ NO ₂ S	1.73	1.27	-	1.53	0.93 137

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Eq. 1
Multifunctional compounds						
464. 1,3-Dinitrobenzene	C ₆ H ₄ N ₂ O ₄	2.41	2.08	-	1.82	1.65
465. 2-Nitrophenol	C ₆ H ₅ NO ₃	1.62	0.20	-	1.62	1.86
466. 3-Nitrophenol	C ₆ H ₅ NO ₃	0.66	0.69	-	1.33	1.12
467. 4-Nitrophenol	C ₆ H ₅ NO ₃	0.63	0.85	-	1.49	1.12
468. 2-Nitroaniline	C ₆ H ₆ N ₂ O ₂	1.97	0.69	-	1.44	1.44
469. 3-Nitroaniline	C ₆ H ₆ N ₂ O ₂	2.06	1.08	-	0.98	0.63
470. 4-Nitroaniline	C ₆ H ₆ N ₂ O ₂	2.28	1.43	-	1.33	0.63
471. <i>m</i> -Phenylenediamine	C ₆ H ₈ N ₂	-0.34	-0.61	-	-0.55	-0.39
472. <i>p</i> -Phenylenediamine	C ₆ H ₈ N ₂	0.47	1.11	-	1.18	-0.39
473. <i>p</i> -Nitrobenzaldehyde	C ₇ H ₅ NO ₃	1.81	1.81	-	1.69	1.38
474. <i>m</i> -Nitrobenzaldehyde	C ₇ H ₅ NO ₃	1.97	1.35	-	1.24	1.38
475. 4-Nitroanisole	C ₇ H ₇ NO ₃	2.41	2.61	-	1.58	1.73
476. Phenylthiourea	C ₇ H ₈ N ₂ S	1.86	1.25	-	1.24	0.50
477. Vanillin	C ₈ H ₈ O ₃	1.18	0.80	-	0.93	0.88
478. Methyl <i>p</i> -hydroxybenzoate	C ₈ H ₈ O ₃	1.84	0.94	-	1.77	1.26
479. Methyl <i>p</i> -amino-benzoate	C ₈ H ₉ NO ₂	1.60	1.07	-	1.16	0.78
480. Phthalimide	C ₈ H ₅ N ₂ O ₂	2.39	-0.14*	-	0.55	-0.92

*Original method [Ref.6] gives 2.40.

TABLE A1 (continued)

Compound	Empirical formula	log 1/S [S.mol/l]			log P	
		Obsd.	Eq. 4'	Eq. 3	Eq. 2	Eq. 1
481. <i>o</i> -Nitroacetanilide	C ₈ H ₈ N ₂ O ₃	1.91	0.70	-	2.42	1.65
482. <i>p</i> -Nitroacetanilide	C ₈ H ₈ N ₂ O ₃	1.91	1.30	-	2.17	0.84
483. Ethyl <i>p</i> -hydroxybenzoate	C ₉ H ₁₀ O ₃	2.22	1.45	-	2.18	1.74
484. <i>p</i> -Acetanilide	C ₉ H ₁₁ NO ₂	1.04	1.35	-	1.45	0.92
485. Ethyl <i>p</i> -aminobenzoate	C ₉ H ₁₁ NO ₂	1.99	1.42	-	1.41	1.26
486. Propyl <i>p</i> -hydroxybenzoate	C ₁₀ H ₁₂ O ₃	2.59	1.87	-	2.54	2.28
487. Phenacetin	C ₁₀ H ₁₃ NO ₂	1.10	2.00	-	2.01	1.41
488. Propyl <i>p</i> -aminobenzoate	C ₁₀ H ₁₃ NO ₂	2.33	1.90	-	1.84	1.80
489. Butyl <i>p</i> -hydroxybenzoate	C ₁₁ H ₁₄ O ₃	2.89	2.22	-	2.86	2.82
490. Butyl <i>p</i> -aminobenzoate	C ₁₁ H ₁₅ NO ₂	2.76	2.33	-	2.23	2.33
491. 3,3'-Dichlorobenzidine	C ₁₂ H ₁₀ Cl ₂ N ₂	4.91	3.08	-	4.34	3.65
492. Pentyl <i>p</i> -aminobenzoate	C ₁₃ H ₁₇ NO ₂	3.35	2.91	-	2.76	2.87
493. Hexyl <i>p</i> -aminobenzoate	C ₁₃ H ₁₉ NO ₂	3.95	3.60	-	3.41	3.41
494. Heptyl <i>p</i> -aminobenzoate	C ₁₄ H ₂₁ NO ₂	4.60	4.35	-	4.10	3.94
495. Octyl <i>p</i> -aminobenzoate	C ₁₅ H ₂₃ NO ₂	5.40	4.92	-	4.62	4.48
496. Nonyl <i>p</i> -aminobenzoate	C ₁₆ H ₂₅ NO ₂	6.00	5.51	-	5.17	5.01
497. Dodecyl <i>p</i> -amino-benzoate	C ₁₉ H ₃₁ NO ₂	7.80	7.46	-	6.98	6.62