Computer Automated log P Calculations Based on an Extended Group Contribution Approach

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A program for the automatic calculation of the logarithm of the partition coefficient between *n*-octanol and water (log *P*) for organic compounds was developed. The log *P* model was derived from a multivariate regression analysis based on a database consisting of 1663 organic molecules with diverse structures. The parameters used in the model are basic functional groups and correction factors which were automatically identified by the Computer Automated Structure Evaluation (CASE) program. The CASE program was used to identify the correction terms for members of each congeneric series with large deviations. This approach was found to be better than our previously reported methodologies and accurate enough to give good log *P* estimations, even for the most complex molecules.

INTRODUCTION

The logarithm of the partition coefficient between *n*-octanol and water (log *P*) has often been used to represent molecular lipophilicity, which seems to be a key factor related to the transport process through cell membranes and to many other biological events.[1-4] Indeed, log *P* has been found to be a crucial parameter in many quantitative structure–bioactivity relationship (QSBR) studies and has been widely used in the practice of today's rational drug design methods.[5,6] Therefore, accessibility to accurate log *P* values for compounds of interest may be essential for the correct prediction of their biological activity. The experimental determination of the log *P* value of a compound is a relatively easy task, although it may be time consuming. However, it was found that there is an increasing need for reliable estimates of log *P* values for new compounds often not synthesized as yet, particularly for drug design purposes.

Several approaches for the estimations of log *P* values have been proposed;[7] all of them are directly or indirectly based on the chemical structure of the compounds. One of the earliest approaches with wide applicability is known as the fragmental constant method pioneered by Rekker et al. and based on the assumption that log *P* has an additive–constitutive nature.[8] These authors used a "reductionist approach" to derive the fragmental contribution to calculate the log *P* values. Leo and Hansch developed a similar method based on fragment constants by a "constructionist approach" at about the same time.[9,10] These approaches work well for many simple compounds but have limitations for a number of complex compounds where correction factors have to be introduced. Thus, major efforts have been made to include a large number of correction factors to improve the accuracy of the calculations.[11,12]

Meanwhile, both Klopman's[13,14] and Crippen's[15,16] groups have been using atomic and group contributions for the calculations of log *P* values. Their approaches employ multiple regression analysis to establish a statistical model based on a learning database. An example of this approach was recently published by Klopman and Wang, who used the Computer Automated Structure Evaluation (CASE) program to develop a model for the calculations of log *P*, in which simple atomic types and star centered fragments were used as descriptors. Good results were obtained for a database consisting of 935 organic compounds (r^2 = 0.93, SD = 0.39).

Molecular properties have also been used as descriptors to correlate with log *P* values. Klopman and Iroff used atomic charges as parameters to estimate the log *P* values for simple organic compounds.[17] Bodor et al. have recently developed two log *P* estimation models in which charge densities, molecular surfaces, molecular volumes, ovalities, molecular weights, dipoles of molecules, etc., were used as regression parameters.[18,19] In their recent publication, a nonlinear equation was obtained with 18 molecular parameters for a database of 302 compounds. Good results were obtained (r^2 = 0.978, SD = 0.31), although the applicability of this approach needs to be verified outside the relatively small database used in the study.

An attempt to estimate the log *P* values of some simple organic compounds using Monte Carlo simulation has been also reported.[20-22] This approach demands a great amount of computer time and is difficult to parametrize for the *n*-octanol/water system. Although this approach is not practical at the present time, it is a promising approach for the future.

Among all the current log *P* estimation approaches, the group contribution approach shows several advantages. It is conceptually simple and able to give fast and rather accurate estimations for many organic compounds. Poor estimations for certain compounds using group contribution alone were found to be primarily due to the interaction between groups in these compounds. Therefore, the inclusion of some correction factors representing group interactions should improve the accuracy of the log *P* estimation. Identification of these interactions (correction factors) normally requires detailed studies on the chemical structures and is somewhat *ad hoc*, as demonstrated by Leo and Hansch.[9,11]

In this paper, we employed the CASE program[23,24] to automatically identify these correction factors. Then, we combined the basic group parameters and correction factors to develop a log *P* estimation model.

METHODS

The establishment of an error free learning database is extremely important for the developmment of a reliable log *P* estimation model. The log *P* values reported in the literature were determined by various methods under different exper-

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imental conditions. Therefore, some care has to be taken in the process of selecting entries for the learning database. Factors such as the solvent system, buffer solutions, and consistency of data have to be considered. For example, in cases where the experimental log P value of the same compound is reported by different sources, the deviation should not be greater than 0.4 log unit.

The predictive ability and applicability of a log P estimation model is strongly affected by the size of the learning database. Hence, we extended our previous database of 935 compounds to 1663 compounds. These compounds mainly came from Hansch and Leo's compilation[9,10] with the addition of a number of compounds from the collection of Suzuki and Kudo[25] and Viswanadhan et al.[28,29]

The molecular structures were encoded using the Klopman Line Notation (KLN) code.[26] A set of basic group parameters were defined, and a program was developed to automatically identify the occurrence of each group parameter in the compounds. The basic group parameters consist of two fundamental types: (1) heavy atoms with both their hybridization and the number of hydrogen(s) attached to them and (2) fundamental functional groups (OH, CHO, COOH, COO, $CONH_2$, CONH, CON, CON=, CO, CS, NO, NO_2, PO, SO, SO_2, NH_2, NH, CN, SH, etc.). In some cases, the nearest heavy atoms are also specified. The log P values and occurrence of the group parameters for all the compounds of the database were then submitted to a multivariate linear regression analysis. An equation correlating the log P values to the basic group parameters was obtained in the form of eq 1,

$$\log P = a + \sum b_i B_i \qquad (1)$$

where a is a constant, b_i is the contribution coefficient of the ith group, and B_i is the number of occurrences of the ith group. This equation implies that the effects of interactions between groups are negligible. The significance of each parameter and the equation resulting from their use was evaluated by our analysis of their statistical t and F values, respectively.

Although eq 1 gave reasonably good log P retrofit values for many compounds of the database, there still was a significant number of compounds showing unacceptably high deviations. This was interpreted as an indication that the interactions between some groups in these compounds have a substantial effect on their log P values. We postulated that most of these effects could be due to substructures not represented by our set of basic group parameters. The CASE methodology[24] then could be used to identify these substructures which may be responsible for the large error when eq 1 is used.

The CASE methodology has been described on a number of occasions.[23,24] Basically, the CASE program is an artificial intelligence system capable of identifying structural descriptors that may be associated with the properties of the molecules which are examined, such as biological activity or physicochemical property. A general scheme of the program is shown in Figure 1.

Molecular structures and the index of activity are required by the program as the input. A break-point activity value is chosen between the active and inactive molecules of the learning set to ensure a suitable distribution between active and inactive molecules in the data set for the discriminant analysis. Specifically, CASE takes each molecule of the learning set and breaks it into all possible linear fragments of 2–10 connected heavy atoms. These fragments are labeled as active or inactive, depending on whether or not the parent molecule is active. The occurrence of these fragments then

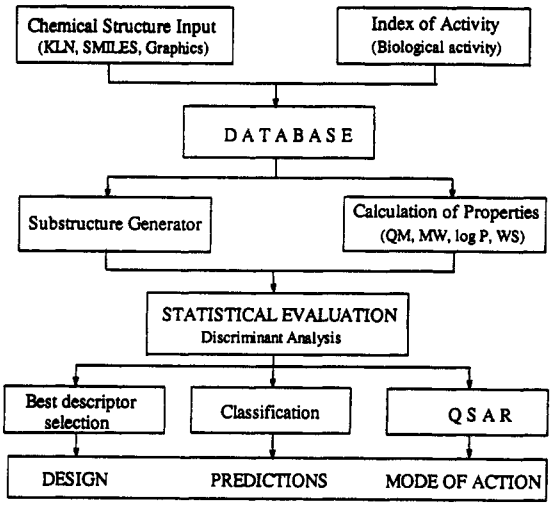


Figure 1. General scheme of the CASE program.

is submitted to a series of statistical analyses to identify those whose distribution is significantly skewed toward either actives or inactives in the entire database. Furthermore, these significant fragments are used as descriptors in a quantitative structure–activity relationship (QSAR) analysis to yield a linear regression equation that best describes the activity of the compounds in the database.

In this study, we are interested in finding substructures responsible for the calculation error in eq 1 using the CASE program. To do so, we took the difference between the log P value estimated from eq 1 and the experimental value entered as input for the CASE analysis. Subsequently, in the fragment generation step, the fragments are labeled as active if they originate from compounds with positive error or inactive if they originate from compounds with negative error. The significant fragments identified by the CASE analysis were subsequently used for the development of the final log P estimation model in addition to the basic group parameters. These additional substructure parameters enable the new log P model to account for effects of group interaction and serve as correction features. Hence, the final log P estimation model obtained is of the form

$$\log P = a + \sum b_i B_i + \sum c_j C_j \qquad (2)$$

where a, b_i, and c_j are regression coefficients, B_i is the number of occurrences of the ith basic group, and C_j is the number of occurrences of the jth correction factor identified by the CASE program.

RESULTS AND DISCUSSION

(1) log P Estimation Model Using Group Contribution Alone. Our log P calculation model was established on the basis of a learning database of 1663 compounds with diverse structures. A graphics program GMK[27] was used to ensure that the structures entered in the program were correct.

The initial model was established on the basis of the basic group contribution parameters alone. There are 68 fundamental group parameters, as shown in Table 1. Of these, 64 were found significant enough to be used in the linear regression analysis. The model generated a r^2 value equal to 0.838 and showed a standard deviation equal to 0.577. The standard error of 0.58 is fairly good considering the size of the database and the number of parameters used.

The 1663 compounds were divided into 12 classes on the basis of their chemical structure. The log P estimation error for each class of compounds is listed in Table 2, and a histogram

Table 1. List of Fundamental Group Parameters

param	remarks	param	remarks
1. $-CH_3$		35. $-C^*OO-$	
2. $-CH_2-$		36. $-CONH_2$	
3. $-CH<$		37. $-CONH-$	
4. $>C<$		38. $-CON<$	
5. $=CH_2$		39. $-CON=$	
6. $=CH-$	not in –CHO	40. $-CO-$	not in –COOH, –COO–, $-CONH_{2(1,0)}-$
7. $=C<$	not in –CO–, –CS–	41. $-C^*O-$	not in $-C^*OO-$
8. $=C=$		42. $-NO$	not in $-NO_2$
9. $-C\equiv CH$	including $HC\equiv CH$	43. $-PO$	not in $-PO_4$
10. $-C\equiv$	not in $-C\equiv N$, $-C\equiv CH$	44. $-SO-$	not in $-SO_2$
11. $-C^*H_2-$		45. $-NH_2$	primary
12. $-C^*H<$		46. $-NH_2$	secondary, tertiary
13. $>C^*<$		47. $-NH_2$	aniline
14. $=C^*H-$		48. $-NH_2$	the other, not in $CONH_2$
15. $=C^*<$		49. $-NH-$	not in –CONH–
16. –F	connected to C_{arom}	50. $-N<$	not in –CON<
17. –F	not connected to C_{arom}	51. $-N^*H-$	not in $-CON^*H-$
18. –Cl	connected to C_{arom}	52. $-N^*<$	not in $-CON^*<$
19. –Cl	not connected to C_{arom}	53. $-C\equiv N$	connected to C_{arom}
20. –Br	connected to C_{arom}	54. $-C\equiv N$	not connected to C_{arom}
21. –Br	not connected to C_{arom}	55. $=NH$	
22. –I	connected to C_{arom}	56. $=N-$	
23. –I	not connected to C_{arom}	57. $=N^*-$	including aromatic N
24. –OH	primary alcohol	58. $-NO_2$	connected to C_{arom}
25. –OH	secondary alcohol	59. $-NO_2$	not connected to C_{arom}
26. –OH	tertiary alcohol	60. –SH	
27. –OH	phenol	61. –S–	
28. –OH	the others	62. $-S^*-$	
29. $-O^*-$	not in ester	63. $=S$	not in $-N=C=S$
30. –O–	not in ester	64. –CS–	
31. –CHO	aldehyde	65. $-SO_2$	
32. –COOH	connected to C_{arom}	66. $-S^*O_2$	
33. –COOH	not connected to C_{arom}	67. $-P=$	not in $-P=O$
34. –COO–		68. $-P=(<)$	

[a] An asterisk indicates the atom in a ring system; C_{arom} refers to an aromatic carbon atom; the symbol in the parentheses indicates the open valence, not filled by hydrogen.

Table 2. Estimation Result for Different Classes of Compounds

compd class	no. of compds	std dev: group contribution	std dev: final model
aliphatic hydrocarbon	28	1.14	0.28
aromatic hydrocarbon	52	0.77	0.20
alcohol, ether, phenol	74	0.36	0.31
ketone, aldehyde	27	0.33	0.31
acid, ester	43	0.32	0.30
amine, nitrile	66	0.62	0.38
amide, anilide	23	0.59	0.39
sulfur-containing hydrocarbon	9	0.54	0.36
nitro-containing hydrocarbon	18	0.35	0.35
amino acid	10	1.03	0.24
halogen hydrocarbon	54	0.39	0.43
multifunctional compounds	1259	0.58	0.40
all	1663	0.58	0.38

of the estimation error between the experimental and calculated log P values is shown in Figure 2. As can be seen in Figure 2, there are a number of compounds with unacceptable deviations. Table 2 shows that the compounds with the largest errors are primarily aliphatic and aromatic hydrocarbons, amino acids, and chemicals with multiple functional groups.

The contributions of the basic groups used in our log P model were obtained without consideration of the interactions between these groups. Our results show that log P calculations using basic group contribution alone are usually satisfactory for simple compounds, such as monofunctional compounds. However, when this model is applied to compounds containing multiple functional groups, correction factors need to be included to account for the possible interactions between these groups.

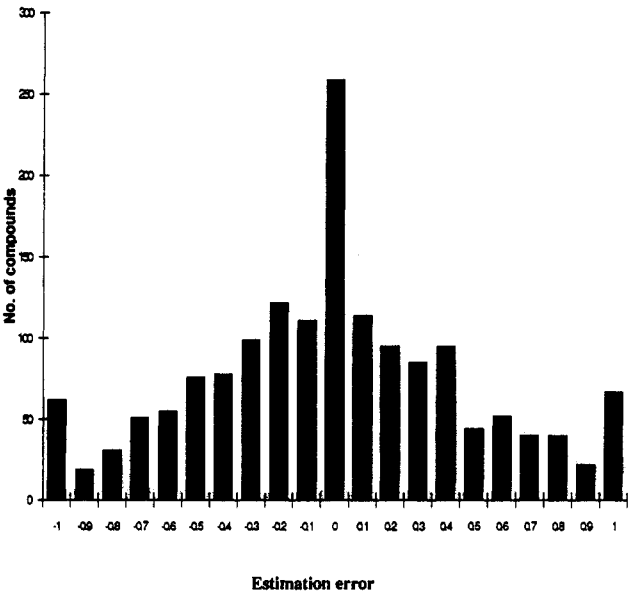


Figure 2. Estimation error distribution.

(2) Final log P Estimation Model. The CASE program identified 25 statistically significant fragments (parameters 69–93) responsible for the large estimation errors. Besides the CASE correction factors, five other additional correction parameters (parameters 94–98) were included in our model to account for the large estimation errors seen in alkanes, unsaturated hydrocarbons, and compounds with folding capability.

The log P program automatically tabulated the 98 parameters, as shown in Table 3. Since four basic group parameters have zero occurrence in our database, their log P contribution

Table 3. Contribution Values to the log P of the Basic Group Set and the Correction Factors[a]

param	no. of compds	freq of occurrence	contribution	remarks
1. –CH_3	855	1391	0.661	
2. –CH_2–	610	1180	0.415	
3. –CH<	138	169	0.104	
4. >C<	99	107	–0.107	
5. =CH_2	31	37	0.553	
6. =CH–	70	108	0.315	not in –CHO
7. =C<	39	39	0.470	not in –CO–, –CS–
8. =C=	21	22	1.748	
9. –C≡CH	4	4	0.262	including HC≡CH
10. –C≡	2	4	0.131	not in –C≡N, –C≡CH
11. –C*H_2–	148	420	0.360	
12. –C*H<	107	287	0.104	
13. >C*<	27	31	0.064	
14. =C*H–	1331	5946	0.380	
15. =C*<	1322	3065	0.129	not in –C*O–
16. –F	36	45	0.468	connected to C_{arom}
17. –F	81	212	0.487	not connected to C_{arom}
18. –Cl	147	214	0.905	connected to C_{arom}
19. –Cl	47	108	0.713	not connected to C_{arom}
20. –Br	58	79	1.088	connected to C_{arom}
21. –Br	23	25	1.021	not connected to C_{arom}
22. –I	25	26	1.442	connected to C_{arom}
23. –I	6	6	1.209	not connected to C_{arom}
24. –OH	118	120	–0.681	primary alcohol
25. –OH	65	78	–0.575	secondary alcohol
26. –OH	8	9	–0.415	tertiary alcohol
27. –OH	185	196	0.135	phenol
28. –OH	16	16	–0.190	the others
29. –O*–	67	73	0.103	not in ester
30. –O–	235	270	–0.402	not in ester
31. –CHO	15	15	0.009	aldehyde
32. –COOH	72	73	0.467	connected to C_{arom}
33. –COOH	141	148	–0.263	not connected to C_{arom}
34. –COO–	195	199	–0.414	
35. –C*OO–	7	8	–0.874	
36. –$CONH_2$	86	92	–0.795	
37. –CONH–	239	325	–1.006	
38. –CON<	94	109	–1.283	
39. –CON=	17	18	–1.661	
40. –CO–	68	70	–0.493	not in –COOH, –COO–, –$CONH_{2(1,0)}$–
41. –C*O–	28	41	–0.187	not in –C*OO–
42. –NO	36	39	–0.469	not in –NO_2
43. –PO				not in –PO_4
44. –SO–	5	5	–1.320	not in –SO_2
45. –NH_2	36	36	–0.894	primary
46. –NH_2	21	21	–0.759	secondary, tertiary
47. –NH_2	132	139	–0.402	aniline
48. –NH_2	70	73	0.050	the other, not in –$CONH_2$
49. –NH–	94	95	0.021	not in –CONH–
50. –N<	42	44	–0.937	not in –CON<
51. –N*H–	73	77	–0.160	not in –CON*H–
52. –N*<	111	122	–1.027	not in –CON*<
53. –C≡N	28	28	–0.067	connected to C_{arom}
54. –C≡N	43	45	0.072	not connected to C_{arom}
55. =NH				
56. =N–	71	74	0.739	
57. =N*–	63	102	–0.034	including aromatic N
58. –NO_2	140	160	0.220	connected to C_{arom}
59. –NO_2	9	9	0.079	not connected to C_{arom}
60. –SH	5	5	0.875	
61. –S–	37	38	0.485	
62. –S*–	24	24	0.812	
63. =S				not in –N=C=S
64. –CS–	9	9	–0.042	
65. –SO_2	50	50	–0.818	
66. –S*O_2	3	3	–0.984	
67. –P=				not in –P=O
68. –P=(<)	4	4	–0.450	
69. HO–C=N–	5	5	–1.133	
70. HO–CO–C=N–	3	3	–3.578	
71. –NH–N=CH–X	7	7	0.363	X not N=
72. HCO–X	12	12	0.736	X not C
73. $NH_{2(1,0)}$–CO–$NH_{2(1,0)}$	89	182	0.510	
74. $OH_{(0)}$–CO–$NH_{2(1,0)}$	82	83	0.652	
75. –CO–$NH_{(0)}$–CO–	46	116	0.541	
76. –$CH_{2(1,0)}$–NH–$CH_{2(1,0)}$–	35	72	–0.367	
77. –$CH_{2(1,0)}$–O–$CH_{2(1,0)}$–	69	148	–0.121	
78. –N=C($NH_{2(1)}$)–N=	16	24	–0.185	
79. HO–C=C–CO–OH	9	10	0.419	

Table 3. (Continued)

param	no. of compds	freq of occurrence	contribution	remarks
80. HO–C=C–CO–	27	27	0.730	
81. HO–CO–$CH_{2(1)}$–$NH_{2(1)}$	13	13	−1.846	
82. =NH(0)–N=N–N=	14	15	0.326	including =$NH_{(0)}$–N=N–$CH_{(0)}$–, =$NH_{(0)}$–N=$CH_{(0)}$–N=
83. –C–N(–NH_2)–C=N	7	7	0.178	
84. HO–CO–CH_2–O–	67	67	0.261	
85. $NH_{2(1)}$–CH_2–CH_2–OH	16	17	−0.324	
86. $NH_{2(1)}$–CO–N–NO	8	8	0.704	
87. –N=$CH_{(0)}$–$CH_{(0)}$=C–OH	10	12	−0.494	
88. NO_2–C=$CH_{(0)}$–$CH_{(0)}$=C–OH	3	4	0.302	
89. NO_2–C=$CH_{(0)}$–$CH_{(0)}$=C–NH_2	8	14	0.185	
90. NH2–C=$CH_{(0)}$–$CH_{(0)}$=C–CO–OH	23	47	−0.530	including NH_2–C=$CH_{(0)}$–C–CO–OH
91. $NH_{2(1)}$–C=$CH_{(0)}$–$CH_{(0)}$=C–SO_2–$NH_{2(1)}$	14	28	−0.466	
92. –CO–NH–C=$CH_{(0)}$–$CH_{(0)}$=C–OH	16	32	−0.187	
93. CH_3–CH_2–CH_2–CH_2–CH_2–CH_2–	14	14	0.824	not in the alkane
94. OH–$(CH_2)_n$–pyridine	9	12	−0.650	$n \geq 3$
95. NH_2–$(CH_2)_n$–pyridine	9	12	−0.545	$n \geq 3$
96. NH_2–CO–$(CH_2)_n$–pyridine	12	16	−0.903	$n \geq 2$
97. no. of atoms in alkane	13	13	0.095	including cycloalkane
98. unsaturated hydrocarbon	67	67	0.872	
constant			−0.703	

[a] An asterisk indicates the atom in a ring system; C_{arom} refers to an aromatic carbon atom; a symbol in the parentheses indicates the open valence, not filled by hydrogen; a number in the parentheses indicates the acceptable number of hydrogen atoms.

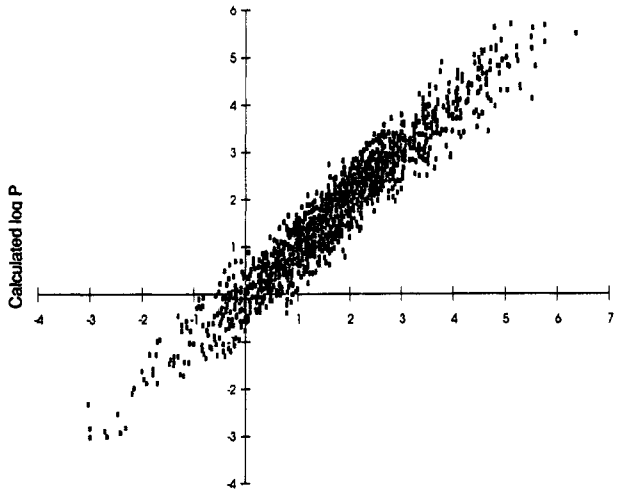


Figure 3. Correlation between the experimental and calculated log *P*.

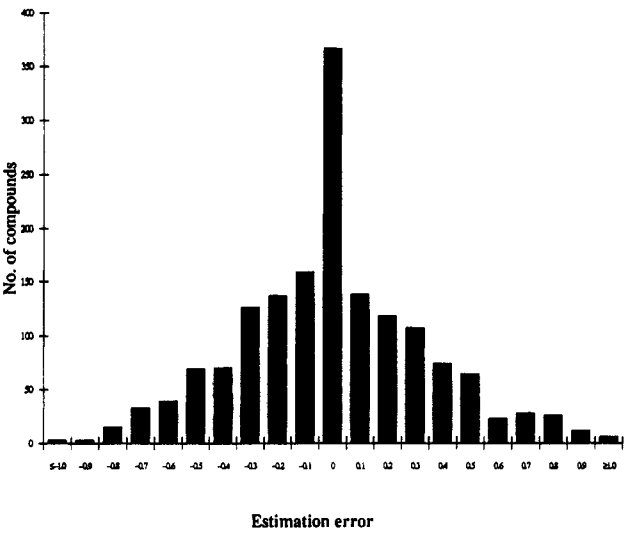


Figure 4. Distribution of estimation error.

values could not be evaluated. The final log *P* estimation model was obtained by correlating the remaining 94 parameters with the log *P* values through a multivariate linear-regression analysis (n = 1663, r^2 = 0.928, SD = 0.3817, F(94, 1568) = 217.77). The standard deviation of 0.38 is within the experimental error range of 0.4 in spite of the fact that a relatively small number of parameters were used in our model for such a large database.

A plot of the experimental log *P* values vs the calculated log *P* values for all the compounds in the database is shown in Figure 3. This figure shows good agreement between the experimental and calculated log *P* values for the 1663 compounds with diverse structures. The histogram of estimation errors is shown in Figure 4, where a near-Gausian error distribution curve centered at zero is seen.

The experimental and calculated log *P* values of the 1663 compounds, as well as the estimation errors, have been summarized in Table 4. There are 71 compounds showing deviations greater than or equal to 0.8 log unit, as shown in Table 5. To improve the calculation for these outliers will require the development of new correction factors. We found that each of these 71 outliers contain at least one unique fragment in its structure. The inclusion of these unique fragments would definitely improve the accuracy of the log *P* estimation. However, we did not include these unique fragments in our final log *P* model because (1) they are not statistically significant and their value based on one compound may not lead to a stable correlation and (2) in some compounds, a number of unique fragments exists, which makes it difficult to decide which of these should be used as the correction factor. Nevertheless, in the future when more compounds containing these unique fragments become available, their contribution to the log *P* values may be evaluated and hence be included in our log *P* model.

Table 2 also shows the average deviation for the 12 classes of compounds, as defined before, in the final model. As can be seen, the final model gives accurate log *P* values not only for the simple compounds but also for the complex ones. Comparing these values in Table 2, it can be seen that the accuracy of the calculated log *P* values for amino acids, hydrocarbons, and multifunctional compounds was greatly improved by the inclusion of these correction factors. Overall, the standard deviation has been reduced by about 0.2 log unit from 0.58 to 0.38, and the r^2 value has been increased from 0.84 to 0.93.

Table 4. Experimental, Calculated log *P* Values, and Estimation Error

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Aliphatic Hydrocarbons			
1. C_2H_4	ethylene	1.13	1.27	0.14
2. C_2H_6	ethane	1.81	1.38	−0.43
3. C_3H_4	propyne	0.94	1.09	0.15
4. C_3H_6	propylene	1.77	1.70	−0.07
5. C_3H_6	cyclopropane	1.72	1.23	−0.49
6. C_3H_8	propane	2.36	2.08	−0.28
7. C_4H_6	1,3-butadiene	1.99	1.90	−0.09
8. C_4H_6	2-butyne	1.46	1.75	0.29
9. C_4H_8	isobutylene	2.34	2.51	0.17
10. C_4H_8	2-butene	2.31	2.12	−0.19
11. C_4H_8	1-butene	2.40	2.11	−0.29
12. C_4H_{10}	isobutane	2.76	2.71	−0.05
13. C_4H_{10}	butane	2.89	2.78	−0.11
14. C_5H_8	1-pentyne	1.98	1.92	−0.06
15. C_5H_{10}	cyclopentane	3.00	2.52	−0.48
16. C_5H_{12}	neopentane	3.11	3.45	0.34
17. C_5H_{12}	pentane	3.62	3.48	−0.14
18. C_6H_8	1,4-cyclohexadiene	2.30	2.41	0.11
19. C_6H_8	1,3-cyclohexadiene	2.47	2.41	−0.06
20. C_6H_{10}	cyclohexene	2.86	2.37	−0.49
21. C_6H_{10}	1,5-hexadiene	2.45	2.73	0.28
22. C_6H_{12}	cyclohexane	3.44	3.16	−0.28
23. C_6H_{14}	*n*-hexane	4.11	4.18	0.07
24. C_6H_{14}	2,3-dimethylbutane	3.85	4.05	0.20
25. C_6H_{14}	2,2-dimethylbutane	3.82	4.15	0.33
26. C_8H_{18}	*n*-octane	5.18	5.57	0.39
27. $C_{10}H_8$	azulene	3.20	3.47	0.27
28. $C_{14}H_{10}$	diphenylacetylene	4.78	4.49	−0.29
	Aromatic Hydrocarbons			
29. C_6H_6	benzene	2.13	2.45	0.32
30. C_7H_8	toluene	2.69	2.86	0.17
31. C_8H_6	ethynylbenzene	2.53	2.46	−0.07
32. C_8H_8	styrene	3.16	3.06	−0.10
33. C_8H_{10}	ethylbenzene	3.15	3.27	0.12
34. C_8H_{10}	*p*-xylene	3.18	3.27	0.09
35. C_8H_{10}	*m*-xylene	3.20	3.27	0.07
36. C_8H_{10}	*o*-xylene	3.13	3.27	0.14
37. C_9H_8	indene	2.92	3.07	0.15
38. C_9H_{10}	indane	3.33	3.03	−0.30
39. C_9H_{10}	1-phenyl-1-propene	3.35	3.49	0.14
40. C_9H_{10}	cyclopropylbenzene	3.27	3.02	−0.25
41. C_9H_{10}	allylbenzene	3.23	3.48	0.25
42. C_9H_{12}	1,3,5-trimethylbenzene	3.42	3.68	0.26
43. C_9H_{12}	1-ethyl-2-methylbenzene	3.53	3.68	0.15
44. C_9H_{12}	1,2,3-trimethylbenzene	3.55	3.68	0.13
45. C_9H_{12}	propylbenzene	3.68	3.69	0.01
46. C_9H_{12}	isopropylbenzene	3.66	3.62	−0.04
47. C_9H_{12}	1,2,4-trimethylbenzene	3.65	3.68	0.03
48. $C_{10}H_8$	naphthalene	3.35	3.47	0.12
49. $C_{10}H_{14}$	1,2,4,5-tetramethylbenzene	4.00	4.09	0.09
50. $C_{10}H_{14}$	*tert*-butylbenzene	4.11	4.07	−0.04
51. $C_{10}H_{14}$	*p*-cymene	4.10	4.03	−0.07
52. $C_{10}H_{14}$	butylbenzene	4.26	4.10	−0.16
53. $C_{11}H_{10}$	2-methylnaphthalene	3.86	3.88	0.02
54. $C_{11}H_{10}$	1-methylnaphthalene	3.87	3.88	0.01
55. $C_{12}H_8$	acenaphthylene	4.03	3.72	−0.31
56. $C_{12}H_{10}$	acenaphthene	3.92	3.68	−0.24
57. $C_{12}H_{10}$	biphenyl	4.09	4.23	0.14
58. $C_{12}H_{12}$	2,6-dimethylnaphthalene	4.31	4.29	−0.02
59. $C_{12}H_{12}$	2,3-dimethylnaphthalene	4.40	4.29	−0.11
60. $C_{12}H_{12}$	1,8-dimethylnaphthalene	4.26	4.29	0.03
61. $C_{12}H_{12}$	1,7-dimethylnaphthalene	4.44	4.29	−0.15
62. $C_{12}H_{12}$	1,5-dimethylnaphthalene	4.38	4.29	−0.09
63. $C_{12}H_{12}$	1,4-dimethylnaphthalene	4.37	4.29	−0.08
64. $C_{12}H_{12}$	1,3-dimethylnaphthalene	4.42	4.29	−0.13
65. $C_{12}H_{12}$	1,2-dimethylnaphthalene	4.31	4.29	−0.02
66. $C_{12}H_{12}$	2-ethylnaphthalene	4.38	4.29	−0.09
67. $C_{12}H_{12}$	1-ethylnaphthalene	4.39	4.29	−0.10
68. $C_{12}H_{18}$	hexamethylbenzene	4.31	4.91	0.60
69. $C_{13}H_{10}$	fluorene	4.18	4.08	−0.10
70. $C_{13}H_{12}$	diphenylmethane	4.14	4.64	0.50
71. $C_{13}H_{14}$	1,4,5-trimethylnaphthalene	4.90	4.70	−0.20
72. $C_{13}H_{14}$	2,3,6-trimethylnaphthalene	4.73	4.70	−0.03
73. $C_{14}H_{10}$	phenanthrene	4.57	4.48	−0.09
74. $C_{14}H_{10}$	anthracene	4.54	4.48	−0.06
75. $C_{14}H_{12}$	1-methylfluorene	4.97	4.49	−0.48
76. $C_{14}H_{12}$	stilbene	4.81	4.85	0.04

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Aromatic Hydrocarbons			
77. $C_{14}H_{12}$	9,10-dihydroanthracene	4.25	4.44	0.19
78. $C_{14}H_{14}$	diphenylethane	4.80	5.05	0.25
79. $C_{16}H_{10}$	pyrene	5.18	4.74	−0.44
80. $C_{18}H_{12}$	benz[*a*]anthracene	5.61	5.50	−0.11
	Alcohols, Ethers, and Phenols			
81. CH_4O	methanol	−0.66	−0.72	−0.06
82. C_2H_4O	ethylene oxide	−0.30	−0.12	0.18
83. C_2H_6O	dimethyl ether	0.10	−0.02	−0.12
84. C_2H_6O	ethanol	−0.31	−0.31	0.00
85. C_3H_6O	allyl alcohol	0.17	−0.10	−0.27
86. C_3H_8O	2-propanol	0.05	0.15	0.10
87. C_3H_8O	1-propanol	0.34	0.11	−0.23
88. C_4H_4O	furan	1.34	0.92	−0.42
89. C_4H_6O	2,5-dihydrofuran	0.46	0.64	0.18
90. C_4H_8O	ethylvinyl ether	1.04	0.84	−0.20
91. C_4H_8O	tetrahydrofuran	0.41	0.60	0.19
92. $C_4H_{10}O$	diethyl ether	0.89	0.81	−0.08
93. $C_4H_{10}O$	*tert*-butyl alcohol	0.37	0.76	0.39
94. $C_4H_{10}O$	*sec*-butyl alcohol	0.61	0.56	−0.05
95. $C_4H_{10}O$	isobutyl alcohol	0.65	0.46	−0.19
96. $C_4H_{10}O$	butanol	0.88	0.52	−0.36
97. $C_5H_{12}O$	2-methyl-2-butanol	0.89	1.17	0.28
98. $C_5H_{12}O$	2,2-dimethylpropanol	1.36	0.91	−0.45
99. $C_5H_{12}O$	isopentyl alcohol	1.42	0.87	−0.55
100. $C_5H_{12}O$	3-pentanol	1.21	0.98	−0.23
101. $C_5H_{12}O$	pentanol	1.40	0.94	−0.46
102. $C_5H_{12}O$	3-methyl-2-butanol	1.28	0.91	−0.37
103. C_6H_6O	phenol	1.46	1.46	0.00
104. $C_6H_{12}O$	cyclohexanol	1.23	0.63	−0.60
105. $C_6H_{14}O$	butyl ethyl ether	2.03	1.64	−0.39
106. $C_6H_{14}O$	dipropyl ether	2.03	1.64	−0.39
107. $C_6H_{14}O$	3,3-dimethyl-2-butanol	1.48	1.36	−0.12
108. $C_6H_{14}O$	hexanol	2.03	2.18	0.15
109. C_7H_8O	anisole	2.10	1.58	−0.51
110. C_7H_8O	*p*-cresol	1.94	1.87	−0.07
111. C_7H_8O	*o*-cresol	1.95	1.87	−0.08
112. C_7H_8O	*m*-cresol	1.96	1.87	−0.09
113. C_7H_8O	benzyl alcohol	1.10	1.06	−0.04
114. C_8H_6O	benzofuran	2.67	1.94	−0.73
115. $C_8H_{10}O$	ethoxybenzene	2.51	2.00	−0.51
116. $C_8H_{10}O$	*p*-methylbenzyl alcohol	1.59	1.47	−0.12
117. $C_8H_{10}O$	*o*-methylbenzyl alcohol	1.58	1.47	−0.11
118. $C_8H_{10}O$	*m*-methylbenzyl alcohol	1.60	1.47	−0.13
119. $C_8H_{10}O$	*p*-ethylphenol	2.26	2.29	0.03
120. $C_8H_{10}O$	*o*-ethylphenyl	2.47	2.29	−0.18
121. $C_8H_{10}O$	*m*-ethylphenol	2.40	2.29	−0.11
122. $C_8H_{10}O$	2-phenyl-1-ethanol	1.36	1.47	0.11
123. $C_8H_{10}O$	3,5-dimethylphenol	2.35	2.28	−0.07
124. $C_8H_{10}O$	3,4-dimethylphenol	2.23	2.28	0.05
125. $C_8H_{10}O$	2,6-dimethylphenol	2.36	2.28	−0.08
126. $C_8H_{10}O$	2,5-dimethylphenol	2.33	2.28	−0.05
127. $C_8H_{10}O$	2,4-dimethylphenol	2.30	2.28	−0.02
128. $C_8H_{10}O$	benzyl methyl ether	1.35	1.76	0.41
129. $C_8H_{18}O$	octanol	3.15	3.01	−0.14
130. $C_9H_{10}O$	cinnamyl alcohol	1.95	1.69	−0.26
131. $C_9H_{10}O$	allyl phenyl ether	2.94	2.21	−0.73
132. $C_9H_{12}O$	phenyl propyl ether	3.18	2.41	−0.77
133. $C_9H_{12}O$	2-prop-2-yl-1-phenol	2.88	2.64	−0.24
134. $C_9H_{12}O$	2-prop-1-yl-1-phenol	2.93	2.70	−0.23
135. $C_9H_{12}O$	γ-phenylpropyl alcohol	1.85	1.89	0.04
136. $C_{10}H_8O$	2-naphthol	2.84	2.48	−0.36
137. $C_{10}H_8O$	1-naphthol	2.98	2.48	−0.50
138. $C_{10}H_{12}O$	phenylcyclopropylcarbinol	1.95	1.68	−0.27
139. $C_{10}H_{14}O$	1-methoxy-3-phenylpropane	2.70	2.59	−0.11
140. $C_{10}H_{14}O$	*o*-(1-methylpropyl)phenol	3.27	3.05	−0.22
141. $C_{10}H_{14}O$	*p*-(1,1-dimethylethyl)phenol	2.94	3.09	0.15
142. $C_{10}H_{14}O$	thymol	3.30	3.05	−0.25
143. $C_{10}H_{14}O$	δ-phenylbutyl alcohol	2.35	2.30	−0.05
144. $C_{10}H_{14}O$	thymol	3.30	3.05	−0.25
145. $C_{10}H_{14}O$	*o*-(1,1-dimethylethyl)phenol	3.31	3.09	−0.22
146. $C_{10}H_{16}O$	1-hydroxyladamantane	2.14	1.42	−0.72
147. $C_{12}H_{10}O$	*p*-phenylphenol	3.20	3.24	0.04
148. $C_{12}H_{10}O$	*o*-phenylphenol	3.09	3.24	0.15
149. $C_{12}H_{10}O$	*m*-phenylphenol	3.23	3.24	0.01
150. $C_{12}H_{26}O$	1-dodecanol	5.13	4.67	−0.46
151. $C_{13}H_{12}O$	diphenylmethyl alcohol	2.67	2.88	0.21
152. $C_{13}H_{12}O$	benzyl phenyl ether	3.79	3.37	−0.42

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Alcohols, Ethers, and Phenols			
153. $C_{14}H_{14}O$	phenyl-*p*-tolylcarbinol	3.13	3.29	0.16
154. $C_{14}H_{14}O$	phenyl-*o*-tolylcarbinol	3.06	3.29	0.23
	Aldehydes and Ketones			
155. C_3H_6O	propionaldehyde	0.59	0.36	−0.23
156. C_3O_6O	acetone	−0.24	0.13	0.37
157. C_4H_8O	butyaldehyde	0.88	0.78	−0.10
158. C_4H_8O	2-butanone	0.29	0.54	0.25
159. $C_5H_{10}O$	2-pentanone	0.91	0.96	0.05
160. C_6H_8O	1-hexyn-5-one	0.58	0.56	−0.02
161. $C_6H_{10}O$	1-hexen-5-one	1.02	1.16	0.14
162. $C_6H_{10}O$	cyclohexanone	0.81	0.91	0.10
163. $C_6H_{12}O$	2-hexanone	1.38	1.37	−0.01
164. $C_6H_{12}O$	hexaldehyde	1.78	1.61	−0.17
165. C_7H_6O	benzaldehyde	1.48	1.32	−0.16
166. $C_7H_{12}O$	4-cyclopropyl-2-butanone	1.50	1.12	−0.38
167. $C_7H_{14}O$	2-heptanone	1.98	1.79	−0.19
168. C_8H_8O	acetophenone	1.58	1.49	−0.09
169. C_8H_8	phenylacetaldehyde	1.78	1.73	−0.05
170. C_8H_8O	*o*-methylbenzaldehyde	2.26	1.73	−0.53
171. $C_8H_{16}O$	2-octanone	2.76	3.03	0.27
172. C_9H_8O	cinnamaldehyde	1.90	1.95	0.05
173. C_9H_8O	acrylophenone	1.88	1.70	−0.18
174. $C_9H_{10}O$	propiophenone	2.19	1.91	−0.28
175. $C_9H_{10}O$	*p*-methylacetophenone	2.28	1.90	−0.38
176. $C_9H_{18}O$	2-nonanone	3.18	3.44	0.26
177. $C_{10}H_{10}O$	methyl styryl ketone	2.07	2.12	0.05
178. $C_{11}H_{14}O$	5-phenyl-2-pentanone	2.42	2.74	0.32
179. $C_{13}H_8O$	9-fluorenone	3.58	2.66	−0.92
180. $C_{13}H_{10}O$	benzophenone	3.18	2.86	−0.32
181. $C_{15}H_{12}O$	benzalacetophenone	3.08	3.49	0.41
	Acids and Esters			
182. CH_2O_2	formic acid	−0.54	−0.23	0.31
183. $C_2H_4O_2$	acetic acid	−0.17	−0.30	−0.13
184. $C_3H_6O_2$	methyl acetate	0.18	0.21	0.03
185. $C_3H_6O_2$	propionic acid	0.33	0.11	−0.22
186. $C_4H_6O_2$	crotonic acid	0.72	0.32	−0.40
187. $C_4H_8O_2$	propyl formate	0.83	1.11	0.28
188. $C_4H_8O_2$	ethyl acetate	0.73	0.62	−0.11
189. $C_4H_8O_2$	butyric acid	0.79	0.53	−0.26
190. $C_5H_{10}O_2$	ethyl propionate	1.21	1.04	−0.17
191. $C_6H_{12}O_2$	hexanoic acid	1.88	1.36	−0.52
192. $C_7H_6O_2$	phenyl formate	1.26	1.65	0.39
193. $C_7H_6O_2$	benzoic acid	1.81	1.79	−0.02
194. $C_8H_8O_2$	*p*-toluic acid	2.27	2.20	−0.07
195. $C_8H_8O_2$	*m*-toluic acid	2.37	2.20	−0.17
196. $C_8H_8O_2$	benzoic acid methyl ester	2.12	1.57	−0.55
197. $C_8H_8O_2$	acetic acid phenyl ester	1.49	1.57	0.08
198. $C_8H_8O_2$	phenylacetic acid	1.41	1.48	0.07
199. $C_8H_{16}O_2$	valproic acid	2.75	2.12	−0.63
200. $C_9H_8O_2$	cinnamic acid	2.08	1.69	−0.39
201. $C_9H_{10}O_2$	*m*-tolyl acetate	2.09	1.98	−0.11
202. $C_9H_{10}O_2$	*p*-tolyl acetate	2.11	1.98	−0.13
203. $C_9H_{10}O_2$	ethyl benzoate	2.64	1.99	−0.65
204. $C_9H_{10}O_2$	acetic acid benzyl ester	1.96	1.99	0.03
205. $C_9H_{10}O_2$	phenylacetic acid methyl ester	1.83	1.99	0.16
206. $C_9H_{10}O_2$	(*p*-methylphenyl)acetic acid	1.86	1.89	0.03
207. $C_9H_{10}O_2$	*o*-tolyl acetate	2.11	1.98	−0.13
208. $C_9H_{10}O_2$	3-phenylpropionic acid	1.84	1.89	0.05
209. $C_{10}H_{10}O_2$	cinnamic acid methyl ester	2.62	2.20	−0.42
210. $C_{10}H_{12}O_2$	β-phenylpropionic acid methyl ester	2.32	2.40	0.08
211. $C_{10}H_{12}O_2$	phenylacetic acid ethyl ester	2.42	2.40	−0.02
212. $C_{10}H_{12}O_2$	4-ethylphenyl acetate	2.56	2.40	−0.16
213. $C_{10}H_{12}O_2$	2-ethylphenyl acetate	2.42	2.40	−0.02
214. $C_{10}H_{12}O_2$	4-phenylbutyric acid	2.42	2.31	−0.11
215. $C_{10}H_{12}O_2$	acetic acid β-phenylethyl ester	2.30	2.40	0.10
216. $C_{10}H_{20}O_2$	decanoic acid	4.09	3.84	−0.25
217. $C_{11}H_8O_2$	1-naphthonic acid	3.10	2.81	−0.29
218. $C_{11}H_{12}O_2$	cinnamic acid ethyl ester	2.99	2.62	−0.37
219. $C_{11}H_{14}O_2$	2-isopropylphenyl acetate	2.78	2.75	−0.03
220. $C_{11}H_{14}O_2$	4-phenylbutyric acid methyl ester	2.77	2.82	0.05
221. $C_{12}H_{24}O_2$	dodecanoic acid	4.20	4.67	0.47
222. $C_{13}H_{10}O_2$	phenyl benzoate	3.59	2.94	−0.65
223. $C_{14}H_{12}O_2$	diphenylacetic acid	3.05	3.19	0.14
224. $C_{14}H_{12}O_2$	benzyl benzoate	3.97	3.35	−0.62
	Amines and Nitriles			
225. CH_5N	methylamine	−0.57	−0.94	−0.37
226. C_2H_3N	acetonitrile	−0.34	0.03	0.37
227. C_2H_7N	ethylamine	−0.13	−0.52	−0.39

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Amines and Nitriles			
228. C_3H_5N	propionitrile	0.16	0.45	0.29
229. C_3H_7N	allylamine	0.03	−0.31	−0.34
230. C_3H_9N	trimethylamine	0.27	0.34	0.07
231. C_3H_9N	isopropylamine	−0.03	−0.03	0.00
232. C_3H_9N	propylamine	0.48	−0.11	−0.59
233. C_3H_9N	methylethylamine	0.15	0.32	0.17
234. $C_4H_{11}N$	diethylamine	0.57	0.74	0.17
235. $C_4H_{11}N$	butylamine	0.81	0.31	−0.50
236. $C_4H_{11}N$	ethyldimethylamine	0.70	0.76	0.06
237. $C_4H_{11}N$	*sec*-butylamine	0.74	0.38	−0.36
238. $C_4H_{11}N$	isobutylamine	0.88	0.24	−0.64
239. $C_4H_{11}N$	*tert*-butylamine	0.40	0.42	0.02
240. $C_5H_{11}N$	ethylallylamine	0.81	0.94	0.13
241. $C_5H_{13}N$	butylmethylamine	1.33	1.15	−0.18
242. $C_5H_{13}N$	amylamine	1.45	0.72	−0.73
243. C_6H_7N	aniline	0.90	0.92	0.02
244. $C_6H_{11}N$	diallylamine	1.11	1.15	0.04
245. $C_6H_{13}N$	propylallylamine	1.33	1.36	0.03
246. $C_6H_{13}N$	cyclohexylamine	1.49	0.44	−1.05
247. $C_6H_{15}N$	triethylamine	1.44	1.59	0.15
248. $C_6H_{15}N$	butyldimethylamine	1.70	1.59	−0.11
249. $C_6H_{15}N$	dipropylamine	1.73	1.57	−0.16
250. $C_6H_{15}N$	hexylamine	2.06	1.96	−0.10
251. C_7H_5N	benzonitrile	1.56	1.26	−0.30
252. C_7H_9N	*N*-methylaniline	1.82	2.01	0.19
253. C_7H_9N	*p*-toluidine	1.39	1.33	−0.06
254. C_7H_9N	*o*-toluidine	1.29	1.33	0.04
255. C_7H_9N	*m*-toluidine	1.42	1.33	−0.09
256. C_7H_9N	benzylamine	1.09	0.85	−0.24
257. $C_7H_{17}N$	propylbutylamine	2.12	1.98	−0.14
258. $C_7H_{17}N$	propyl-*sec*-butylamine	1.91	1.92	0.01
259. $C_7H_{17}N$	propylisobutylamine	2.07	1.92	−0.15
260. $C_7H_{17}N$	heptylamine	2.57	2.38	−0.19
261. C_8H_7N	phenylacetonitrile	1.56	1.81	0.25
262. $C_8H_{11}N$	2-ethylaniline	1.74	1.75	0.01
263. $C_8H_{11}N$	*N,N*-dimethylaniline	2.31	1.71	−0.60
264. $C_8H_{11}N$	*N*-ethylaniline	2.16	2.42	0.26
265. $C_8H_{11}N$	β-phenylethylamine	1.41	1.26	−0.15
266. $C_8H_{11}N$	*N*-methyl-*o*-toluidine	2.16	2.42	0.26
267. $C_8H_{11}N$	*N*-methyl-*p*-toluidine	2.15	2.42	0.27
268. $C_8H_{11}N$	methylbenzylamine	1.52	1.69	0.17
269. $C_8H_{19}N$	dibutylamine	2.68	2.40	−0.28
270. $C_8H_{19}N$	2-ethylhexylamine	2.82	2.04	−0.78
271. $C_8H_{19}N$	ethyldiisopropylamine	2.68	2.29	−0.39
272. C_9H_7N	cinnamonitrile	1.96	2.03	0.07
273. $C_9H_{13}N$	amphetamine	1.76	1.75	−0.01
274. $C_9H_{13}N$	*N*-propylaniline	2.45	2.84	0.39
275. $C_9H_{13}N$	γ-phenylpropylamine	1.83	1.68	−0.15
276. $C_9H_{13}N$	*N,N*-dimethyl-*o*-toluidine	2.85	2.12	−0.73
277. $C_9H_{13}N$	*N,N*-dimethyl-*m*-toluidine	2.80	2.12	−0.68
278. $C_9H_{13}N$	*N,N*-dimethyl-*p*-toluidine	2.61	2.12	−0.49
279. $C_9H_{21}N$	tripropylamine	2.79	2.83	0.04
280. $C_9H_{21}N$	2-ethylhexylamine	2.68	2.32	−0.36
281. $C_{10}H_9N$	1-naphthamine	2.25	1.94	−0.31
282. $C_{10}H_9N$	2-naphthamine	2.28	1.94	−0.34
283. $C_{10}H_{15}N$	*N,N*-diethylaniline	3.31	2.54	−0.77
284. $C_{10}H_{15}N$	δ-phenylbutylamine	2.40	2.09	−0.31
285. $C_{11}H_{17}N$	γ-phenylpropyl-dimethylamine	2.73	2.96	0.23
286. $C_{12}H_{11}N$	2-aminobiphenyl	3.34	2.70	−0.64
287. $C_{12}H_{11}N$	diphenylamine	3.50	3.37	−0.13
288. $C_{13}H_{13}N$	*N*-benzylaniline	3.13	3.79	0.66
289. $C_{13}H_{13}N$	diphenylmethylamine	3.16	3.08	−0.08
290. $C_{14}H_{15}N$	*N*-methyl-*N*-benzylaniline	4.22	3.49	−0.73
	Amides and Anilides			
291. C_3H_7ON	*N*-methylacetamide	−1.05	−0.39	0.66
292. C_4H_9ON	butylamide	−0.21	−0.01	0.20
293. C_4H_9ON	*N,N*-dimethylacetamide	−0.77	0.00	0.77
294. C_7H_7ON	benzamide	0.64	0.53	−0.11
295. C_7H_7ON	formanilide	1.15	1.05	−0.10
296. C_8H_9ON	acetanilide	1.16	0.98	−0.18
297. C_8H_9ON	*N*-methylformanilide	1.09	1.44	0.35
298. C_8H_9ON	*p*-methylformanilide	1.61	1.47	−0.14
299. C_8H_9ON	*m*-methylbenzamide	1.18	0.94	−0.24
300. C_8H_9ON	phenylacetamide	0.45	0.94	0.49
301. $C_8H_{15}ON$	allylisopropylacetamide	1.14	1.32	0.18
302. $C_8H_{17}ON$	propylisopropylacetamide	1.48	1.52	0.04
303. C_9H_9ON	cinnamamide	1.41	1.16	−0.25

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Amides and Anilides			
304. $C_9H_{11}ON$	propionanilide	1.61	1.40	−0.21
305. $C_9H_{11}ON$	γ-phenylpropionamide	1.03	1.36	0.33
306. $C_9H_{11}ON$	*N,N*-dimethylbenzamide	0.62	1.37	0.75
307. $C_9H_{11}ON$	*N*-methylacetanilide	1.07	1.37	0.30
308. $C_9H_{13}ON$	*p*-methoxy-*N,N*-dimethylaniline	1.42	1.72	0.30
309. $C_{10}H_{13}ON$	*p*-isopropylbenzamide	2.14	1.71	−0.43
310. $C_{10}H_{13}ON$	butyranilide	2.05	1.81	−0.24
311. $C_{10}H_{13}ON$	isobutyranilide	2.02	1.75	−0.27
312. $C_{13}H_{11}ON$	benzanilide	2.70	2.35	−0.35
313. $C_{15}H_{13}ON$	cinnamanilide	3.61	2.98	−0.63
	S-Containing Hydrocarbons			
314. C_4H_4S	thiophene	1.81	1.63	−0.18
315. $C_4H_{10}S$	butanethiol	2.28	2.08	−0.20
316. $C_4H_{10}S$	diethyl sulfide	1.95	1.93	−0.02
317. C_6H_6S	thiophenol	2.52	2.20	−0.32
318. C_7H_8S	methylthiobenzene	2.74	2.47	−0.27
319. C_8H_6S	benzothiophene	3.12	2.65	−0.47
320. $C_8H_{10}S$	phenylethyl sulfide	3.20	2.89	−0.31
321. $C_{10}H_8S$	2-phenylthiophene	3.74	3.41	−0.33
322. $C_{12}H_{10}S$	diphenyl sulfide	4.45	3.84	−0.61
	Nitro Hydrocarbons			
323. CH_3O_2N	nitromethane	0.08	0.04	−0.04
324. $C_2H_5O_2N$	nitroethane	0.18	0.45	0.27
325. $C_3H_7O_2N$	nitropropane	0.65	0.87	0.22
326. $C_4H_9O_2N$	2-methyl-2-nitropropane	1.01	1.25	0.24
327. $C_4H_9O_2N$	nitrobutane	1.47	1.28	−0.19
328. $C_5H_{11}O_2N$	nitropentane	2.01	1.70	−0.31
329. $C_6H_5O_2N$	nitrobenzene	1.85	1.54	−0.31
330. $C_7H_7O_2N$	*p*-nitrotoluene	2.37	1.95	−0.42
331. $C_7H_7O_2N$	*o*-nitrotoluene	2.30	1.95	−0.35
332. $C^7H_7O_2N$	*m*-nitrotoluene	2.45	1.95	−0.50
333. $C_7H_7O_2N$	α-nitrotoluene	1.75	1.96	0.21
334. $C_8H_7O_2N$	β-nitrostyrene	2.24	2.17	−0.07
335. $C_8H_9O_2N$	1,3-dimethyl-2-nitrobenzene	2.95	2.37	−0.58
336. $C_8H_9O_2N$	β-nitroethylbenzene	2.08	2.37	0.29
337. $C_9H_9O_2N$	4-methyl-β-nitrostyrene	2.66	2.58	−0.08
338. $C_9H_9O_2N$	2-methyl-β-nitrostyrene	2.63	2.58	−0.05
339. $C_9H_9O_2N$	β-methyl-β-nitrostyrene	2.52	2.99	0.47
340. $C_{10}H_7O_2N$	1-nitronaphthalene	3.19	2.56	−0.63
	Amino Acids			
341. $C_2H_5O_2N$	glycine	−3.00	−3.29	−0.29
342. $C_3H_7O_2N$	alanine	−2.83	−2.80	0.03
343. $C_5H_{11}O_2N$	valine	−2.10	−2.04	0.06
344. $C_5H_{11}O_2NS$	methionine	−1.87	−1.49	0.38
345. $C_5H_{12}O_2N_2$	ornithine	−2.89	−3.12	−0.23
346. $C_6H_9O_2N_3$	histidine	−2.52	−2.32	0.20
347. $C_6H_{13}O_2N$	isoleucine	−1.69	−1.62	0.07
348. $C_6H_{13}O_2N$	leucine	−1.57	−1.62	−0.05
349. $C_6H_{14}O_2N_2$	lysine	−2.82	−2.70	0.12
350. $C_9H_{11}O_2N$	phenylalanine	−1.43	−1.02	0.41
	Halogenated Hydrocarbons			
351. CCl_4	carbon tetrachloride	2.83	2.04	−0.79
352. $CHCl_3$	chloroform	1.97	1.54	−0.43
353. CH_2F_2	difluoromethane	0.20	0.69	0.49
354. CH_2Cl_2	dichloromethane	1.25	1.14	−0.11
355. CH_3F	methyl fluoride	0.51	0.44	−0.07
356. CH_3Cl	methyl chloride	0.91	0.67	−0.24
357. CH_3Br	methyl bromide	1.19	0.98	−0.21
358. CH_3I	methyl iodide	1.51	1.17	−0.34
359. C_2HCl_3	trichloroethylene	2.29	2.22	−0.07
360. $C_2H_2F_2$	1,1-difluoroethylene	1.24	1.29	0.05
361. $C_2H_3Cl_3$	1,1,1-trichloroethane	2.49	1.99	−0.05
362. C_2H_3Br	vinyl bromide	1.57	1.19	−0.38
363. $C_2H_4F_2$	1,1-difluoroethane	0.75	1.04	0.29
364. $C_2H_4Cl_2$	1,2-dichloroethane	1.48	1.55	0.07
365. $C_2H_4Cl_2$	1,1-dichloroethane	1.79	1.49	−0.30
366. C_2H_5Cl	ethyl chloride	1.43	1.09	−0.34
367. C_2H_5Br	ethyl bromide	1.61	1.39	−0.22
368. C_2H_5I	ethyl iodide	2.00	1.58	−0.42
369. C_3H_5Br	allyl bromide	1.79	1.60	−0.19
370. $C_3H_6Cl_2$	1,3-dichloropropane	2.00	1.97	−0.03
371. C_3H_7Cl	2-chloropropane	1.90	1.44	−0.46
372. C_3H_7Br	1-bromopropane	2.10	1.81	−0.29
373. C_3H_7Cl	chloropropane	2.04	1.50	−0.54
374. C_4H_9Br	1-bromobutane	2.75	2.22	−0.53
375. C_4H_9Cl	1-chlorobutane	2.55	1.92	−0.63

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Halogenated Hydrocarbons			
376. $C_5H_{11}F$	1-fluoropentane	2.33	2.10	−0.23
377. $C_5H_{11}Br$	1-bromopentane	3.37	2.64	−0.73
378. C_6F_6	hexafluorobenzene	2.22	2.88	0.66
379. $C_6H_4Cl_2$	*p*-dichlorobenzene	3.39	2.88	−0.51
380. $C_6H_4Cl_2$	*o*-dichlorobenzene	3.38	2.88	−0.50
381. $C_6H_4Cl_2$	*m*-dichlorobenzene	3.38	2.88	−0.50
382. $C_6H_4Br_2$	*o*-dibromobenzene	3.64	3.25	−0.39
383. $C_6H_4Br_2$	*m*-dibromobenzene	3.75	3.25	−0.50
384. C_6H_5F	fluorobenzene	2.27	1.79	−0.48
385. C_6H_5Cl	chlorobenzene	2.84	2.23	−0.61
386. C_6H_5Br	bromobenzene	2.99	2.41	−0.58
387. $C_6H_6Cl_6$	hexachlorocyclohexane	3.72	4.19	0.47
388. $C_6H_{13}Br$	1-bromohexane	3.80	3.88	0.08
389. $C_7H_5F_3$	α,α,α-trifluorotoluene	2.79	2.68	−0.11
390. $C_7H_5Cl_3$	α,α,α-trichlorotoluene	2.92	3.36	0.44
391. C_7H_7Cl	*p*-chlorotoluene	3.33	2.64	−0.69
392. C_7H_7Cl	*o*-chlorotoluene	3.42	2.64	−0.78
393. C_7H_7Cl	*m*-chlorotoluene	3.42	2.64	−0.78
394. C_7H_7Br	α-bromotoluene	2.92	2.76	−0.16
395. $C_7H_9Cl_5$	1-methylpentachlorocyclohexane	4.04	4.14	0.10
396. C_8H_9Cl	2-chloro-1-ethylbenzene	2.95	2.87	−0.08
397. C_8H_9Br	β-phenylethyl bromide	3.09	3.18	0.09
398. $C_9H_{11}F$	γ-phenylpropyl fluoride	2.95	3.06	0.11
399. $C_9H_{11}Cl$	γ-phenylpropyl chloride	3.55	3.28	−0.27
400. $C_9H_{11}Br$	γ-phenylpropyl bromide	3.72	3.59	−0.13
401. $C_{10}H_9Cl_3$	α-(2,2,2-trichloroethyl)styrene	4.56	4.39	−0.17
402. $C_{12}H_9Cl$	4-chlorobiphenyl	4.61	4.01	−0.60
403. $C_{12}H_9Cl$	3-chlorobiphenyl	4.71	4.01	−0.70
404. $C_{12}H_9Cl$	2-chlorobiphenyl	4.59	4.01	−0.58
	Nucleosides			
405. $C_{10}H_{13}O_4N_5$	Ado	−1.23	−2.13	−0.90
406. $C_{10}H_{13}O_3N_5$	dAdo	−0.54	−1.29	−0.75
407. $C_{10}H_{13}O_2N_5$	ddAdo	−0.21	−0.46	−0.25
408. $C_{10}H_{11}O_2N_5$	ddeAdo	−0.35	−0.42	−0.07
409. $C_{10}H_{12}O_2N_5F$	FddAdo	0.08	−0.23	−0.31
410. $C_{10}H_{13}O_5N_5$	Guo	−1.89	−3.09	−1.20
411. $C_{10}H_{13}O_4N_5$	dGuo	−1.30	−2.26	−0.96
412. $C_{10}H_{13}O_3N_5$	ddGuo	−1.00	−1.43	−0.43
413. $C_{10}H_{11}O_3N_5$	ddeGuo	−1.21	−1.39	−0.18
414. $C_{10}H_{16}O_3N_6$	dDAPR	−0.52	−1.38	−0.86
415. $C_{10}H_{16}O_2N_6$	ddDAPR	−0.46	−0.55	−0.09
416. $C_{10}H_{15}O_2N_6F$	FddDAPR	0.05	−0.32	−0.37
417. $C_9H_{12}O_6N_2$	Urd	−1.71	−2.28	−0.57
418. $C_9H_{12}O_5N_2$	dUrd	−1.50	−1.44	0.06
419. $C_9H_{12}O_4N_2$	ddUrd	−0.88	−0.61	0.27
420. $C_9H_{10}O_4N_2$	ddeUrd	−1.07	−0.57	0.50
421. $C_9H_{11}O_4N_2F$	FddUrd	−0.48	−0.38	0.10
422. $C_{10}H_{14}O_5N_2$	dThd	−1.17	−1.03	0.14
423. $C_{10}H_{14}O_4N_2$	ddThd	−0.63	−0.20	0.43
424. $C_{10}H_{12}O_4O_2$	ddeThd	−0.81	−0.16	0.65
425. $C_{10}H_{13}O_4N_2F$	FddThd	−0.27	0.03	0.30
426. $C_9H_{13}O_5N_3$	Cyd	−2.51	−2.86	−0.35
427. $C_9H_{13}O_4N_3$	dCyd	−1.77	−2.03	−0.26
428. $C_9H_{13}O_3N_3$	ddCyd	−1.30	−1.20	0.10
429. $C_9H_{11}O_3N_3$	ddeCyd	−1.42	−1.16	0.26
430. $C_9H_{12}O_3N_3F$	FddCyd	−0.91	−0.97	−0.06
431. $C_{10}H_{13}O_2N_4F$	F6ddP	0.00	0.28	0.28
432. $C_{10}H_{14}O_2N_5F$	F62AddP	−0.05	−0.11	−0.06
433. $C_{10}H_{13}O_2N_4Br$	Br6ddP	0.35	0.81	0.46
434. $C_{10}H_{14}O_2N_5Br$	Br62AddP	0.33	0.42	0.09
435. $C_{10}H_{13}O_2N_4Cl$	Cl6ddP	0.23	0.50	0.27
436. $C_{10}H_{14}O_2N_5Cl$	Cl62AddP	0.21	0.11	−0.10
437. $C_{10}H_{13}O_2N_4I$	I6ddP	0.52	1.00	0.48
438. $C_{10}H_{14}O_2N_5I$	I62AddP	0.52	0.61	0.09
439. $C_{10}H_{12}O_3N_4$	ddI	−1.24	−1.55	−0.31
	Nucleobases			
440. $C_5H_5N_5$	adenine	−0.09	0.23	0.32
441. $C_4H_4N_6$	adenine, 8Aza	−0.96	−0.11	0.85
442. $C_8H_{11}N_5$	9-propyladenine	0.74	0.50	−0.24
443. $C_9H_{13}N_5$	9-butyladenine	1.25	0.92	−0.33
444. $C_{10}H_{15}N_5$	9-pentyladenine	1.79	1.33	−0.46
445. $C_{10}H_{15}ON_5$	9-(1-(hydroxymethyl)butyl))adenine	0.66	0.34	−0.32
446. $C_4H_5ON_3$	cytosine	−1.73	−1.45	0.28
447. $C_5H_7ON_5$	guanine	−0.91	−1.17	−0.26
448. $C_4H_4ON_6$	guanine, 8Aza	−0.71	−1.14	−0.43
449. $C_5H_4ON_4$	hypoxanthine	−1.11	−0.89	0.22
450. $C_5H_4N_4$	purine	−0.37	0.53	0.90

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_f[c]
	Nucleobases			
451. $C_5H_7N_5S$	thioguanine	−0.07	−0.37	−0.30
452. $C_5H_6O_2N_2$	thymine	−0.62	−0.45	0.17
453. $C_4H_4O_2N_2$	uracil	−1.07	−0.86	0.21
454. $C_3H_3O_2N_3$	uracil, 5Aza	−1.87	−1.91	−0.04
455. $C_3H_3O_2N_3$	uracil, 6Aza	−0.59	−0.91	−0.32
456. $C_4H_3O_2N_2F$	5-fluorouracil	−0.95	−0.62	0.33
457. $C_4H_3O_2N_2Cl$	5-chlorouracil	−0.35	−0.40	−0.05
458. $C_4H_3O_2N_2Br$	5-bromouracil	−0.21	−0.09	0.12
459. $C_4H_4ON_2S$	2-thiouracil	−0.28	−0.30	−0.02
460. $C_5H_6O_2N_2$	1-methyluracil	−1.20	−0.48	0.72
461. $C_5H_4O_3N_2$	5-formyluracil	−1.03	−1.12	−0.09
462. $C_6H_8O_2N_2$	1,3-dimethyluracil	0.00	−0.37	−0.37
463. $C_5H_7O_2N_3$	5-ethyl-6-azauracil	0.22	−0.45	−0.67
	Multifunctional Compounds			
464. $CH_4O_2N_2$	hydroxyurea	−1.27	−1.67	−0.40
465. $C_2F_4Cl_2$	1,2-dichloro-1,1,2,2-tetrafluoroethane	2.82	2.46	−0.36
466. $C_2HN_3Br_2$	4,5-dibromo-1,2,3-triazole	2.44	1.90	−0.54
467. $C_2HN_3Br_2$	3,5-dibromo-1,2,4-triazole	2.24	1.90	−0.34
468. $C_2H_2ONF_3$	trifluoroacetamide	0.12	−0.14	−0.26
469. $C_2H_2ONCl_3$	2,2,2-trichloroacetamide	1.04	0.53	−0.51
470. $C_2H_3OF_3$	2,2,2-trifluoroethanol	0.32	0.38	0.06
471. $C_2H_3OCl_3$	2,2,2-trichloroethanol	1.35	1.06	−0.29
472. $C_2H_3O_2Br$	bromoacetic acid	0.41	0.47	0.06
473. C_2H_4ONF	fluoroacetamide	−1.05	−0.60	0.45
474. C_2H_4ONCl	chloroacetamide	−0.53	−0.37	0.16
475. C_2H_4ONBr	bromoacetamide	−0.52	−0.06	0.46
476. C_2H_4ONI	iodoacetamide	−0.19	0.12	0.31
477. $C_2H_4O_2S$	mercaptoacetic acid	0.09	0.32	0.23
478. $C_2H_4O_3$	hydroxyacetic acid	−1.11	−1.23	−0.12
479. C_2H_5ON	acetaldoxime	−0.12	0.82	0.94
480. C_2H_5OF	2-fluoroethanol	−0.92	−0.07	0.85
481. C_2H_5OCl	2-chloroethanol	0.03	0.16	0.13
482. C_2H_5OBr	2-bromoethanol	0.23	0.47	0.24
483. $C_2H_5O_2N_3$	1-methyl-1-nitrosourea	−0.10	−0.13	−0.03
484. $C_2H_5O_3N$	2-nitroethanol	−0.42	−0.48	−0.06
485. $C_2H_6S_2$	dimethyl disulfide	1.77	1.59	−0.18
486. C_2H_6OS	methyl sulfoxide	−1.35	−0.70	0.65
487. $C_2H_6N_2$	*N*-nitrosodimethylamine	−0.57	−0.05	0.52
488. $C_2H_6O_2N_2$	1-methyl-1-hydroxyurea	−0.46	−1.29	−0.83
489. C_2H_7ON	2-hydroxylethylamine	−1.31	−1.77	−0.46
490. $C_3HN_2Br_3$	2,4,5-tribromoimidazole	1.96	2.79	0.83
491. $C_3H_4N_2$	imidazole	−0.08	0.28	0.36
492. $C_3H_4N_2$	pyrazole	0.13	0.64	0.51
493. C_3H_9ON	1-amino-2-propanol	−0.96	−1.32	−0.36
494. $C_3H_8O_2$	dimethoxymethane	0.00	−0.25	−0.25
495. C_3H_3NS	thiazole	0.44	1.25	0.81
496. $C_3H_3N_2I$	4-iodopyrazole	1.70	1.83	0.13
497. C_3H_3ON	isoxazole	0.08	0.54	0.46
498. $C_3H_3OF_5$	2,2,3,3,3-pentafluoropropanol	1.23	1.25	0.02
499. $C_3H_3O_2N_3$	4-nitropyrazole	0.59	0.61	0.02
500. $C_3H_3O_2N_3$	5-nitroimidazole	−0.16	0.24	0.40
501. $C_3H_4O_2N_2$	hydantoin	−1.69	−1.26	0.43
502. C_3H_5NS	ethyl isothiocyanate	1.47	2.12	0.65
503. $C_3H_5OF_3$	1,1,1-trifluoro-2-propanol	0.71	0.84	0.13
504. $C_3H_5O_2Br$	α-bromopropionic acid	0.92	0.82	−0.10
505. $C_3H_6N_2S$	ethylenethiourea	−0.66	−0.35	0.31
506. $C_3H_6O_2S$	3-mercaptopropionic acid	0.43	0.74	0.31
507. $C_3H_6O_2N_3Cl$	1-(2-chloroethyl)-1-nitrosourea	0.57	0.76	0.19
508. $C_3H_6O_3$	hydroxypropionic acid	−0.62	−0.82	−0.02
509. $C_3H_7O_2N$	methyl *N*-methylcarbamate	−0.06	−0.15	−0.09
510. $C_3H_7O_2N$	urethane	−0.15	−0.18	−0.03
511. $C_3H_8ON_2$	*N*-ethylurea	−0.74	−0.41	0.33
512. $C_3H_8O_2N_2$	1-ethyl-1-hydroxyurea	−0.10	−0.87	−0.77
513. $C_3H_8O_2N_2$	3-ethyl-1-hydroxyurea	−0.76	−0.81	−0.05
514. $C_3H_8O_3$	glycerol	−1.79	−1.71	0.08
515. $C_3H_9O_4P$	trimethyl phosphate	−0.52	−0.43	0.09
516. $C_4H_3N_3$	4-cyanopyrazole	0.24	0.32	0.08
517. C_4H_5N	pyrrole	0.75	0.66	−0.09
518. $C_4H_4N_2$	pyrazine	−0.22	0.82	1.04
519. $C_4H_4N_2$	pyrimidine	−0.40	0.82	1.22
520. $C_4H_4ON_2$	pyrazin-2-one	−1.49	−1.31	0.18
521. $C_4H_4ON_2$	2-pyrimidone	−1.62	−1.95	−0.33
522. $C_4H_4ON_2$	4-pyrimidone	−1.38	−1.31	0.07
523. $C_4H_4O_3N_2$	barbituric acid	−1.44	−1.18	0.26
524. $C_4H_5N_3$	2-aminopyrazine	−0.07	0.16	0.23
525. $C_4H_5N_3$	2-aminopyrimidine	−0.22	−0.21	0.01
526. $C_4H_5ON_3$	2-amino-4-pyrimidone	−0.99	−1.70	−0.71

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
527. $C_4H_5ON_3S$	3-(methylthio)-4-amino-1.2.4-triazin-5-one	0.38	–0.15	–0.53
528. $C_4H_5O_2F_3$	2,2,2-trifluoroethyl acetate	1.18	1.31	0.13
529. $C_4H_5O_2N_3$	2-methylimidazole	0.49	0.66	0.17
530. C_4H_6OS	γ-thiobutyrolactone	0.60	1.00	0.40
531. $C_4H_6O_2$	γ-butyrolactone	–0.64	–0.50	0.14
532. $C_4H_6O_3N_4S_2$	2-(acetylamino)-1,3,4-thiadiazole-5-sulfamide	–0.26	–0.75	–0.49
533. $C_4H_6O_4$	succinic acid	–0.59	–0.40	0.19
534. $C_4H_6O_5$	malic acid	–1.26	–1.28	–0.02
535. C_4H_7NS	2-azacyclopentathione	–0.05	0.17	0.22
536. $C_4H_7OCl_3$	β,β,β-trichloro-*tert*-butyl alcohol	2.03	2.13	0.10
537. $C_4H_7O_2Br$	α-bromobutyric acid	1.42	1.24	–0.18
538. $C_4H_7O_4PCl_2$	dichlorovinyl phosphate-*O,O*-dimethyl	1.40	1.12	–0.28
539. $C_4H_8N_2$	2-methyl-2-imidazoline	0.52	0.61	0.09
540. C_4H_8ONBr	*N*-ethylbromoacetamide	0.34	0.80	0.46
541. $C_4H_8ON_2$	*N*-nitrosopyrrolidine	–0.19	–0.02	0.17
542. $C_4H_8ON_2S$	*N*-nitroso-4-thiomorpholine	0.40	0.79	0.39
543. $C_4H_8O_2$	1,4-dioxane	–0.27	0.46	0.73
544. $C_4H_8O_2N_2$	*N*-nitrosomorpholine	–0.44	–0.16	0.28
545. $C_4H_8O_2N_4$	*N,N'*-dinitrosopiperazine	–0.85	–0.78	0.07
546. $C_4H_8O_3$	α-hydroxybutyric acid	–0.36	–0.36	0.00
547. C_4H_9N	pyrrolidine	0.46	–0.16	–0.62
548. C_4H_9ON	morpholine	–1.08	–0.30	0.78
549. $C_4H_9O_2N_3$	1-nitroso-1,3,3-trimethylurea	0.36	0.71	0.35
550. $C_4H_{10}N_2$	piperazine	–1.17	–1.05	0.12
551. $C_4H_{10}ON_2$	*N*-nitrosodiethylamine	0.48	0.78	0.30
552. $C_4H_{10}O_2$	2,3-butanediol	–0.92	–0.32	0.60
553. $C_4H_{10}O_2$	2-ethoxyethanol	–0.54	–0.12	0.42
554. $C_4H_{11}O_2N$	bis(2-hydroxyethyl)amine	–1.43	–1.77	–0.34
555. $C_4H_{10}O_2N_2$	1-hydroxy-3-propylurea	–0.22	–0.39	–0.17
556. C_5BCl_5	2,3,4,5,6-pentachloropyridine	3.53	4.47	0.94
557. $C_5H_3NCl_2$	2,3-dichloropyridine	2.11	2.50	0.39
558. $C_5H_3NCl_2$	2,5-dichloropyrimidine	2.40	2.50	0.10
559. $C_5H_3NCl_2$	2,6-dichloropyridine	2.15	2.50	0.35
560. $C_5H_3NCl_2$	3,5-dichloropyridine	2.56	2.50	–0.06
561. C_5H_4NCl	2-chloropyridine	1.28	1.85	0.57
562. C_5H_4NCl	3-chloropyridine	1.33	1.85	0.52
563. C_5H_4NBr	2-bromopyridine	1.42	2.03	0.61
564. C_5H_4NBr	3-bromopyridine	1.60	2.03	0.43
565. C_5H_4NBr	4-bromopyrdine	1.54	2.03	0.49
566. $C_5H_4ON_4$	hypoxanthine	–1.31	–1.21	0.10
567. $C_5H_4O_2N_2$	2-nitropyridine	0.48	1.16	0.68
568. $C_5H_4O_2N_2$	3-nitropyridine	0.60	1.16	0.56
569. $C_5H_4O_3N_4$	uric acid	–2.92	–2.35	0.57
570. C_5H_5N	pyridine	0.64	1.20	0.56
571. C_5H_5ON	2-hydroxypyridine	–0.58	–0.05	0.53
572. C_5H_5ON	pyridine 1-oxide	–1.30	–0.23	1.07
573. $C_5H_5O_2F_5$	pentafluoropropionic acid ethyl ester	2.12	2.18	0.06
574. $C_5H_6N_2$	2-aminopyridine	0.58	0.54	–0.04
575. $C_5H_6N_2$	2-methylpyrazine	0.23	1.23	1.00
576. $C_5H_6N_2$	3-aminopyridine	0.11	0.54	0.43
577. $C_5H_6N_2$	4-aminopyridine	0.28	0.54	0.26
578. $C_5H_7O_3N_3$	1-methyl-2-(hydroxymethyl)-5-nitroimidazo	–0.03	–0.48	–0.45
579. $C_5H_8ON_4S$	3-methylthio-4-amino-6-methyl-1,2,4-triazin-5-one	–0.16	0.24	0.40
580. $C_5H_8O_2$	acetylacetone	0.34	0.05	–0.29
581. $C_5H_8O_2$	δ-valerolactone	–0.35	–0.14	0.21
582. $C_5H_8O_2N_2$	*N*-nitroso-4-piperidone	–0.47	–0.21	0.26
583. $C_5H_8O_3N_2$	1,3-diacetylurea	–0.68	–0.22	0.46
584. C_5H_9NS	butyl thiocyanate	2.03	1.76	–0.27
585. $C_5H_{10}ON_2$	*N*-nitrosopiperidine	0.63	0.34	–0.29
586. $C_5H_{10}O_2N_2$	3-hydroxy-*N*-nitrosopiperidine	–0.47	–0.49	–0.02
587. $C_5H_{10}O_2N_2$	4-hydroxy-*N*-nitrosopiperidine	–0.89	–0.49	0.40
588. $C_5H_{10}O_2N_4$	2-methyl-*N,N'*-dinitrosopiperazine	–0.28	–0.37	–0.09
589. $C_5H_{10}O_5$	D-ribose	–2.32	–2.42	–0.10
590. $C_5H_{10}O_5$	L-arabinose	–3.02	–2.37	0.65
591. $C_5H_{11}N$	piperidine	0.85	0.20	–0.65
592. $C_5H_{11}ON$	4-methylmorpholine	–0.33	0.23	0.56
593. $C_5H_{12}ON_2$	*N*-butylurea	0.41	0.42	0.01
594. $C_5H_{11}ON_3$	4-methyl-*N*-nitrosopiperazine	0.20	–0.39	–0.59
595. $C_5H_{11}O_2N$	propyl *N*-methylcarbamate	0.95	0.68	–0.27
596. $C_5H_{12}O_2$	1-isopropoxyethanol	0.05	0.23	0.18
597. $C_5H_{12}O_2$	diethoxymethane	0.84	0.58	–0.26
598. $C_5H_{12}O_2N_2$	1-hydroxy-3-butylurea	0.32	0.02	–0.30
599. C_6HOF_5	pentafluorophenol	3.23	2.55	–0.68
600. C_6HOCl_5	pentachlorophenol	5.12	4.73	–0.39
601. $C_6H_2OCl_4$	2,3,4,6-tetrachlorophenol	4.10	4.08	–0.02
602. $C_6H_3OCl_3$	2,4,5-trichlorophenol	3.72	3.42	–0.30
603. $C_6H_3OCl_3$	2,4,6-trichlorophenol	3.38	3.42	0.04

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
604. $C_6H_3OBr_3$	2,4,6-tribromophenol	3.96	3.97	0.01
605. $C_6H_3O_2Br_3$	2,4,6-tribromoresorcinol	4.37	3.86	–0.51
606. $C_6H_3O_3NCl_2$	2,6-dichloro-4-nitrophenol	2.94	3.11	0.17
607. $C_6H_3O_3NBr_2$	2,6-dibromo-4-nitrophenol	3.05	3.47	0.42
608. $C_6H_3O_6B_3$	1,3,5-trinitrobenzene	1.18	1.48	0.30
609. $C_6H_4N_2$	2-cyanopyridine	0.50	0.88	0.38
610. $C_6H_4N_2$	3-cyanopyridine	0.36	0.88	0.52
611. $C_6H_4N_2$	4-cyanopyridine	0.46	0.88	0.42
612. $C_6H_4OCl_2$	2,5-dichlorophenol	3.20	2.77	–0.43
613. $C_6H_4OCl_2$	2,4-dichlorophenol	3.30	2.77	–0.53
614. $C_6H_4OBr_2$	2,4-dibromophenol	3.22	3.13	–0.09
615. $C_6H_4O_2$	quinone	0.20	0.44	0.24
616. $C_6H_4O_2NCl$	*p*-chloronitrobenzene	2.39	2.20	–0.19
617. $C_6H_4O_2NCl$	3-chloro-1-nitrobenzene	2.46	2.20	–0.26
618. $C_6H_4O_2NCl$	2-chloro-1-nitrobenzene	2.24	2.20	–0.04
619. $C_6H_4O_2NBr$	4-bromo-1-nitrobenzene	2.55	2.38	–0.17
620. $C_6H_4O_2NBr$	3-bromo-1-nitrobenzene	2.64	2.38	–0.26
621. $C_6H_4O_2NI$	3-iodonitrobenzene	2.94	2.74	–0.20
622. $C_6H_4O_4N_2$	*m*-dinitrobenzene	1.49	1.51	0.02
623. $C_6H_4O_4N_2$	*o*-dinitrobenzene	1.58	1.51	–0.07
624. $C_6H_4O_4N_2$	*p*-dinitrobenzene	1.49	1.51	0.02
625. $C_6H_4O_5N_2$	3,5-dinitrophenol	2.32	1.77	–0.55
626. $C_6H_4O_5N_2$	2,4-dinitrophenol	1.51	1.77	0.26
627. $C_6H_4O_5N_2$	2,6-dinitrophenol	1.25	1.40	0.15
628. $C_6H_4O_5N_2$	2,5-dinitrophenol	1.75	1.58	–0.17
629. $C_6H_5N_3$	benzotriazole	1.34	1.24	–0.10
630. C_6H_5I	iodobenzene	3.25	2.77	–0.48
631. $C_6H_5NCl_2$	2,3-dichloroaniline	2.78	2.23	–0.55
632. $C_6H_5NCl_2$	3,4-dichloroaniline	2.69	2.23	–0.46
633. C_6H_5OF	*p*-fluorophenol	1.79	1.68	–0.11
634. C_6H_5OF	*m*-fluorophenol	1.93	1.68	–0.25
635. C_6H_5OF	*o*-fluorophenol	1.71	1.68	–0.03
636. C_6H_5OCl	*p*-chlorophenol	2.35	2.11	–0.24
637. C_6H_5OCl	*o*-chlorophenol	2.15	2.11	–0.04
638. C_6H_5OCl	*m*-chlorophenol	2.50	2.11	–0.39
639. C_6H_5OBr	*o*-bromophenol	2.35	2.30	–0.05
640. C_6H_5OBr	*p*-bromophenol	2.43	2.30	–0.13
641. C_6H_5OBr	*m*-bromophenol	2.63	2.30	–0.33
642. C_6H_5OI	*m*-iodophenol	2.93	2.65	–0.28
643. C_6H_5OI	*o*-iodophenol	2.65	2.65	0.00
644. C_6H_5OI	*p*-iodophenol	2.91	2.65	–0.26
645. $C_6H_5O_2N$	*N*-hydroxybenzoquinone	1.08	1.31	0.23
646. $C_6H_5O_2N$	picolinic acid	–1.98	–2.17	–0.19
647. $C_6H_5O_2NSCl_2$	3,4-dichlorobenzenesulfonamide	1.44	1.86	0.42
648. $C_6H_5O_3N$	3-hydroxypicolinic acid	–1.27	–1.86	–0.59
649. $C_6H_5O_3N$	*m*-nitrophenol	2.01	1.61	–0.40
650. $C_6H_5O_3N$	*o*-nitrophenol	1.79	1.43	–0.36
651. $C_6H_5O_3N$	*p*-nitrophenol	1.91	1.80	–0.11
652. $C_6H_5O_4N$	2-nitroresorcinol	1.36	1.31	–0.05
653. C_6H_6NF	*m*-fluoroaniline	1.30	1.14	–0.16
654. C_6H_6NF	*o*-fluoroaniline	1.26	1.14	–0.12
655. C_6H_6NF	*p*-fluoroaniline	1.15	1.14	–0.01
656. C_6H_6NCl	*m*-chloroaniline	1.88	1.58	–0.30
657. C_6H_6NCl	*o*-chloroaniline	1.90	1.58	–0.32
658. C_6H_6NCl	*p*-chloroaniline	1.83	1.58	–0.25
659. C_6H_6NBr	*m*-bromoaniline	2.10	1.76	–0.34
660. C_6H_6NBr	*o*-bromoaniline	2.29	1.76	–0.53
661. C_6H_6NBr	*p*-bromoaniline	2.26	1.76	–0.50
662. $C_6H_6ON_2$	nicotinamide	–0.37	0.15	0.52
663. $C_6H_6ON_3F$	2-fluoroisoniazide	–0.11	0.21	0.32
664. $C_6H_6ON_3Cl$	2-chloroisoniazide	0.11	0.64	0.53
665. $C_6H_6O_2$	*p*-dihydroxybenzene	0.59	1.34	0.75
666. $C_6H_6O_2$	*m*-dihydroxybenzene	0.80	1.34	0.54
667. $C_6H_6O_2$	*o*-dihydroxybenzene	0.88	1.34	0.46
668. $C_6H_6O_2N_2$	3-hydroxypicolinamide	0.65	0.76	0.11
669. $C_6H_6O_2N_2$	*m*-nitroaniline	1.37	1.19	–0.18
670. $C_6H_6O_2N_2$	*o*-nitroaniline	1.44	0.89	–0.55
671. $C_6H_6O_2N_2$	*p*-nitroaniline	1.39	1.49	0.10
672. $C_6H_6O_2NSCl$	*m*-chlorobenzenesulfonamide	1.29	1.21	–0.08
673. $C_6H_6O_2NSCl$	*o*-chlorobenzenesulfonamide	0.74	1.21	0.47
674. $C_6H_6O_2NSCl$	*p*-chlorobenzenesulfonamice	0.84	1.21	0.37
675. $C_6H_6O_2NSBr$	*p*-bromobenzenesulfonamide	1.36	1.39	0.03
676. $C_6H_6O_4N_2S$	*o*-nitrobenzenesulfonamide	0.34	0.53	0.19
677. $C_6H_6O_4N_2S$	*p*-nitrobenzenesulfonamide	0.64	0.53	–0.11
678. $C_6H_6O_4N_2S$	*m*-nitrobenzenesulfonamide	0.55	0.53	–0.02
679. C_6H_7N	2-methylpyridine	1.11	1.61	0.50
680. C_6H_7N	3-methylpyridine	1.20	1.61	0.41
681. C_6H_7N	4-methylpyridine	1.22	1.61	0.39

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
682. C_6H_7O	*N*-phenylhydroxyamine	0.79	1.16	0.37
683. C_6H_7ON	*m*-aminophenol	0.17	0.81	0.64
684. C_6H_7ON	α-pyridylmethanol	0.06	0.68	0.62
685. C_6H_7ON	β-pyridylmethanol	−0.02	0.68	0.70
686. C_6H_7ON	γ-pyridylmethanol	0.06	0.68	0.62
687. C_6H_7ON	*o*-aminophenol	0.57	0.81	0.24
688. C_6H_7ON	*p*-aminophenol	0.04	0.81	0.77
689. $C_6H_7ON_3$	6-aminonicotinamide	0.70	−0.50	−1.20
690. $C_6H_7ON_3$	isoniazid	−1.14	−0.01	1.13
691. $C_6H_7OCl_5$	1-hydroxypentachlorocyclohexane	2.54	2.91	0.37
692. $C_6H_7O_2NS$	benzenesulfonamide	0.31	0.56	0.25
693. $C_6H_7O_3NS$	*p*-phenolsulfonamide	0.06	0.44	0.38
694. $C_6H_8N_2$	2-amino-4-picoline	0.56	0.95	0.39
695. $C_6H_8N_2$	α-pyridilmethylamine	−0.21	0.47	0.68
696. $C_6H_8N_2$	β-pyridylmethylamine	−0.32	0.47	0.79
697. $C_6H_8N_2$	γ-pyridylmethylamine	−0.38	0.47	0.85
698. $C_6H_8N_2$	2-amino-5-methylpyridine	1.02	0.95	−0.07
699. $C_6H_8N_2$	4,6-dimethylpyrimidine	0.62	1.64	1.02
700. $C_6H_8N_2$	*o*-diaminobenzene	0.15	0.27	0.12
701. $C_6H_8O_2N_2S$	*m*-aminobenzenesulfonamide	−1.20	−0.10	1.10
702. $C_6H_8O_2N_2S$	*N*-phenylsulfamide	0.40	0.58	0.18
703. $C_6H_8O_2N_2S$	sulfanilamide	−0.78	−1.03	−0.25
704. $C_6H_8O_4N_4$	romidazole	−0.38	−0.16	0.22
705. $C_6H_8O_7$	citric acid	−1.72	−1.18	0.54
706. $C_6H_9O_3N$	trimethadione	−0.37	−0.36	0.01
707. $C_6H_9O_3N_3$	metronidazole	−0.10	−0.06	0.04
708. $C_6H_{10}O_3$	4-ketovaleric acid methyl ester	−0.13	0.54	0.67
709. $C_6H_{10}O_4$	adipic acid	0.08	0.43	0.35
710. $C_6H_{11}NS$	2-azacycloheptanthion	0.75	0.90	0.15
711. $C_6H_{11}ON$	2-azacycloheptanone	−0.19	0.09	0.28
712. $C_6H_{11}O_2N_2Cl$	α-chloroisovalerylurea	1.00	0.84	−0.16
713. $C_6H_{12}ON_2$	2-methyl-*N*-nitrosopiperidine	0.71	0.75	0.04
714. $C_6H_{12}ON_2$	3-methyl-*N*-nitrosopiperidine	0.99	0.75	−0.24
715. $C_6H_{12}ON_2$	4-methyl-*N*-nitrosopiperidine	1.05	0.75	−0.30
716. $C_6H_{13}O_2N$	pentyl carbamate	1.35	1.06	−0.29
717. $C_6H_{13}O_2N$	*tert*-pentyl carbamate	0.94	1.03	0.09
718. $C_6H_{12}O_2N_2$	2,6-dimethyl-*N*-nitrosomorpholine	0.32	0.65	0.33
719. $C_6H_{12}O_2N_4$	2,6-dimethyl-*N,N'*-dinitrosopiperazine	0.08	0.03	−0.05
720. $C_6H_{13}O_2N_3$	1-nitroso-3,3-diethyl-1-methylurea	1.11	1.54	0.43
721. $C_6H_{14}O_2$	2-butoxyethanol	0.83	0.71	−0.12
722. $C_6H_{14}O_2$	diethylacetal	0.84	0.93	0.09
723. $C_6H_{14}ON_2$	1-nitrosodiisopropylamine	1.63	1.46	−0.17
724. $C_6H_{14}ON_2$	*N*-nitrosodipropylamine	1.63	1.61	−0.02
725. $C_6H_{16}N_2$	*N,N,N',N'*-tetramethylethylenediamine	0.30	0.90	0.60
726. $C_7HN_2Cl_5$	2,4,5,6,7-pentachlorobenzimidazole	4.53	4.56	0.03
727. C_7H_4NSBr	*p*-bromophenyl isothiocyanate	4.03	3.91	−0.12
728. $C_7H_4N_4$	phenylenetetrazole	0.14	0.50	0.36
729. $C_7H_4O_2N_2$	3-cyano-1-nitrobenzene	1.17	1.23	0.06
730. $C_7H_4O_2N_2$	4-cyano-1-nitrobenzene	1.19	1.23	0.04
731. $C_7H_4O_2N_2S$	4-nitrophenyl isothiocyanate	3.62	3.04	−0.58
732. $C_7H_4O_3I_2$	3,5-diiodosalicylic acid	4.56	4.48	−0.08
733. C_7H_5NS	phenyl isothiocyanate	3.28	3.07	−0.21
734. C_7H_5NS	phenyl thiocyanate	2.54	1.88	−0.66
735. C_7H_5NS	benzothiazole	2.02	2.27	0.25
736. $C_7H_5F_3S$	trifluoromethylthiobenzene	3.57	3.16	−0.41
737. $C_7H_5N_4Cl$	1-phenyl-4-chlorotetrazole	1.48	1.98	0.50
738. $C_7H_5SCl_3$	trichloromethylthiobenzene	3.78	3.84	0.06
739. C_7H_5ON	*o*-cyanophenol	1.61	1.14	−0.47
740. C_7H_5ON	*m*-cyanophenol	1.70	1.14	−0.56
741. C_7H_5ON	*p*-cyanophenol	1.60	1.14	−0.46
742. $C_7H_5ON_2Cl$	zoxazolamine	2.46	1.56	−0.90
743. $C_7H_5OF_3$	trifluoromethoxybenzene	3.17	2.28	−0.89
744. $C_7H_5OF_3$	*m*-trifluoromethylphenol	2.95	2.56	−0.39
745. $C_7H_5OF_3$	*o*-trifluoromethylphenol	2.80	2.56	−0.24
746. $C_7H_5O_2F$	*m*-fluorobenzoic acid	2.15	2.01	−0.14
747. $C_7H_5O_2F$	*p*-fluorobenzoic acid	2.07	2.01	−0.06
748. $C_7H_5O_2Cl$	*m*-chlorobenzoic acid	2.68	2.45	−0.23
749. $C_7H_5O_2Cl$	*o*-chlorobenzoic acid	1.98	2.45	0.47
750. $C_7H_5O_2Cl$	*p*-chlorobenzoic acid	2.65	2.45	−0.20
751. $C_7H_5O_2Br$	*m*-bromobenzoic acid	2.87	2.63	−0.24
752. $C_7H_5O_2Br$	*p*-bromobenzoic acid	2.86	2.63	−0.23
753. $C_7H_5O_2I$	*m*-iodobenzoic acid	3.13	2.98	−0.15
754. $C_7H_5O_2I$	*o*-iodobenzoic acid	2.40	2.98	0.58
755. $C_7H_5O_2I$	*p*-iodobenzoic acid	3.02	2.98	−0.04
756. $C_7H_5O_2F_3S$	phenyl trifluoromethyl sulfone	2.68	1.86	−0.82
757. $C_7H_5O_3Br$	5-bromosalicylic acid	2.87	2.93	0.06
758. $C_7H_5O_4N$	*m*-nitrobenzoic acid	1.83	1.76	−0.07
759. $C_7H_5O_4N$	*p*-nitrobenzoic acid	1.89	1.76	−0.13

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
760. $C_7H_5O_5N$	5-nitrosalicylic acid	2.34	2.43	0.09
761. $C_7H_5O_5N_3$	3,5-dinitrobenzamide	0.83	0.47	–0.36
762. $C_7H_6NF_3$	*p*-trifluoromethylaniline	1.95	2.03	0.08
763. $C_7H_6N_2$	7-azaindole	1.82	1.29	–0.53
764. $C_7H_6N_2$	benzimidazole	1.46	1.29	–0.17
765. $C_7H_6N_2$	4-cyano-2-methylpyridine	0.81	1.29	0.48
766. $C_7H_6N_2$	2-cyano-6-methylpyridine	0.84	1.29	0.45
767. $C_7H_6N_2$	indazole	1.82	1.66	–0.16
768. $C_7H_6N_2S$	*o*-phenylenethiourea	1.66	0.71	–0.95
769. $C_7H_6N_4$	1-phenyltetrazole	1.09	1.00	–0.09
770. C_7H_6ONF	*m*-fluorobenzamide	0.91	0.75	–0.16
771. C_7H_6ONF	*p*-fluorobenzamide	0.91	0.75	–0.16
772. C_7H_6ONCl	*m*-chlorobenzamide	1.51	1.18	–0.33
773. C_7H_6OBCl	*p*-chlorobenzamide	1.51	1.18	–0.33
744. C_7H_6ONBr	*m*-bromobenzamide	1.65	1.37	–0.28
775. C_7H_6ONBr	*p*-bromobenzamide	1.76	1.37	–0.39
776. C_7H_6ONI	*p*-iodobenzamide	1.99	1.72	–0.27
777. $C_7H_6O_2$	1,2-methylenedioxybenzene	2.08	1.64	–0.44
778. $C_7H_6O_2$	*o*-hydroxybenzaldehyde	1.70	1.93	0.23
779. $C_7H_6O_2$	tropolone	0.53	0.95	0.42
780. $C_7H_6O_2NF$	2-fluoro-4-aminobenzoic acid	0.46	0.29	–0.17
781. $C_7H_6O_2NF$	3-fluoro-4-aminobenzoic acid	0.58	0.29	–0.29
782. $C_7H_6O_2NCl$	2-chloro-4-aminobenzoic acid	0.50	0.73	0.23
783. $C_7H_6O_2NCl$	3-chloro-4-aminobenzoic acid	1.52	0.73	–0.79
784. $C_7H_6O_2NBr$	2-bromo-4-aminobenzoic acid	0.66	0.92	0.26
785. $C_7H_6O_2NBr$	3-bromo-4-aminobenzoic acid	1.40	0.92	–0.48
786. $C_7H_6O_2NI$	2-iodo-4-aminobenzoic acid	0.82	1.27	0.45
787. $C_7H_6O_2NI$	3-iodo-4-aminobenzoic acid	1.53	1.27	–0.26
788. $C_7H_6O_2N_2S$	*p*-cyanobenzenesulfonamide	0.23	0.24	0.01
789. $C_7H_6O_3$	salicylic acid	2.26	2.09	–0.17
790. $C_7H_6O_3$	*m*-hydroxybenzoic acid	1.50	1.68	0.18
791. $C_7H_6O_3$	*p*-hydroxybenzoic acid	1.58	1.68	0.10
792. $C_7H_6O_3N_2$	*m*-nitrobenzamide	0.77	0.50	–0.27
793. $C_7H_6O_3N_2$	*p*-nitrobenzamide	0.82	0.50	–0.32
794. $C_7H_6O_3N_2$	*p*-nitroformanilide	1.43	1.02	–0.41
795. $C_7H_6O_4$	2,4-dihydroxybenzoic acid	1.44	1.98	0.54
796. $C_7H_6O_4$	2,6-dihydroxybenzoic acid	2.20	2.40	0.20
797. $C_7H_6O_4$	2,5-dihydroxybenzoic acid	1.74	1.98	0.24
798. $C_7H_6O_4N_2$	2,4-dinitrotoluene	1.98	1.92	–0.06
799. $C_7H_6O_4N_2$	2-nitro-4-aminobenzoic acid	0.38	0.35	–0.03
800. C_7H_7NS	thiobenzamide	1.49	1.33	–0.16
801. $C_7H_7N_3$	1-methylbenzotriazole	1.13	1.03	–0.10
802. C_7H_7ON	2-acetylpyridine	0.83	1.11	0.28
803. C_7H_7ON	4-acetylpyridine	0.54	1.11	0.57
804. C_7H_7ON	3-acetylpyridine	0.43	1.11	0.68
805. C_7N_7ON	benzaldoxime	1.75	2.19	0.44
806. C_7H_7OCl	2-methyl-4-chlorophenol	2.78	2.52	–0.26
807. C_7H_7OCl	3-methyl-4-chlorophenol	3.10	2.52	–0.58
808. C_7H_7OCl	*m*-chlorobenzyl alcohol	1.94	1.71	–0.23
809. C_7H_7OCl	*p*-chlorobenzyl alcohol	1.96	1.71	–0.25
810. $C_7H_7O_2N$	isonicotinic acid methyl ester	0.87	1.19	0.32
811. $C_7H_7O_2N$	nicotinic acid methyl ester	0.81	1.19	0.38
812. $C_7H_7O_2N$	*m*-hydroxybenzamide	0.39	0.41	0.02
813. $C_7H_7O_2N$	*p*-hydroxybenzamide	0.25	0.41	0.16
814. $C_7H_7O_2N$	benzohydroxamic acid	0.26	0.13	–0.13
815. $C_7H_7O_2N$	salicylamide	0.89	1.14	0.25
816. $C_7H_7O_2N$	*p*-aminobenzoic acid	0.68	0.08	–0.60
817. $C_7H_7O_2N$	*o*-aminobenzoic acid	1.21	1.14	–0.07
818. $C_7H_7O_2FS$	*p*-fluorosulfonyltoluene	2.74	1.40	–1.34
819. $C_7H_7O_3N$	3-hydroxy-4-aminobenzoic acid	–0.32	–0.04	0.28
820. $C_7H_7O_3N$	*p*-aminosalicylic acid	0.87	0.38	–0.49
821. $C_7H_7O_3N$	*m*-nitrobenzyl alcohol	1.21	1.03	–0.18
822. $C_7H_7O_3N$	*p*-nitrobenzyl alcohol	1.26	1.03	–0.23
823. $C_7H_7O_3N$	*p*-nitroanisole	2.03	1.55	–0.48
824. $C_7H_7O_3N$	*m*-nitroanisole	2.16	1.55	–0.61
825. $C_7H_8ON_2$	*m*-aminobenzamide	0.33	–0.12	–0.45
826. $C_7H_8ON_2$	*p*-aminobenzamide	0.02	–0.12	–0.14
827. $C_7H_8ON_2$	benzoylhydrazine	0.19	0.37	0.18
828. $C_7H_8ON_2$	2-acetaminopyridine	0.61	0.60	–0.01
829. $C_7H_8ON_2$	3-acetaminopyridine	0.41	0.60	0.19
830. $C_7H_8ON_2$	4-acetaminopyridine	0.59	0.60	0.01
831. $C_7H_8ON_2$	α-pyridylethanamide	–0.65	–0.34	0.31
832. $C_7H_8ON_2$	β-pyridylethanamide	–0.71	–0.34	0.37
833. $C_7H_8ON_2$	γ-pyridylethanamide	–0.65	–1.24	–0.59
834. $C_7H_8ON_2$	phenylurea	0.82	0.54	–0.28
835. $C_7H_8ON_2S$	phenylthiourea	0.73	1.03	0.30
836. C_7H_8OS	methyl phenyl sulfoxide	0.55	0.67	0.12
837. C_7H_8OS	*p*-(methylthio)phenol	1.78	2.36	0.58

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
838. $C_7H_8O_2$	*m*-hydroxybenzyl alcohol	0.49	0.94	0.45
839. $C_7H_8O_2$	*o*-hydroxybenzyl alcohol	0.73	0.94	0.21
840. $C_7H_8O_2$	*p*-hydroxybenzyl alcohol	0.25	0.94	0.69
841. $C_7H_8O_2$	*o*-methoxyphenol	1.32	1.47	0.15
842. $C_7H_8O_2$	*m*-methoxyphenol	1.58	1.47	−0.11
843. $C_7H_8O_2$	*p*-methoxyphenol	1.34	1.47	0.13
844. $C_7H_8O_2N_2$	2,4-diaminobenzoic acid	−1.14	−0.58	0.56
845. $C_7H_8O_2N_2$	3,4-diaminobenzoic acid	−0.70	−1.11	−0.41
846. $C_7H_8O_2N_2$	*p*-nitro-*N*-methylaniline	2.04	1.98	−0.06
847. $C_7H_8O_2S$	methyl phenyl sulfone	0.47	1.17	0.70
848. $C_7H_8O_2S$	2-carboxylic acid ethyl thiophene	2.33	2.04	−0.29
849. $C_7H_8O_2N_4$	3,7-dimethylxanthine	−0.78	−1.24	−0.46
850. $C_7H_8O_3$	furoic acid ethyl ester	1.52	1.33	−0.19
851. C_7H_9N	2-ethylpyridine	1.69	2.02	0.33
852. C_7H_9N	2,6-lutidine	1.68	2.02	0.34
853. C_7H_9NS	*m*-(methylthio)aniline	1.45	1.82	0.37
854. C_7H_9NS	*o*-(methylthio)aniline	1.20	1.82	0.62
855. $C_7H_9SCl_5$	1-(methylthio)pentachlorocyclohexane	3.75	4.63	0.88
856. C_7H_9ON	2-(α-pyridyl)ethanol	0.12	1.09	0.97
857. C_7H_9ON	2-(β-pyridyl)ethanol	0.12	1.09	0.97
858. C_7H_9ON	2-(γ-pyridyl)ethanol	0.10	1.09	0.99
859. C_7H_9ON	*m*-aminobenzyl alcohol	−0.05	0.41	0.46
860. C_7H_9ON	*m*-methoxyaniline	0.93	0.93	0.00
861. C_7H_9ON	*o*-methoxyaniline	0.95	0.93	−0.02
862. C_7H_9ON	*p*-methoxyaniline	0.95	0.93	−0.02
863. $C_7H_9ON_3$	2-methylisoniazide	−0.37	0.40	0.77
864. $C_7H_9OCl_5$	1-hydroxy-1-methyl-2,3,4,5,6-pentachlorocyclohexane	2.94	3.69	0.75
865. $C_7H_9O_2N_3$	2-methoxyisoniazide	−0.10	0.00	0.10
866. $C_7H_9O_2NS$	*m*-methylbenzenesulfonamide	0.85	0.97	0.12
867. $C_7H_9O_2NS$	*o*-methylbenzenesulfonamide	0.84	0.97	0.13
868. $C_7H_9O_2NS$	*p*-methylbenzenesulfonamide	0.82	0.97	0.15
869. $C_7H_{10}N_2$	2-(α-pyridyl)ethylamine	0.08	0.88	0.80
870. $C_7H_{10}N_2$	2-(β-pyridyl)ethylamine	0.00	0.88	0.88
871. $C^7H_{10}N_2$	1-(γ-pyridyl)ethylamine	−0.01	0.88	0.89
872. $C_7H_{10}OCl_4$	2-methoxy-3,4,5,6-tetrachlorocyclohexane	2.99	3.04	0.05
873. $C_7H_{11}O_2N_3$	ipromidazole	1.06	1.22	0.16
874. $C_7H_{10}O_3N_3Cl$	ormidazole	0.60	0.75	0.15
875. $C_7H_{11}O_4N_3$	DA3838	−0.63	−0.53	0.10
876. $C_7H_{12}ON_2$	1,3-diallylurea	0.64	0.87	0.23
877. $C_7H_{12}ON_4S$	3-(methylthio)-4-amino-6-prop-1-yl-1,2,4-triazine-5-one	1.01	1.07	0.06
878. $C_7H_{12}O_2N_4$	3-methoxy-4-amino-6-isopropyl-1,2,4-triazine-5-one	−0.06	0.12	0.18
879. $C_7H_{13}N$	quinuclidine	1.20	0.53	−0.67
880. $C_7H_{13}NS$	2-azacyclooctanethione	1.00	1.26	0.26
881. $C_7H_{13}ON$	2-azacyclooctanone	0.24	0.45	0.21
882. $C_7H_{13}O_2N_2Br$	carbromal	1.54	1.66	0.12
883. $C_7H_{14}ON_2$	2,6-dimethyl-*N*-nitrosopiperidine	1.36	1.15	−0.21
884. $C_7H_{14}ON_2$	3,5-dimethyl-*N*-nitrosopiperidine	1.53	1.15	−0.38
885. $C_7H_{15}O_3N_3$	1-nitrosotriethylurea	1.54	1.06	−0.48
886. $C_8HN_2F_3Cl_4$	4,5,6,7-tetrachloro-2-trifluoromethylbenzimidazole	3.97	5.01	1.04
887. $C_8HN_2F_3Br_4$	4,5,6,7-tetrabromo-2-trifluoromethylbenzimidazole	4.81	5.75	0.94
888. $C_8H_2N_2F_3Cl_3$	4,5,7-trichloro-2-trifluoromethylbenzimidazole	3.78	4.36	0.58
889. $C_8H_2N_2F_3Br_3$	4,5,6-tribromo-2-trifluoromethylbenzimidazole	4.08	4.91	0.83
890. $C_8H_3N_2F_3Cl_2$	4,7-dichloro-2-trifluoromethylbenzimidzole	2.87	3.70	0.83
891. $C_8H_3N_2F_3Cl_2$	4,5-dichloro-2-trifluoromethylbenzimidazole	3.49	3.70	0.21
892. $C_8H_3N_2F_3Cl_2$	4,6-dichloro-2-trifluoromethylbenzimidazole	3.49	3.70	0.21
893. $C_8H_3N_2F_3Cl_2$	5,6-dichloro-2-trifluoromethylbenzimidazole	3.99	3.70	−0.29
894. $C_8H_3N_2F_3Br_2$	5,6-dibromo-2-trifluoromethylbenzimidazole	4.15	4.07	−0.08
895. $C_8H_3O_2N_3F_3Cl$	5-chloro-6-nitro-2-trifluoromethylbenzimidazole	3.21	3.02	−0.19
896. $C_8H_4N_2F_3Cl$	5-chloro-2-trifluoromethylbenzimidazole	3.39	3.05	−0.34
897. $C_8H_4N_2F_3Cl$	4-chloro-2-trifluoromethylbenzimidazole	2.93	3.05	0.12
898. $C_8H_4N_2F_3Br$	5-bromo-2-trifluoromethylbenzimidazole	3.57	3.23	−0.34
899. $C_8H_4O_2N_3F_3$	5-nitro-2-trifluoromethylbenzimidazole	2.68	2.37	−0.31
900. $C_8H_4O_3$	phthalic anhydride	−0.62	−0.67	−0.05
901. $C_8H_5N_2Cl$	2-chloroquinoxaline	2.23	2.49	0.26
902. $C_8H_5N_2Cl$	5-chloroquinoxaline	1.75	2.49	0.74
903. $C_8H_5N_2Cl$	6-chloroquinoxaline	2.10	2.49	0.39
904. $C_8H_5N_2F_3$	2-trifluoromethylbenzimidazole	2.67	2.40	−0.27
905. $C_8H_5ONF_3Br$	*p*-trifluoroacetamide bromobenzene	3.34	2.51	−0.83
906. $C_8H_5OF_3$	trifluoroacetophenone	2.15	2.19	0.04
907. $C_8H_5O_2N$	*m*-cyanobenzoic acid	1.48	1.47	−0.01
908. $C_8H_5O_2N$	*p*-cyanobenzoic acid	1.56	1.47	−0.09
909. $C_8H_5O_2NS$	4-carboxyphenyl isothiocyanate	3.52	3.29	−0.23
910. $C_8H_5O_2F_3$	*m*-trifluoromethylbenzoic acid	2.95	2.90	−0.05
911. $C_8H_5O_2NCl_2$	2,4-dichloro-β-nitrostyrene	3.26	3.48	0.22
912. $C_8H_5O_3Cl_3$	2,4,5-trichlorophenoxyacetic acid	3.36	3.30	−0.06
913. $C_8H_5O_4N_2Cl$	2-chloro-5-nitro-β-nitrostyrene	2.23	2.80	0.57
914. C_8H_6NBr	5-bromoindole	3.00	2.51	−0.49
915. $C_8H_6N_2$	quinoxaline	1.32	1.83	0.51

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
916. $C_8H_6ONF_3$	*p*-trifluoromethylbenzamide	1.71	1.63	−0.08
917. $C_8H_6ONF_3$	trifluoroacetanilide	2.21	1.67	−0.54
918. $C_8H_6ON_2$	cinnoin-4-one	0.82	1.25	0.43
919. $C_8H_6ON_2$	*m*-cyanobenzamide	0.52	0.21	−0.31
920. $C_8H_6ON_2$	*p*-cyanobenzamide	0.48	0.21	−0.27
921. $C_8H_6ON_2$	*p*-cyanoformanilide	1.08	0.74	−0.34
922. $C_8H_6ON_2$	quinazolin-4-one	0.77	0.41	−0.36
923. $C_8H_6O_2N_2$	quinazoline-2,4-dione	0.55	0.16	−0.39
924. $C_8H_6O_2N_2$	quinazoline-2,3-dione	0.20	1.07	0.87
925. $C_8H_6O_2NCl$	4-chloro-β-nitrostyrene	2.44	2.83	0.39
926. $C_8H_6O_2NCl$	3-chloro-β-nitrostyrene	2.57	2.83	0.26
927. $C_8H_6O_2NCl$	4-chloro-β-nitrostyrene	2.85	2.83	−0.02
928. $C_8H_6O_3$	piperonal	1.05	1.38	0.33
929. $C_8H_6O_3FCl$	3-chloro-5-flurophenoxyacetic acid	2.20	2.21	0.01
930. $C_8H_6O_3Cl_2$	2,4-dichlorophenoxyacetic acid	2.81	2.64	−0.17
931. $C_8H_6O_3Cl_2$	3,4-dichlorophenoxyacetic acid	2.81	2.64	−0.17
932. $C_8H_6O_3ClBr$	3-bromo-4-chlorophenoxyacetic acid	2.75	2.83	0.08
933. $C_8H_6O_3FI$	3-iodo-5-fluorophenoxyacetic acid	2.42	2.74	0.32
934. $C_8H_6O_3ClI$	3-iodo-4-chlorophenoxyacetic acid	3.10	3.18	0.08
935. $C_8H_6O_4$	*m*-phthalic acid	1.66	2.01	0.35
936. $C_8H_6O_4N_2$	2,β-dinitrostyrene	1.80	2.14	0.34
937. $C_8H_6O_4N_2$	3,β-dinitrostyrene	1.82	2.14	0.32
938. $C_8H_6O_4N_2$	4,β-dinitrostyrene	1.89	2.14	0.25
939. $C_8H_6O_5NCl$	3-nitro-4-chlorophenoxyacetic acid	1.85	1.96	0.11
940. C_8H_7N	indole	2.14	1.67	−0.47
941. C_8H_7NS	benzyl isothiocyanate	2.83	3.49	0.66
942. C_8H_7NS	benzyl thiocyanate	1.99	2.30	0.31
943. C_8H_7NS	4-methylphenyl isothiocyanate	3.92	3.48	−0.44
944. $C_8H_7N_2SCl$	5-chloro-2-methylthiobenzimidazole	3.22	2.84	−0.38
945. $C_8H_7ON_3$	2-aminoquinazolin-4-one	0.60	0.21	−0.39
946. C_8H_7OCl	*p*-chloroacetophenone	2.35	2.15	−0.20
947. C_8H_7OBr	*p*-bromoacetophenone	2.43	2.33	−0.10
948. $C_8H_7O_2F$	2-fluorophenyl acetate	1.76	1.79	0.03
949. $C_8H_7O_2F$	3-fluorophenyl acetate	1.74	1.79	0.05
950. $C_8H_7O_2F$	*m*-flurophenylacetic acid	1.65	1.69	0.04
951. $C_8H_7O_2F$	*o*-flurophenylacetic acid	1.50	1.69	0.19
952. $C_8H_7O_2F$	*p*-flurophenylacetic acid	1.55	1.69	0.14
953. $C_8H_7O_2Cl$	3-chlorophenyl acetate	2.32	2.23	−0.09
954. $C_8H_7O_2Cl$	*p*-chlorophenylacetic acid	2.12	2.13	0.01
955. $C_8H_7O_2Cl$	*m*-chlorophenylacetic acid	2.09	2.13	0.04
956. $C_8H_7O_2Cl$	2-chlorophenyl acetate	2.18	2.23	0.05
957. $C_8H_7O_2Br$	2-bromophenyl acetate	2.20	2.41	0.21
958. $C_8H_7O_2Br$	*m*-bromophenylacetic acid	2.37	2.31	−0.06
959. $C_8H_7O_2Br$	*p*-bromophenylacetic acid	2.31	2.31	0.00
960. $C_8H_7O_2I$	2-iodophenyl acetate	2.55	2.76	0.21
961. $C_8H_7O_2I$	*m*-iodophenoxylacetic acid	2.62	2.67	0.05
962. $C_8H_7O_2I$	*p*-iodophenoxylacetic acid	2.64	2.67	0.03
963. $C_8H_7O_2NCl_2$	2,3-dichlorophenyl *N*-methylcarbamate	2.48	2.53	0.05
964. $C_8H_7O_2NCl_2$	2,5-dichlorophenyl *N*-methylcarbamate	2.44	2.53	0.09
965. $C_8H_7O_2NCl_2$	3,4-dichlorophenyl *N*-methylcarbamate	2.80	2.53	−0.27
966. $C_8H_7O_2NCl_2$	3,5-dichlorophenyl *N*-methylcarbamate	3.03	2.53	−0.50
967. $C_8H_7O_2Br_3$	2-(2,4,6-tribromophenoxy)ethanol	3.42	3.58	0.16
968. $C_8H_7O_3N$	*m*-acetylnitrobenzene	1.42	1.46	0.04
969. $C_8H_7O_3N$	*p*-acetylnitrobenzene	1.49	1.46	−0.03
970. $C_8H_7O_3N$	3-hydroxy-β-nitrostyrene	2.07	2.06	−0.01
971. $C_8H_7O_3N$	4-hydroxy-β-nitrostyrene	2.12	2.06	−0.06
972. $C_8H_7O_3F$	*m*-flurophenoxyacetic acid	1.48	1.55	0.07
973. $C_8H_7O_3F$	*o*-flurophenoxyacetic acid	1.26	1.55	0.29
974. $C_8H_7O_3F$	*p*-flurophenoxyacetic acid	1.41	1.55	0.14
975. $C_8H_7O_3Cl$	*m*-chlorophenoxyacetic acid	2.03	1.99	−0.04
976. $C_8H_7O_3Cl$	*o*-chlorophenoxyacetic acid	2.02	1.99	−0.03
977. $C_8H_7O_3Cl$	*p*-chlorophenoxyacetic acid	1.99	1.99	0.00
978. $C_8H_7O_3Br$	2-bromophenoxyacetic acid	2.10	2.17	0.07
979. $C_8H_7O_3Br$	3-bromophenoxyacetic acid	2.22	2.17	−0.05
980. $C_8H_7O_3Br$	4-bromophenoxyacetic acid	2.45	2.17	−0.28
981. $C_8H_7O_3I$	2-iodophenoxyacetic acid	2.44	2.53	0.09
982. $C_8H_7O_3I$	3-iodophenoxyacetic acid	2.19	2.53	0.34
983. $C_8H_7O_3I$	4-iodophenoxyacetic acid	2.69	2.53	−0.16
984. $C_8H_7O_4N$	2-nitrophenyl acetate	1.55	1.54	−0.01
985. $C_8H_7O_4N$	3-nitrophenyl acetate	1.82	1.54	−0.28
986. $C_8H_7O_4N$	4-nitrophenyl acetate	1.49	1.54	0.05
987. $C_8H_7O_4N$	*m*-nitrophenylacetic acid	1.45	1.45	0.00
988. $C_8H_7O_4N$	*p*-nitrophenylacetic acid	1.39	1.45	0.06
989. $C_8H_7O_4FS$	*p*-(fluorosulfonyl)phenylacetic acid	1.84	0.90	−0.94
990. $C_8H_7O_5N$	*m*-nitrophenoxyacetic acid	1.37	1.30	−0.07
991. $C_8H_7O_5N$	*o*-nitrophenoxyacetic acid	1.22	1.30	0.08
992. $C_8H_7O_5N$	*p*-nitrophenoxyacetic acid	1.48	1.30	−0.18
993. $C_8H_7O_5N_3$	3,5-dinitro-4-methylbenzamide	0.68	0.88	0.20

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
994. $C_8H_8N_4$	hydrazaline	1.00	1.65	0.65
995. C_8H_8OS	acetylthiobenzene	2.23	1.98	–0.25
996. C_8H_8ONF	*p*-fluoroacetanilide	1.47	1.20	–0.27
997. C_8H_8ONCl	*p*-chloroacetanilide	1.87	1.63	–0.24
998. C_8H_8ONI	*p*-iodoacetanilide	2.46	2.17	–0.29
999. $C_8H_8O_2$	*m*-acetylphenol	1.39	1.38	–0.01
1000. $C_8H_8O_2$	*p*-acetylphenol	1.35	1.38	0.03
1001. $C_8H_8O_2$	*o*-hydroxyacetophone	1.92	2.11	0.19
1002. $C_8H_8O_2$	*p*-methoxybenzaldehyde	1.59	1.32	–0.27
1003. $C_8H_8O_2$	1,4-benzodioxane	2.01	2.00	–0.01
1004. $C_8H_8O_2S$	phenylthioacetic acid	1.91	1.96	0.05
1005. $C_8H_8O_2S$	*p*-(methylthio)benzoic acid	2.74	2.69	–0.05
1006. $C_8H_8O_2N_2$	isophthalamide	–0.21	–0.52	–0.31
1007. $C_8H_8O_2NF$	2-fluorophenyl *N*-methylcarbamate	1.25	1.44	0.19
1008. $C_8H_8O_2NF$	3-fluorophenyl *N*-methylcarbamate	1.48	1.44	–0.04
1009. $C_8H_8O_2NF$	4-fluorophenyl *N*-methylcarbamate	1.28	1.44	0.16
1010. $C_8H_8O_2NCl$	4-chlorophenyl *N*-methylcarbamate	2.01	1.87	–0.14
1011. $C_8H_8O_2NCl$	2-chlorophenyl *N*-methylcarbamate	1.64	1.87	0.23
1012. $C_8H_8O_2NCl$	3-chlorophenyl *N*-methylcarbamate	2.03	1.87	–0.16
1013. $C_8H_8O_2NBr$	3-bromophenyl *N*-methylcarbamate	2.25	2.06	–0.19
1014. $C_8H_8O_2NBr$	4-bromophenyl *N*-methylcarbamate	2.17	2.06	–0.11
1015. $C_8H_8O_2NBr$	2-bromophenyl *N*-methylcarbamate	1.77	2.06	0.29
1016. $C_8H_8O_2NI$	2-iodophenyl *N*-methylcarbamate	1.96	2.41	0.45
1017. $C_8H_8O_2NI$	3-iodophenyl *N*-methylcarbamate	2.52	2.41	–0.11
1018. $C_8H_8O_2NI$	4-iodophenyl *N*-methylcarbamate	2.46	2.41	–0.05
1019. $C_8H_8O_3$	vanillin	1.31	1.21	–0.10
1020. $C_8H_8O_3$	*m*-carbomethoxyphenol	1.89	1.46	–0.43
1021. $C_8H_8O_3$	*m*-hydroxyphenyl acetate	1.23	1.46	0.23
1022. $C_8H_8O_3$	isovanillin	0.97	1.21	0.24
1023. $C_8H_8O_3$	*m*-methoxybenzoic acid	2.02	1.80	–0.22
1024. $C_8H_8O_3$	*o*-methoxybenzoic acid	1.59	1.80	0.21
1025. $C_8H_8O_3$	*p*-methoxybenzoic acid	1.96	1.80	–0.16
1026. $C_8H_8O_3$	methyl salicyate	2.46	2.19	–0.27
1027. $C_8H_8O_3$	*o*-vanillin	1.37	1.94	0.57
1028. $C_8H_8O_3$	mandelic acid	0.62	0.59	–0.03
1029. $C_8H_8O_3$	phenoxyacetic acid	1.34	1.34	0.00
1030. $C_8H_8O_3$	3,4-methylenedioxy benzyl alcohol	1.05	1.12	0.07
1031. $C_8H_8O_3$	*p*-hydroxybenzoic acid methyl ester	1.96	1.46	–0.50
1032. $C_8H_8O_3$	*m*-hydroxyphenylacetic acid	0.85	1.36	0.51
1033. $C_8H_8O_3$	*p*-hydroxyphenylacetic acid	1.96	1.36	–0.60
1034. $C_8H_8O_3NCl$	3-amino-4-chlorophenoxyacetic acid	1.16	1.34	0.18
1035. $C_8H_8O_3N_2$	*p*-nitroacetanilide	1.66	0.95	–0.71
1036. $C_8H_8O_4$	*m*-hydroxyphenoxyacetic acid	0.76	1.22	0.46
1037. $C_8H_8O_4$	*o*-hydroxyphenoxyacetic acid	0.85	1.22	0.37
1038. $C_8H_8O_4$	*p*-hydroxyphenoxyacetic acid	0.65	1.22	0.57
1039. $C_8H_8O_4S$	*p*-methylsulfonylbenzoic acid	0.67	1.38	0.71
1040. $C_8H_8O_4N_2$	2-nitrophenyl *N*-methylcarbamate	1.02	1.19	0.17
1041. $C_8H_8O_4N_2$	3-nitrophenyl *N*-methylcarbamate	1.39	1.19	–0.20
1042. $C_8H_8O_4N_2$	4-nitrophenyl *N*-methylcarbamate	1.47	1.19	–0.28
1043. C_8H_9NS	thioacetanilide	1.71	1.96	0.25
1044. C_8H_9ON	*p*-aminoacetophone	0.41	0.84	0.43
1045. C_8H_9ON	ethyl 4-pyridyl ketone	0.77	1.53	0.76
1046. C_8H_9ON	*o*-methylbenzaldoxime	2.53	2.60	0.07
1047. $C_8H_9O_2N$	*p*-aminophenyl acetate	–0.16	0.92	1.08
1048. $C_8H_9O_2N$	*m*-hydroxyacetoanilide	0.73	0.86	0.13
1049. $C_8H_9O_2N$	*o*-hydroxyacetoanilide	0.72	0.86	0.14
1050. $C_8H_9O_2N$	*p*-hydroxyacetoanilide	0.36	0.49	0.13
1051. $C_8H_9O_2N$	*m*-methoxyformanilide	1.25	1.06	–0.19
1052. $C_8H_9O_2N$	*p*-methoxyformanilide	1.03	1.06	0.03
1053. $C_8H_9O_2N$	3-methyl-4-aminobenzoic acid	0.54	0.49	–0.05
1054. $C_8H_9O_2N$	nicotinic acid ethyl ester	1.32	1.61	0.29
1055. $C_8H_9O_2N$	isonicotinic acid ethyl ester	1.43	1.61	0.18
1056. $C_8H_9O_2N$	phenoxyacetamide	0.76	0.54	–0.22
1057. $C_8H_9O_2N$	picolinic acid ethyl ester	0.87	1.61	0.74
1058. $C_8H_9O_2N$	phenyl *N*-methylcarbamate	1.24	1.59	0.35
1059. $C_8H_9O_2N$	*N*-phenyl glycine	0.62	–0.35	–0.97
1060. $C_8H_9O_2N$	2-methyl-4-aminobenzoic acid	0.31	0.49	0.18
1061. $C_8H_9O_2N$	*p*-methoxybenzamide	0.86	0.54	–0.32
1062. $C_8H_9O_2N$	*o*-methoxybenzamide	0.87	0.54	–0.33
1063. $C_8H_9O_2N$	*m*-methoxybenzamide	0.94	0.54	–0.40
1064. $C_8H_9O_2Cl_5$	1-acetoxy-2,3,4,5,6-pentachlorocyclohexane	3.40	3.73	0.33
1065. $C_8H_9O_3N$	2-methoxy-4-aminobenzoic acid	–0.38	0.09	0.47
1066. $C_8H_9O_3N$	*p*-nitrophenetole	2.53	1.97	–0.56
1067. $C_8H_{10}N_2S$	1-methyl-1-phenyl-2-thiourea	0.85	1.06	0.21
1068. $C_8H_{10}ON_2$	β-(α-pyridyl)propanamide	–0.27	0.08	0.35
1069. $C_8H_{10}ON_2$	β-(β-pyridyl)propanamide	–0.26	0.08	0.34
1070. $C_8H_{10}ON_2$	β-(γ-pyridyl)propanamide	–0.25	–0.83	–0.58
1071. $C_8H_{10}O_2$	1,3-dimethoxybenzene	2.21	1.59	–0.62

Table 4 (Continued)

formula	name	log P_c[a]	log P_c[b]	log P_f[c]
	Multifunctional Compounds			
1072. $C_8H_{10}O_2$	*o*-dimethoxybenzene	2.21	1.59	–0.62
1073. $C_8H_{10}O_2$	*m*-ethoxyphenol	1.98	1.88	–0.10
1074. $C_8H_{10}O_2$	*o*-ethoxyphenol	1.68	1.88	0.20
1075. $C_8H_{10}O_2$	*p*-ethoxyphenol	1.81	1.88	0.07
1976. $C_8H_{10}O_2$	*o*-methoxybenzyl alcohol	1.13	1.07	–0.06
1077. $C_8H_{10}O_2$	*p*-methoxybenzyl alcohol	1.10	1.07	–0.03
1078. $C_8H_{10}O_2$	2-phenoxyethanol	1.16	1.07	–0.09
1079. $C_8H_{10}O_2N_4$	caffeine	–0.07	–0.86	–0.79
1080. $C_8H_{10}O_3N_2S$	sulfanilacetamide	–0.96	–0.53	0.43
1081. $C_8H_{11}N$	4-propylpyridine	2.10	2.44	0.34
1082. $C_8H_{11}ON$	*m*-(dimethylamino)phenol	1.57	1.59	0.02
1083. $C_8H_{11}ON$	3-(α-pyridyl)propanol	0.58	0.86	0.28
1084. $C_8H_{11}ON$	3-(β-pyridyl)propanol	0.60	0.86	0.26
1085. $C_8H_{11}ON$	3-(γ-pyridyl)propanol	0.58	0.21	–0.37
1086. $C_8H_{11}O_2NS$	*N,N*-dimethylbenzenesulfonamide	1.35	0.89	–0.46
1087. $C_8H_{11}O_2NS$	*p*-ethylbenzenesulfonamide	1.31	1.38	0.07
1088. $C_8H_{12}N_2$	3-(α-pyridyl)propylamine	0.49	0.75	0.26
1089. $C_8H_{12}N_2$	3-(β-pyridyl)propylamine	0.44	0.75	0.31
1090. $C_8H_{12}N_2$	3-(γ-pyridyl)propylamine	0.40	0.21	–0.19
1091. $C_8H_{12}O_2Cl_4$	3,6-dimethoxy-1,2,4,5-tetrachlorocyclohexane	3.15	2.81	–0.34
1092. $C_8H_{12}O_3N_2$	barbital	0.65	0.67	0.02
1093. $C_8H_{14}N_2$	4-pentylpyrazole	2.96	2.71	–0.25
1094. $C_8H_{18}ON_2$	*N*-nitrosodibutylamine	1.92	2.44	0.52
1095. $C_9H_5N_3$	6-cyanoquinoxaline	1.01	1.52	0.51
1096. $C_9H_5O_3N_2F$	8-fluoro-4-nitroquinoline 1-oxide	1.00	0.97	–0.03
1097. $C_9H_5O_3N_2Cl$	6-chloro-4-nitroquinoline 1-oxide	1.41	1.41	0.00
1098. $C_9H_5O_5N_3$	4,5-dinitroquinoline 1-oxide	0.95	0.72	–0.23
1099. $C_9H_5O_5N_3$	4,6-dinitroquinoline 1-oxide	0.90	0.72	–0.18
1100. $C_9H_5O_5N_3$	4,8-dinitroquinoline 1-oxide	0.76	0.72	–0.04
1101. C_9H_6NCl	2-chloroquinoline	2.71	2.87	0.16
1102. C_9H_6NCl	6-chloroquinoline	2.73	2.87	0.14
1103. C_9H_6NCl	8-chloroquinoline	2.33	2.87	0.54
1104. C_9H_6NBr	3-bromoquinoline	3.03	3.05	0.02
1105. C_9H_6NBr	6-bromoquinoline	2.83	3.05	0.22
1106. C_9H_6NBr	7-bromoquinoline	2.92	3.05	0.13
1107. C_9H_6ONCl	4-chloro-8-quinolinol	2.67	2.75	0.08
1108. C_9H_6ONCl	4-chloroquinolin 1-oxide	1.08	1.44	0.36
1109. $C_9H_6OF_6$	1,1,1,3,3,3-hexafluoro-2-phenyl-2-propanol	3.41	3.51	0.10
1110. $C_9H_6O_2$	coumarin	1.39	0.96	–0.43
1111. $C_9H_6O_2$	indanedione	0.61	1.06	0.45
1112. $C_9H_6O_2N_2$	3-nitroquinoline	1.97	2.18	0.21
1113. $C_9H_6O_2N_2$	4-nitroquinoline	2.06	2.18	0.12
1114. $C_9H_6O_2N_2$	5-nitroquinoline	1.86	2.18	0.32
1115. $C_9H_6O_2N_2$	6-nitroquinoline	1.84	2.18	0.34
1116. $C_9H_6O_2N_2$	7-nitroquinoline	1.82	2.18	0.36
1117. $C_9H_6O_2N_2$	8-nitroquinoline	1.40	2.18	0.78
1118. $C_9H_6O_3NCl$	3-cyano-4-chlorophenoxyacetic acid	1.56	1.67	0.11
1119. $C_9H_6O_3N_2$	3-nitroquinoline 1-oxide	0.56	0.75	0.19
1120. $C_9H_6O_3N_2$	4-nitroquinoline 1-oxide	1.02	0.75	–0.27
1121. $C_9H_6O_3N_2$	5-nitroquinoline 1-oxide	0.49	0.75	0.26
1122. $C_9H_6O_3N_2$	6-nitroquinoline 1-oxide	0.39	0.75	0.36
1123. $C_9H_6O_3N_2$	7-nitroquinoline 1-oxide	0.36	0.75	0.39
1124. $C_9H_6O_3N_2$	8-nitroquinoline 1-oxide	0.04	0.75	0.71
1125. $C_9H_6O_4$	ninhydrin	0.65	–0.07	–0.72
1126. C_9H_7N	isoquinoline	2.08	2.21	0.13
1127. C_9H_7N	quinoline	2.03	2.21	0.18
1128. C_9H_7ON	quinoline 1-oxide	0.36	0.78	0.42
1129. C_9H_7ON	4-hydroxyquinoline	0.58	1.11	0.53
1130. C_9H_7ON	2-quinolone	1.26	0.83	–0.43
1131. C_9H_7ON	2-quinolinol	1.26	0.96	–0.30
1132. C_9H_7ON	8-quinolinol	2.00	2.10	0.10
1133. $C_9H_7O_2N$	2-cyanophenyl acetate	1.33	1.25	–0.08
1134. $C_9H_7O_2N$	*m*-cyanophenylacetic acid	1.18	1.16	–0.02
1135. $C_9H_7O_2N$	*N*-methylindol-2,3-dione	0.58	0.27	–0.31
1136. $C_9H_7O_2F_3$	3-(trifluoromethyl)phenylacetic acid	2.62	2.58	–0.04
1137. $C_9H_7O_2F_3$	*p*-(trifluoromethyl)phenylacetic acid	2.45	2.58	0.13
1138. $C_9H_7O_3F_3$	*m*-(trifluoromethyl)phenoxyacetic acid	2.36	2.44	0.08
1139. $C_9H_7O_3N$	4-cyanophenoxyacetic acid	0.93	1.02	0.09
1140. $C_9H_7O_3N$	3-cyanophenoxyacetic acid	0.95	1.02	0.07
1141. $C_9H_7O_3F_3S$	*m*-(trifluoromethyl)thiophenoxyacetic acid	2.86	2.92	0.06
1142. $C_9H_7O_4F_3$	*m*-(trifluoromethoxy)phenoxyacetic acid	2.48	2.04	–0.44
1143. $C_9H_7O_5F_3S$	*m*-(trifluoromethyl)sulfonylphenoxyacetic acid	2.19	1.62	–0.57
1144. $C_9H_8N_2$	8-aminoquinoline	1.79	1.56	–0.23
1145. $C_9H_8N_2$	2-aminoquinoline	1.87	1.56	–0.31
1146. $C_9H_8N_2$	3-aminoquinoline	1.63	1.56	–0.07
1147. $C_9H_8N_2$	4-aminoquinoline	1.63	1.56	–0.07
1148. $C_9H_8N_2$	6-aminoquinoline	1.28	1.56	0.28
1149. $C_9H_8N_2$	2-methylquinoxaline	1.61	2.24	0.63

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
1150. $C_9H_8N_2$	5-methylquinoxaline	2.04	2.24	0.20
1151. $C_9H_8N_2$	2-phenylimidazole	1.88	2.05	0.17
1152. $C_9H_8N_2$	5-aminoquinoline	1.16	1.56	0.40
1153. $C_9H_8N_2S$	2-(methylthio)quinoxaline	2.79	2.73	–0.06
1154. $C_9H_8ON_2$	4-aminoquinoline 1-oxide	0.05	0.13	0.08
1155. $C_9H_8ON_2$	2-methoxyquinoxaline	2.31	1.84	–0.47
1156. $C_9H_8ON_2$	3-methylquinazolin-4-one	0.69	0.80	0.11
1157. $C_9H_8O_2N_2$	4-cyanophenyl *N*-methylcarbamate	0.95	0.90	–0.05
1158. $C_9H_8O_2N_2$	3-cyanophenyl *N*-methylcarbamate	0.97	0.90	–0.07
1159. $C_9H_8O_2N_2$	2-cyanophenyl *N*-methylcarbamate	0.86	0.90	0.04
1160. $C_9H_8O_2N_2S$	8-sulfonamidoquinoline	0.36	1.19	0.83
1161. $C_9H_8O_2NSCl_3$	captan	2.35	2.02	–0.33
1162. $C_9H_8O_4$	*m*-carboxyphenylacetic acid	1.14	1.69	0.55
1163. $C_9H_8O_4$	*p*-formylphenoxyacetic acid	0.79	1.08	0.29
1164. $C_9H_8O_4$	acetylsalicylic acid	1.23	1.79	0.56
1165. $C_9H_8O_5$	*m*-carboxyphenoxyacetic acid	1.11	1.55	0.44
1166. C_9H_9N	2-methylindole	2.53	2.08	–0.45
1167. C_9H_9N	3-methylindole	2.60	2.08	–0.52
1168. C_9H_9N	5-methylindole	2.68	2.08	–0.60
1169. C_9H_9N	β-phenylethyl cyanide	1.70	2.23	0.53
1170. C_9H_9NS	2-phenethyl isothiocyanate	3.47	3.90	0.43
1171. C_9H_9NS	1-phenethyl isothiocyanate	3.46	3.84	0.38
1172. C_9H_9ON	5-methoxyindole	2.06	1.68	–0.38
1173. $C_9H_9O_2N$	*p*-acetylformanilide	0.94	0.97	0.03
1174. $C_9H_9O_2N_3S_2$	sulfathiazole	0.05	0.64	0.59
1175. $C_9H_9O_3N$	*o*-(acetylamino)benzoic acid	1.88	1.20	–0.68
1176. $C_9H_9O_3N$	*p*-(acetylamino)benzoic acid	1.31	1.20	–0.11
1177. $C_9H_9O_3N$	4-methoxy-β-nitrostyrene	2.20	2.18	–0.02
1178. $C_9H_9O_3N$	3-methoxy-β-nitrostyrene	2.37	2.18	–0.19
1179. $C_9H_{10}N_2$	5,6-dimethylbenzimidazole	2.35	2.11	–0.24
1180. $C_9H_{10}O_2$	*o*-hydroxypropiophenone	2.54	2.52	–0.02
1181. $C_9H_{10}O_2$	*p*-hydroxypropiophenone	2.03	1.79	–0.24
1182. $C_9H_{10}O_2$	*p*-methoxyacetophenone	1.82	1.50	–0.32
1183. $C_9H_{10}O_2N_2$	*p*-(acetylamino)benzamide	0.01	–0.07	–0.08
1184. $C_9H_{10}O_3$	4-methoxyphenyl acetate	1.54	1.58	0.04
1185. $C_9H_{10}O_3$	*m*-methoxyphenylacetic acid	1.50	1.49	–0.01
1186. $C_9H_{10}O_3$	*p*-methoxyphenylacetic acid	1.42	1.49	0.07
1187. $C_9H_{10}O_3$	*m*-methylphenoxyacetic acid	1.78	1.75	–0.03
1188. $C_9H_{10}O_3$	*o*-methylphenoxyacetic acid	1.98	1.75	–0.23
1189. $C_9H_{10}O_3$	*p*-methylphenoxyacetic acid	1.86	1.75	–0.11
1190. $C_9H_{10}O_3$	2-methoxyphenyl acetate	1.38	1.58	0.20
1191. $C_9H_{10}O_3$	*p*-hydroxybenzoic acid ethyl ester	2.43	1.87	–0.56
1192. $C_9H_{10}O_3S$	3-methylthiophenoxyacetic acid	1.90	2.23	0.33
1193. $C_9H_{10}O_4$	2-methoxyphenoxyacetic acid	0.98	1.34	0.36
1194. $C_9H_{10}O_4$	4-methoxyphenoxyacetic acid	1.23	1.34	0.11
1195. $C_9H_{10}O_4$	3-methoxyphenoxyacetic acid	1.38	1.34	–0.04
1196. $C_9H_{10}O_4N_2$	3-ureidophenoxyacetic acid	0.26	0.30	0.04
1197. $C_9H_{11}N$	1,2,3,4-tetrahydroquinoline	2.29	1.99	–0.30
1198. $C_9H_{11}I$	γ-phenylpropyliodine	3.90	3.78	–0.12
1199. $C_9H_{11}N_3$	1-propylbenzotriazole	2.13	1.86	–0.27
1200. $C_9H_{11}N_3$	1-isopropylbenzotriazole	1.98	1.80	–0.18
1201. $C_9H_{11}ON_2Cl$	1,1-dimethyl-3-(*m*-chlorophenyl)urea	2.00	2.03	0.03
1202. $C_9H_{11}ON_2Cl$	1,1-dimethyl-3-(*p*-chlorophenyl)urea	1.94	2.03	0.09
1203. $C_9H_{11}ON_2Br$	1,1-dimethyl-3-(*p*-bromophenyl)urea	2.19	2.22	0.03
1204. $C_9H_{11}O_2NS$	4-(methylthio)phenyl *N*-methylcarbamate	1.92	2.11	0.19
1205. $C_9H_{11}O_2NS$	2-(methylthio)phenyl *N*-methylcarbamate	1.51	2.11	0.60
1206. $C_9H_{11}O_2N$	*o*-tolyl *N*-methylcarbamate	1.46	1.63	0.17
1207. $C_9H_{11}O_2N$	*p*-tolyl *N*-methylcarbamate	1.66	1.63	–0.03
1208. $C_9H_{11}O_2N$	phenyl *N,N*-dimethylcarbamate	1.69	1.60	–0.09
1209. $C_9H_{11}O_2N$	*p*-ethoxybenzamide	1.30	0.95	–0.35
1210. $C_9H_{11}O_2N$	*o*-methoxylacetanilide	0.98	0.99	0.01
1211. $C_9H_{11}O_2N$	*p*-methoxylacetanilide	1.14	0.99	–0.15
1212. $C_9H_{11}O_2N$	2-methyl-4-hydroxyacetanilide	0.66	0.90	0.24
1213. $C_9H_{11}O_2N$	3-methyl-4-hydroxyacetanilide	1.28	0.90	–0.38
1214. $C_9H_{11}O_2N$	ethyl *N*-phenylcarbamate	2.30	2.01	–0.29
1215. $C_9H_{11}O_3N$	2-ethoxy-4-aminobenzoic acid	0.16	0.50	0.34
1216. $C_9H_{11}O_3N$	2-methoxyphenyl *N*-methylcarbamate	0.81	1.23	0.42
1217. $C_9H_{11}O_3N$	3-methoxyphenyl *N*-methylcarbamate	1.30	1.23	–0.07
1218. $C_9H_{11}O_3N$	4-methoxyphenyl *N*-methylcarbamate	1.20	1.23	0.03
1219. $C_9H_{11}O_3N_3$	1,1-dimethyl-3-(*p*-nitrophenyl)urea	1.51	1.35	–0.16
1220. $C_9H_{11}O_4N$	*N*-maleoyl-3-aminopropionic acid ethyl ester	0.41	0.06	–0.35
1221. $C_9H_{11}O_5N_2F$	2′-deoxy-5-fluorouridine	–1.38	–1.21	0.17
1222. $C_9H_{11}O_5N_2Br$	2′-deoxy-5-bromouridine	–0.29	–0.67	–0.38
1223. $C_9H_{12}ON_2$	*m*-(dimethylamino)benzamide	0.95	0.66	–0.29
1224. $C_9H_{12}ON_2$	*p*-(dimethylamino)benzamide	1.14	0.66	–0.48
1225. $C_9H_{12}ON_2$	1-phenyl-3-ethylurea	1.64	1.41	–0.23
1226. $C_9H_{12}ON_2$	1,1-dimethyl-3-phenylurea	1.04	1.38	0.34
1227. $C_9H_{12}ON_2$	1,3-dimethyl-1-phenylurea	1.02	1.38	0.36

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
1228. $C_9H_{12}ON_2$	γ-(β-pyridyl)butanamide	−0.08	0.49	0.57
1229. $C_9H_{12}ON_2$	γ-(γ-pyridyl)butanamide	−0.09	−0.41	−0.32
1230. $C_9H_{12}O_2$	*o*-isopropoxyphenol	2.09	2.23	0.14
1231. $C_9H_{12}O_3$	phenylglycerol	0.70	0.12	−0.58
1232. $C_9H_{12}O_3$	1,2,3-trimethoxybenzene	1.53	1.60	0.07
1233. $C_9H_{12}O_3N_2$	5-allyl-5-ethylbarbituric acid	0.95	0.88	−0.07
1234. $C_9H_{12}O_3N_2S$	*N*-ethyl-4-sulfamylbenzamide	0.03	0.38	0.35
1235. $C_9H_{13}ON$	*N,N*-dimethyl-*o*-anisidine	1.63	1.72	0.09
1236. $C_9H_{13}ON$	4-(α-pyridyl)butanol	0.86	1.27	0.41
1237. $C_9H_{13}ON$	4-(β-pyridyl)butanol	0.92	1.27	0.35
1238. $C_9H_{13}ON$	4-(γ-pyridyl)butanol	0.90	0.62	−0.28
1239. $C_9H_{13}O_2NS$	*p*-propylbenzenesulfonamide	1.64	1.80	0.16
1240. $C_9H_{14}N_2$	4-(α-pyridyl)butylamine	0.86	1.17	0.31
1241. $C_9H_{14}N_2$	4-(β-pyridyl)butylamine	0.88	1.17	0.29
1242. $C_9H_{14}N_2$	4-(γ-pyridyl)butylamine	0.86	0.62	−0.24
1243. $C_9H_{14}O_3N_2$	probarbital	0.97	1.02	0.05
1244. $C_9H_{14}O_3N_2$	*N*-methyl-5-butylbarbituric acid	1.10	0.57	−0.53
1245. $C_9H_{14}O_3N_4$	nimorazole	0.07	0.48	0.41
1246. $C_9H_{16}ON_4S$	3-(methylthio)-4-amino-6-isopentyl-1,2,4-triazin-5-one	1.85	1.84	−0.01
1247. $C_9H_{16}ON_4S$	3-(propylthio)-4-amino-6-isopropyl-1,2,4-triazin-5-one	2.12	1.84	−0.28
1248. $C_9H_{16}ON_4S$	3-(isopropylthio)-4-amino-6-isorpopyl-1,2,4-triazin-5-one	2.06	1.77	−0.29
1249. $C_9H_{16}O_2N_3Cl$	1-(2-chloroethyl)-3-cyclohexyl-1-nitrosourea	2.83	2.45	−0.38
1250. $C_9H_{16}O_3N_3Cl$	1-(2-chloroethyl)-3-(4-hydroxycyhexyl)-1-nitrosourea	1.05	1.62	0.57
1251. $C_9H_{16}O_4$	azelaic acid	1.57	1.68	0.11
1252. $C_9H_{18}ON_2$	4-*tert*-butyl-*N*-nitrosopiperidine	1.96	1.96	0.00
1253. $C_9H_{18}ON_2$	2,2,6,6-tetramethyl-*N*-nitrosopiperidine	2.49	2.39	−0.10
1254. $C_9H_{18}O_4N_2$	meprobamate	0.70	1.06	0.36
1255. $C_9H_{20}ON_2$	1,3-dibutyrylurea	1.40	2.12	0.72
1256. $C_{10}H_5O_2Cl$	2-chloro-1,4-naphthoquinone	2.15	1.92	−0.23
1257. $C_{10}H_6NF_3$	7-(trifluoromethyl)quinoline	3.02	3.32	0.30
1258. $C_{10}H_6NF_3$	8-(triflurometlhyl)quinoline	2.50	3.32	0.82
1259. $C_{10}H_6N_2$	benzal malononitrile	2.12	2.25	0.13
1260. $C_{10}H_6ONF_3$	4-hydroxy-7-(trifluroethyl)quinoline	2.05	2.21	0.16
1261. $C_{10}H_6O_2$	1,4-naphthoquinone	1.78	1.46	−0.32
1262. $C_{10}H_6O_2NCl$	2-chloro-3-amino-1,4-naphthoquinone	2.12	1.72	−0.40
1263. $C_{10}H_6O_2N_3Cl_3$	1-(2,4,5-trichlorophenylhydrazono)-1-cyanoacetic acid methyl ester	5.15	4.84	−0.31
1264. $C_{10}H_6O_2N_3Cl_3$	1-(3,4,5-trichlorophenylhydrazone)-1-cyanoacetic acid methyl ester	5.22	4.84	−0.38
1265. $C_{10}H_6O_3$	2-hydroxy-1,4-naphthoquinone	1.38	1.02	−0.36
1266. $C_{10}H_7ON_3Cl_2$	1-(3,4-dichlorophenylhydrazone)-1-cyanoacetone	4.56	4.10	−0.46
1267. $C_{10}H_7ON_3Cl_2$	1-(3,5-dichlorophenylhydrazone)-1-cyanoacetone	4.68	4.10	−0.58
1268. $C_{10}H_7O_2N$	2-nitroso-1-naphthol	2.57	2.50	−0.07
1269. $C_{10}H_7O_2N$	1-nitroso-2-naphthol	2.28	2.50	0.22
1270. $C_{10}H_7O_2N_3Cl_2$	1-(3,5-dichlorophenylhydrazone)-1-cyanoacetic acid methyl ester	4.50	4.18	−0.32
1271. $C_{10}H_7O_5N_5$	1-(2,4-dinitrophenylhydrazone)-1-cyanoacetone	3.41	2.73	−0.68
1272. $C_{10}H_8ON_2$	*N*-formyl-*p*-cyanostyrlamine	1.58	1.37	−0.21
1273. $C_{10}H_8ON_3Cl$	1-(4-chlorophenylhydrazono)-1-cyanoacetone	4.13	3.45	−0.68
1274. $C_{10}H_8ON_3Cl$	1-(2-chlorophenylhydrazono)-1-cyanoacetone	4.01	3.45	−0.56
1275. $C_{10}H_8ON_3Cl$	1-(3-chlorophenylhydrazono)-1-cyanoacetone	3.91	3.45	−0.46
1276. $C_{10}H_8O_2N_3Cl$	1-(3-chlorophenylhydrazono)-1-cyanoacetic acid methyl ester	3.56	3.53	−0.03
1277. $C_{10}H_8O_3$	hymecromone	1.58	1.25	−0.33
1278. $C_{10}H_8O_3N_2$	2-methyl-4-nitroquinoline 1-oxide	1.25	1.16	−0.09
1279. $C_{10}H_8O_3N_2$	3-methyl-4-nitroquinoline 1-oxide	1.06	1.16	0.10
1280. $C_{10}H_8O_3N_2$	5-methyl-4-nitroquinoline 1-0xide	1.36	1.16	−0.20
1281. $C_{10}H_8O_3N_2$	6-methyl-4-nitroquinoline 1-oxide	1.43	1.16	−0.27
1282. $C_{10}H_8O_3N_2$	7-methyl-4-nitroquinoline 1-oxide	1.42	1.16	−0.26
1283. $C_{10}H_8O_3N_2$	8-methyl-4-nitroquinoline 1-ozide	1.59	1.16	−0.43
1284. $C_{10}H_9N$	8-methylquinoline	2.60	2.62	0.02
1285. $C_{10}H_9N$	7-methylquinoline	2.47	2.62	0.15
1286. $C_{10}H_9N$	8-methylquinoline	2.60	2.62	0.02
1287. $C_{10}H_9N$	2-methylquinoline	2.59	2.62	0.03
1288. $C_{10}H_9N$	6-methylquinoline	2.57	2.62	0.05
1289. $C_{10}H_9ON$	7-methoxyquinoline	2.37	2.22	−0.15
1290. $C_{10}H_9ON$	*N*-methyl-α-quinolone	1.45	1.21	−0.24
1291. $C_{10}H_9ON$	*N*-methyl-4-quinolone	0.44	1.28	0.84
1292. $C_{10}H_9ON$	4-methyl-8-quinolinol	2.36	2.01	−0.35
1293. $C_{10}H_9ON$	5-methyl-8-quinolinol	2.37	2.01	−0.36
1294. $C_{10}H_9ON$	2-methyl-8-quinolinol	2.33	2.01	−0.32
1295. $C_{10}H_9ON$	6-methoxyquinoline	2.20	2.22	0.02
1296. $C_{10}H_9ON$	8-methoxyquinoline	1.84	2.22	0.38
1297. $C_{10}H_9O_2N$	indole-3-acetic acid	1.41	1.57	0.16
1298. $C_{10}H_9O_2N$	5-methoxyl-8-quinolinol	2.06	1.61	−0.45
1299. $C_{10}H_9O_2N$	4-methyl-5,8-dihydroxyquinoline	1.59	1.90	0.31
1300. $C_{10}H_9O_2N_3$	1-phenylhydrazono-1-cyanoacetic acid methyl ester	2.59	2.87	0.28
1301. $C_{10}H_9O_2N_2F$	3-fluorobenzalmalonamide	0.10	0.48	0.38
1302. $C_{10}H_9O_2N_2SCl$	3-cyclopropyl-2,4-benzothiadiazine 1,1-dioxide	1.98	1.50	−0.48
1303. $C_{10}H_9O_4N_3S$	2-*N,N*-dimethylamino-6-(5-NO_2-2-furyl)-1,3-thiazin-4-one	0.55	0.78	0.23
1304. $C_{10}H_9O_4N_2F_3$	1-(2-trifluoroacetamido)-2-(*p*-nitrophenyl)ethanol	1.46	1.59	0.13
1305. $C_{10}H_{10}N_2$	6,7-dimethylquinoxaline	2.29	2.65	0.36

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_T[c]
	Multifunctional Compounds			
1306. $TC_{10}H_{10}ON_2$	benzalcyanoacetamide	1.50	1.12	–0.38
1307. $C_{10}H_{10}ON_4S$	3-(methylthio)-4-amino-6-phenyl-1,2,4-triazin-5-one	1.66	1.61	–0.05
1308. $C_{10}H_{10}O_2N_2$	*N,N*-dimethylquinoxaline-2,3-dione	0.08	–0.17	–0.25
1309. $C_{10}H_{10}O_2N_2$	benzalmalonamide	–0.13	0.52	0.65
1310. $C_{10}H_{10}O_2N_6$	azanidazole	0.85	0.66	–0.19
1311. $C_{10}H_{10}O_2N_4S$	sulfadiazine	–0.08	–0.16	–0.08
1312. $C_{10}H_{10}O_3N_6$	DA3839	–0.30	0.10	0.40
1313. $C_{10}H_{10}O_3N_3SCl$	1,2,4-benzothiadiazine-1,1-O_2-3-Me-6-NH	0.53	0.75	0.22
1314. $C_{10}H_{10}O_4$	4-acetylphenoxyacetic acid	0.87	1.25	0.38
1315. $C_{10}H_{10}O_4$	3-acetylphenoxyacetic acid	0.98	1.25	0.27
1316. $C_{10}H_{10}O_4$	2-acetylphenoxyacetic acid	1.25	1.25	0.00
1317. $C_{10}H_{10}O_4NCl$	3-acetamido-4-chlorophenoxyacetic acid	0.67	1.39	0.72
1318. $C_{10}H_{10}O_5N_2$	*p*-nitromethyl hippurate	0.98	0.95	–0.03
1319. $C_{10}H_{11}N$	1,2-dimethylindole	2.82	1.88	–0.94
1320. $C_{10}H_{11}N$	γ-phenylpropyl cyanide	2.21	2.64	0.43
1321. $C_{10}H_{11}N$	1,2-dimethylindole	2.82	2.49	–0.33
1322. $C_{10}H_{11}ON$	*N*-methyl-α-quinoline	1.45	1.17	–0.28
1323. $C_{10}H_{11}ON_2F_3$	1,1-dimethyl-3-(*m*-(trifluoromethyl)phenyl)urea	2.36	2.48	0.12
1324. $C_{10}H_{11}O_2N$	2-nitro-1-butenylbenzene	2.86	2.99	0.13
1325. $C_{10}H_{11}O_2N$	β-ethyl-β-nitrostyrene	2.86	3.41	0.55
1326. $C_{10}H_{11}O_3N$	3-allyloxy-4-aminobenzoic acid	0.42	0.71	0.29
1327. $C_{10}H_{11}O_3N$	3-acetylphenyl *N*-methylcarbamate	0.90	1.14	0.24
1328. $C_{10}H_{11}O_3N$	4-acetylphenyl *N*-methylcarbamate	1.01	1.14	0.13
1329. $C_{10}H_{11}O_3N$	methyl hippurate	0.82	0.98	0.16
1330. $C_{10}H_{11}O_3N_3S$	sulfamethoxazole	0.88	0.34	–0.54
1331. $C_{10}H_{11}O_4N$	3-carbomethoxyphenyl *N*-methylcarbamate	1.42	1.21	–0.21
1332. $C_{10}H_{11}O_4N$	4-carbomethoxyphenyl *N*-methylcarbamate	1.50	1.21	–0.29
1333. $C_{10}H_{11}O_4N$	*m*-acetamidophenoxyacetic acid	0.48	0.74	0.26
1334. $C_{10}H_{12}ON_2$	2-(γ-hydroxylpropyl)benzimidazole	1.25	1.61	0.36
1335. $C_{10}H_{12}ON_4$	1-(3-carbamylpropyl)benzotriazole	0.37	0.82	0.45
1336. $C_{10}H_{12}O_2N_2$	*m*-diacetamidobenzene	0.50	0.39	–0.11
1337. $C_{10}H_{12}O_2N_2$	4-dimethylamino-β-nitrostyrene	2.67	2.31	–0.36
1338. $C_{10}H_{12}O_2N_2S$	1,2,4-benzothiadiazine	1.25	1.51	0.26
1339. $C_{10}H_{12}O_2NCl$	2,5-dimethyl-4-chlorophenyl *N*-methylcarbamate	2.95	2.69	–0.26
1340. $C_{10}H_{12}O_3$	4-ethoxyphenyl acetate	1.95	2.00	0.05
1341. $C_{10}H_{12}O_3$	ethyl mandelate	0.91	1.52	0.61
1342. $C_{10}H_{12}O_3$	*p*-hydroxybenzoic acid propyl ester	3.04	2.29	–0.75
1343. $C_{10}H_{12}O_3$	*o*-methylphenoxyacetic acid methyl ester	2.08	2.00	–0.08
1344. $C_{10}H_{12}O_3$	3-ethylphenoxyacetic acid	2.25	2.16	–0.09
1345. $C_{10}H_{12}O_3$	2-ethylphenoxyacetic acid	2.65	2.16	–0.49
1346. $C_{10}H_{12}O_3N_2$	*p*-aminohippurate	–0.23	0.33	0.56
1347. $C_{10}H_{12}O_3N_2$	diallylbarbituric acid	1.07	1.08	0.01
1348. $C_{10}H_{13}N_3$	1-*sec*-butylbenzotriazole	2.31	2.22	–0.09
1349. $C_{10}H_{13}ON$	*m*-tolyl *N*-methylcarbamate	1.70	1.78	0.08
1350. $C_{10}H_{13}ON$	*o*-tolyl *N*-methylcarbamate	1.46	1.78	0.32
1351. $C_{10}H_{13}ON$	*p*-tolyl *N*-methylcarbamate	1.66	1.78	0.12
1352. $C_{10}H_{13}ON$	4-phenylbutyramide	1.41	1.77	0.36
1353. $C_{10}H_{13}ON$	*N*-phenylmorpholine	1.36	1.60	0.24
1354. $C_{10}H_{13}O_2N$	4-ethoxyacetanilide	1.58	1.40	–0.18
1355. $C_{10}H_{13}O_2N$	*N,N*-dimethylphenoxyacetamide	0.77	1.38	0.61
1356. $C_{10}H_{13}O_2N$	fusaric acid	–1.29	–0.51	0.78
1357. $C_{10}H_{13}O_2N$	*m*-methoxy-*N,N*-dimethylbenzamide	1.00	1.37	0.37
1358. $C_{10}H_{13}O_2N$	*o*-methoxy-*N,N*-dimethylbenzamide	0.71	1.37	0.66
1359. $C_{10}H_{13}O_2N$	*p*-methoxy-*N,N*-dimethylbenzamide	0.96	1.37	0.41
1360. $C_{10}H_{13}O_2N$	2,3-dimethyl-4-hydroxyacetanilide	1.06	1.31	0.25
1361. $C_{10}H_{13}O_2N$	2,5-dimethyl-4-hydroxyacetanilide	1.09	1.31	0.22
1362. $C_{10}H_{13}O_2N$	2,6-dimethyl-4-hydroxyacetanilide	0.80	1.31	0.51
1363. $C_{10}H_{13}O_2N$	3,5-dimethyl-4-hydroxyacetanilide	1.60	1.31	–0.29
1364. $C_{10}H_{13}O_2N$	3-ethyl-4-hydroxyacetanilide	1.79	1.32	–0.47
1365. $C_{10}H_{13}O_2N$	2-ethylphenyl *N*-methylcarbamate	1.93	2.04	0.11
1366. $C_{10}H_{13}O_2N$	2,3-dimethylphenyl *N*-methylcarbamate	1.95	2.04	0.09
1367. $C_{10}H_{13}O_2N$	2,5-dimethylphenyl *N*-methylcarbamate	2.03	2.04	0.01
1368. $C_{10}H_{13}O_2N$	3-ethylphenyl *N*-methylcarbamate	2.20	2.04	–0.16
1369. $C_{10}H_{13}O_2N$	3,4-methylphenyl *N*-methylcarbamate	2.09	2.04	–0.05
1370. $C_{10}H_{13}O_2N$	3,5-methylphenyl *N*-methylcarbamate	2.23	2.04	–0.19
1371. $C_{10}H_{13}O_2N$	4-ethylphenyl *N*-methylcarbamate	2.23	2.04	–0.19
1372. $C_{10}H_{13}O_2N$	*m*-tolyl *N,N*-dimethylcarbamate	2.05	2.01	–0.04
1373. $C_{10}H_{13}O_2N$	*o*-tolyl *N,N*-dimethylcarbamate	1.86	2.01	0.15
1374. $C_{10}H_{13}O_2N$	*p*-tolyl *N,N*-dimethylcarbamate	2.03	2.01	–0.02
1375. $C_{10}H_{13}O_2NS$	3-methyl-4-methylthiophenyl *N*-methylcarbamate	2.47	2.52	0.05
1376. $C_{10}H_{13}O_3N$	3-methoxyphenyl *N,N*-dimethylcarbamate	1.60	1.61	0.01
1377. $C_{10}H_{13}O_3N$	4-methoxyphenyl *N,N*-dimethylcarbamate	1.53	1.61	0.08
1378. $C_{10}H_{13}O_3N$	2-ethoxyphenyl *N*-methylcarbamate	1.24	1.64	0.40
1379. $C_{10}H_{13}O_3N$	3-ethoxyphenyl *N*-methylcarbamate	1.75	1.64	–0.11
1380. $C_{10}H_{13}O_3N$	4-ethoxyphenyl *N*-methylcarbamate	1.63	1.64	0.01
1381. $C_{10}H_{13}O_3N$	2-propoxy-4-aminobenzoic acid	0.70	0.92	0.22
1382. $C_{10}H_{13}O_4NS$	4-sulfamonylbenzoic acid propyl ester	1.75	1.38	–0.37
1383. $C_{10}H_{14}N_2$	anabasine	0.97	1.59	0.62

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
1384. $C_{10}H_{14}N_2$	nicotine	1.17	1.76	0.59
1385. $C_{10}H_{14}ON_2$	1,1-dimethyl-*p*-tolylurea	1.98	1.79	–0.19
1386. $C_{10}H_{14}ON_2$	γ-(α-pyridyl)pentamide	–0.01	0.84	0.85
1387. $C_{10}H_{14}ON_2$	δ-(α-pyridyl)pentamide	0.39	0.91	0.52
1388. $C_{10}H_{14}ON_2$	δ-(β-pyridyl)pentamide	0.40	0.91	0.51
1389. $C_{10}H_{14}ON_2$	δ-(γ-pyridyl)pentamide	0.42	0.00	–0.42
1390. $C_{10}H_{14}O_2$	camphorquinone	1.52	1.86	0.34
1391. $C_{10}H_{14}O_2N_2$	3-(dimethylamino)phenyl *N*-methylcarbamate	1.43	1.73	0.30
1392. $C_{10}H_{14}O_2NBr$	3,5-dimethoxy-4-bromophenethylamine	2.03	2.11	0.08
1393. $C_{10}H_{14}O_3$	3-(2-tolyloxy)-1,2-propanediol	1.41	1.01	–0.40
1394. $C_{10}H_{14}O_4N_2$	*N*-isopropyl-3-(5-NO_2-2-furyl)acrylamide	1.34	1.69	0.35
1395. $C_{10}H_{14}O_6NP$	*p*-oxon	1.69	1.74	0.05
1396. $C_{10}H_{15}ON$	5-(α-pyridyl)pentanol	1.28	1.69	0.41
1397. $C_{10}H_{15}ON$	5-(β-pyridyl)pentanol	1.41	1.69	0.28
1398. $C_{10}H_{15}ON$	5-(γ-pyridyl)pentanol	1.39	1.04	–0.35
1399. $C_{10}H_{15}ON$	ephedrine	1.56	1.57	0.01
1400. $C_{10}H_{15}O_2NS$	*p*-butylbenzenesulfonamide	2.45	2.21	–0.24
1401. $C_{10}H_{15}O_4P$	*O,O*-diethyl *O*-phenyl phosphate	1.64	1.77	0.13
1402. $C_{10}H_{16}N_2$	5-(α-pyridyl)pentylamine	1.32	1.58	0.26
1403. $C_{10}H_{16}N_2$	5-(β-pyridyl)pentylamine	1.41	1.58	0.17
1404. $C_{10}H_{16}N_2$	5-(γ-pyridyl)pentylamine	1.40	1.04	–0.36
1405. $C_{10}H_{16}O_2N_3Cl$	3-(2-norbornyl)-1-(2-chloroethyl)nitrosoruea	2.98	2.30	–0.68
1406. $C_{10}H_{16}O_3N_2$	5-butyl-5-ethylbarbituric acid	1.89	1.50	–0.39
1407. $C_{10}H_{17}O_2N_5$	DA3804	–0.33	0.25	0.58
1408. $C_{10}H_{18}O_2N_3Cl$	1-(2-chloroethyl)-3-(4-methylcyclohexyl)-1-nitrosourea	3.30	2.85	–0.45
1409. $C_{10}H_{19}O_2N_5$	3-morpholino-4-amino-6-isopropyl-1,2,4-triazin-5-one	0.49	–0.03	–0.52
1410. $C_{11}H_6O_2N_3F_3Cl_2$	1-(2,6-dichloro-4-(trifluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	4.36	5.29	0.93
1411. $C_{11}H_7NS$	1-isothiocyanonaphthalene	4.34	4.09	–0.25
1412. $C_{11}H_7NS$	2-isothiocyanonaphthalene	4.34	4.09	–0.25
1413. $C_{11}H_7ON_3F_3Cl$	1-(2-chloro-5-(trifluoromethyl)phenylhydrazono)-1-cyanoacetone	5.08	4.55	–0.53
1414. $C_{11}H_7O_2N_3F_3Cl$	1-(4-chloro-2-(trifluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	4.66	4.63	–0.03
1415. $C_{11}H_7O_2N_3F_3Cl$	1-(2-chloro-5-(trifluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	4.42	4.63	0.21
1416. $C_{11}H_7O_4N_4F_3$	1-(2-nitro-5-(trifluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	3.44	3.95	0.51
1417. $C_{11}H_8ONCl$	4-acetyl-7-chloroquinoline	2.62	2.78	0.16
1418. $C_{11}H_8ON_3F_3S$	1-(4-(trifluoromethyl)thiophenylhydrazono)-1-cyanoacetone	5.04	4.38	–0.66
1419. $C_{11}H_8O_2$	6-methyl-1,4-naphthoquinone	2.10	1.87	–0.23
1420. $C_{11}H_8O_2N_3F_3$	1-(3-(trifluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	3.78	3.98	0.20
1421. $C_{11}H_8O_2N_3F_3$	1-(2-(trifluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	3.72	3.98	0.26
1422. $C_{11}H_8O_2N_3F_2Cl$	1-(4-chloro-3-(difluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	3.83	4.36	0.53
1423. $C_{11}H_8O_2N_3F_3S$	1-(4-(trifluoromethyl)thiophenylhydrazono)-1-cyanoacetic acid methyl ester	4.27	4.46	0.19
1424. $C_{11}H_8O_2N_3Cl_3$	1-(3,4,5-trichlorophenylhydrazono)-1-cyanoacetic acid ethyl ester	5.03	5.25	0.22
1425. $C_{11}H_8O_2N_3Cl_3$	1-(2,4,5-trichlorophenylhydrazono)-1-cyanoacetic acid ethyl ester	5.21	5.25	0.04
1426. $C_{11}H_8O_3$	2-methyl-3-hydroxyl-1,4-naphthoquinone	1.20	1.43	0.23
1427. $C_{11}H_8O_4N_3F_3S$	1-(4-[(trifluoromethyl)sulfonyl]phenylhydrazono)-1-cyanoacetic acid methyl ester	4.22	3.16	–1.06
1428. $C_{11}H_9N$	4-phenylpyridine	2.45	2.97	0.52
1429. $C_{11}H_9N$	2-phenylpyridine	2.63	2.97	0.34
1430. $C_{11}H_9O_2N_3Cl_2$	1-(3,4-dichlorophenylhydrazono)-1-cyanoacetic acid ethyl ester	4.66	4.60	–0.06
1431. $C_{11}H_9O_2N_3Cl_2$	1-(3,5-dichlorophenylhydrazono)-1-cyanoacetic acid ethyl ester	3.82	4.60	0.78
1432. $C_{11}H_9O_2N_3SCl_2$	*N*-(3,5-dichloro-2-pyridyl)sulfanilamide	1.97	1.90	–0.07
1433. $C_{11}H_9O_2N_3SBr_2$	*N*-(3,5-dibromo-2-pyridyl)sulfanilamide	2.74	2.27	–0.47
1434. $C_{11}H_{10}N_2$	α-methylbenzalmalononitrile	2.10	2.34	0.24
1435. $C_{11}H_{10}O_2N_3Cl$	1-(4-chloro-2-methylphenylhydrazono)-1-cyanoacetic acid methyl ester	4.28	3.94	–0.34
1436. $C_{11}H_{10}O_2N_3Cl$	1-(3-chlorophenylhydrazono)-1-cyanoacetic acid ethyl ester	3.94	3.94	0.00
1437. $C_{11}H_{10}O_2N_3SBr$	*N*-(3-bromo-2-pyridyl)sulfanilamide	1.24	1.43	0.19
1438. $C_{11}H_{11}ON$	4,5-dimethyl-8-quinolinol	2.71	2.92	0.21
1439. $C_{11}H_{11}O_2N$	4-methyl-5-methoxy-8-quinolinol	2.75	2.52	–0.23
1440. $C_{11}H_{11}O_2N_3S$	sulfapyridine	0.00	0.59	0.59
1441. $C_{11}H_{11}O_5N_2Br_3$	tribromamphenicol	2.17	2.61	0.44
1442. $C_{11}H_{12}N_2$	7-(dimethylamino)quinoline	2.71	2.35	–0.36
1443. $C_{11}H_{12}ON_2$	antipyrine	0.23	0.85	0.62
1444. $C_{11}H_{12}O_2N_2$	5-ethyl-5-phenylhydantoin	1.53	1.55	0.02
1445. $C_{11}H_{12}O_2N_4S$	sulfaperine	0.34	0.25	–0.09
1446. $C_{11}H_{12}O_2N_4S$	sulfamerazine	0.14	0.25	0.11
1447. $C_{11}H_{12}O_2N_2$	tryptophan	–1.04	–0.93	0.11
1448. $C_{11}H_{12}O_3$	indanoxylacetic acid	2.33	1.91	–0.42
1449. $C_{11}H_{12}O_5N_2F_2$	difluoramamphenicol	0.42	0.73	0.31
1450. $C_{11}H_{12}O_5N_2Cl_2$	chloramphenicol	1.14	1.18	0.04
1451. $C_{11}H_{13}ON$	1-phenyl-2-acetamidocyclopropane	1.43	1.55	0.12
1452. $C_{11}H_{13}O_2N_3$	1-(4-carboxybutyl)benzotriazole	0.93	1.77	0.84
1453. $C_{11}H_{13}O_3N$	2-acetylphenyl *N,N*-dimethylcarbamate	0.93	1.52	0.59
1454. $C_{11}H_{13}O_3N$	3-acetylphenyl *N,N*-dimethylcarbamate	1.18	1.52	0.34
1455. $C_{11}H_{13}O_3N$	4-propionylphenyl *N*-methylcarbamate	1.55	1.55	0.00
1456. $C_{11}H_{13}O_3N$	3-propionylphenyl *N*-methylcarbamate	1.49	1.55	0.06
1457. $C_{11}H_{14}ON_2$	4-phenyl-*N*-nitrosopiperidine	2.59	2.11	–0.48
1458. $C_{11}H_{14}O_2N_2$	3-methylbenzalmalonamide	0.40	0.66	0.26
1459. $C_{11}H_{14}O_3$	3-isopropylphenoxyacetic acid	2.59	2.51	–0.08
1460. $C_{11}H_{14}O_3$	4-isopropylphenoxyacetic acid	2.69	2.51	–0.18
1461. $C_{11}H_{14}O_3$	3-propylphenoxyacetic acid	2.71	2.58	–0.13

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
1462. $C_{11}H_{14}O_3$	*o*-isopropylphenoxyacetic acid	2.84	2.51	–0.33
1463. $C_{11}H_{14}O_3$	*p*-hydroxybenzoic acid butyl ester	3.57	2.70	–0.87
1464. $C_{11}H_{14}O_3N_2$	3-methoxylbenzalmalonamide	0.01	0.26	0.25
1465. $C_{11}H_{15}N$	*N*-phenylpiperidine	2.78	2.10	–0.68
1466. $C_{11}H_{15}N_3$	1-pentylbenzotriazole	3.22	2.69	–0.53
1467. $C_{11}H_{15}O_2N$	3-isopropyl-4-hydroxyacetanilide	2.20	1.67	–0.53
1468. $C_{11}H_{15}O_2N$	2,4,5-trimethyl-*N*-methylphenylcarbamate	2.52	2.45	–0.07
1469. $C_{11}H_{15}O_2N$	2,3,5-trimethyl-4-hydroxyacetanilide	1.30	1.72	0.42
1470. $C_{11}H_{15}O_2N$	2,3,6-trimethyl-4-hydroxyacetanilide	1.24	1.72	0.48
1471. $C_{11}H_{15}O_2N$	2-amino-5-phenylvaleric acid	–0.36	–0.19	0.17
1472. $C_{11}H_{15}O_2N$	4-butoxybenzamide	2.48	1.78	–0.70
1473. $C_{11}H_{15}O_3N$	2-butoxy-4-aminobenzoic acid	1.24	1.33	0.09
1474. $C_{11}H_{15}O_3N$	baygon	1.58	1.99	0.41
1475. $C_{11}H_{15}O_3N$	3-isopropoxyphenyl *N*-methylcarbamate	1.96	1.99	0.03
1476. $C_{11}H_{16}O_3N_2$	5-allyl-5-butylbarbituric acid	1.35	1.71	0.36
1477. $C_{11}H_{16}O_3N_2$	INPEA	1.28	1.63	0.35
1478. $C_{11}H_{17}N$	*p*-hexylpyridine	4.35	4.51	0.16
1479. $C_{11}H_{17}ON$	*p*-(diethylamino)benzyl alcohol	2.29	2.02	–0.27
1480. $C_{11}H_{17}O_2N$	2,3-dimethoxyamphetamine	1.49	1.76	0.27
1481. $C_{11}H_{17}O_2N$	2,4-dimethoxyamphetamine	1.75	1.76	0.01
1482. $C_{11}H_{17}O_2N$	2,5-dimethoxyamphetamine	1.88	1.76	–0.12
1483. $C_{11}H_{17}O_2N$	3,4-dimethoxyamphetamine	1.00	1.76	0.76
1484. $C_{11}H_{17}O_3N$	mescaline	0.78	1.29	0.51
1485. $C_{11}H_{18}O_3N_2$	5-amyl-5-ethylbarbituric acid	2.24	1.92	–0.32
1486. $C_{11}H_{18}O_3N_2$	amobarbital	2.07	1.85	–0.22
1487. $C_{11}H_{18}O_3N_2$	pentobarbital	2.03	1.85	–0.18
1488. $C_{12}N_8N_2$	1,7-phenanthroline	2.51	2.85	0.34
1489. $C_{12}H_8N_2$	4,7-phenanthroline	2.05	2.85	0.80
1490. $C_{12}H_8N_2$	phenazine	2.84	2.85	0.01
1491. $C_{12}H_9N$	carbazol	3.72	2.69	–1.03
1492. $C_{12}H_9NS$	phenothiazine	3.78	3.50	–0.28
1493. $C_{12}H_9ON$	4-benzoylpyridine	1.98	2.48	0.50
1494. $C_{12}H_9O_3N$	2-acetamido-1,4-naphthoquinone	1.29	0.86	–0.43
1495. $C_{12}H_{10}O_2$	naphthalene-1-acetoxy	2.78	2.59	–0.19
1496. $C_{12}H_{10}O_2$	6,7-dimethyl-1,4-naphthoquinone	2.49	2.28	–0.21
1497. $C_{12}H_{10}ON_2$	diphenylnitrosoamine	3.13	2.69	–0.44
1498. $C_{12}H_{10}O_2S$	diphenyl sulfone	2.40	2.54	0.14
1499. $C_{12}H_{10}O_3$	2-naphthoxyacetic acid	2.53	2.35	–0.18
1500. $C_{12}H_{10}OS$	phenyl sulfoxide	2.06	2.03	–0.03
1501. $C_{12}H_{11}O_2N$	carbaryl	2.34	2.24	–0.10
1502. $C_{12}H_{11}NS$	1-naphthylmethyl isothiocyanate	4.42	4.45	0.03
1503. $C_{12}H_{11}ON$	*o*-phenoxyaniline	2.46	2.30	–0.16
1504. $C_{12}H_{11}ON$	*p*-phenoxyaniline	2.36	2.30	–0.06
1505. $C_{12}H_{12}N_2$	benzidine	1.34	2.05	0.71
1506. $C_{12}H_{12}N_2$	hydrazobenzene	2.94	3.39	0.45
1507. $C_{12}H_{12}ON_2$	harmalol	2.19	2.53	0.34
1508. $C_{12}H_{12}O_2N_2S$	dapsone	0.97	1.23	0.26
1509. $C_{12}H_{13}O_2NS$	vitavax	2.14	2.87	0.73
1510. $C_{12}H_{14}O_2N_4S$	sulfamethazine	0.27	0.66	0.39
1511. $C_{12}H_{16}O_3$	*o*-*tert*-butylphenoxyacetic acid	3.33	2.96	–0.37
1512. $C_{12}H_{16}O_3$	4-*sec*-butylphenoxyacetic acid	3.12	2.93	–0.19
1513. $C_{12}H_{16}O_3$	*o*-*sec*-butylphenoxyacetic acid	3.32	2.93	–0.39
1514. $C_{12}H_{16}O_3$	3-butylphenoxyacetic acid	3.18	2.99	–0.19
1515. $C_{12}H_{16}O_7$	arbutin	–1.35	–0.80	0.55
1516. $C_{12}H_{17}O_2N$	3-*tert*-butyl-4-hydroxyacetanilide	2.85	2.12	–0.73
1517. $C_{12}H_{17}O_2N$	3,5-diethyl-4-hydroxyacetanilide	2.36	2.14	–0.22
1518. $C_{12}H_{17}O_2N$	2-*sec*-butylphenyl *N*-methylcarbamate	2.78	2.81	0.03
1519. $C_{12}H_{17}O_2N$	2-*tert*-butylphenyl *N*-methylcarbamate	2.65	2.84	0.19
1520. $C_{12}H_{17}O_2N$	3-methyl-4-isopropylphenyl *N*-methylcarbamate	3.11	2.80	–0.31
1521. $C_{12}H_{17}O_2N$	3-methyl-5-isopropylphenyl *N*-methylcarbamate	3.10	2.80	–0.30
1522. $C_{12}H_{17}O_2N$	3-methyl-6-isopropylphenyl *N*-methylcarbamate	2.84	2.80	–0.04
1523. $C_{12}H_{17}O_2N$	3-*tert*-butylphenyl *N*-methylcarbamate	2.93	2.84	–0.09
1524. $C_{12}H_{17}O_2N$	4-*sec*-butylphenyl *N*-methylcarbamate	3.20	2.81	–0.39
1525. $C_{12}H_{17}O_2N$	4-*tert*-butylphenyl *N*-methylcarbamate	3.06	2.84	–0.22
1526. $C_{12}H_{17}O_2N$	2,3,5,6-tetramethyl-4-hydroxyacetamide	1.44	2.13	0.69
1527. $C_{12}H_{17}O_2NS$	*N*-methyl-2-butylthiophenylcarbamate	2.98	3.36	0.38
1528. $C_{12}H_{17}O_3N$	bufexamac	1.47	1.80	0.33
1529. $C_{12}H_{17}O_3N$	3-butoxyphenyl *N*-methylcarbamate	2.96	2.47	–0.49
1530. $C_{12}H_{17}O_3N$	4-butoxypheny; *N*-methylcarbamate	2.86	2.47	–0.39
1531. $C_{12}H_{17}O_3N$	2-pentoxy-4-aminobenzoic acid	1.55	1.75	0.20
1532. $C_{12}H_{17}O_3N$	2-isopentoxy-4-aminobenzoic acid	1.47	1.68	0.21
1533. $C_{12}H_{18}O_3N_2S$	butamidotolylsulfonamide	2.34	1.83	–0.51
1534. $C_{12}H_{19}N$	*p*-heptylpyridine	5.00	4.92	–0.08
1535. $C_{13}H_8OS$	thioxanthon	3.99	3.48	–0.51
1536. $C_{13}H_9N$	acridine	3.40	3.23	–0.17
1537. $C_{13}H_9NS$	4-biphenyl isothiocyanate	4.66	4.85	0.19
1538. $C_{13}H_9ONS$	4-isothiocyanodiphenyl ether	4.75	4.45	–0.30
1539. $C_{13}H_9ONS_2$	4-isothiocyanodiphenyl sulfoxide	4.40	3.53	–0.87

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
1540. $C_{13}H_{10}N_2S$	4-isothiocyanodiphenylamine	4.94	4.87	−0.07
1541. $C_{13}H_{10}N_2$	1-aminoacridine	2.47	2.58	0.11
1542. $C_{13}H_{10}N_2$	2-aminoacridine	2.62	2.58	−0.04
1543. $C_{13}H_{10}N_2$	3-aminoacridine	2.19	2.58	0.39
1544. $C_{13}H_{10}N_2$	4-aminoacridine	3.26	2.58	−0.68
1545. $C_{13}H_{10}N_2$	9-aminoacridine	2.74	2.58	−0.16
1546. $C_{13}H_{10}ON_2Cl_2$	1-(3,4-dichlorophenyl)-3-phenylurea	4.70	3.67	−1.03
1547. $C_{13}H_{10}O_2$	*o*-hydroxybenzophenone	3.52	3.47	−0.05
1548. $C_{13}H_{10}O_2$	*p*-hydroxybenzophenone	3.07	2.74	−0.33
1549. $C_{13}H_{10}O_3$	*o*-phenoxybenzoic acid	2.84	3.17	0.33
1550. $C_{13}H_{10}O_3$	*p*-phenoxybenzoic acid	3.21	3.17	−0.04
1551. $C_{13}H_{10}O_3NF$	4-aminosalicylic acid 4-fluorophenyl ester	3.27	3.12	−0.15
1552. $C_{13}H_{10}O_3NF$	4-aminosalicylic acid 2-fluorophenyl ester	3.29	3.12	−0.17
1553. $C_{13}H_{10}O_3NF$	4-aminosalicylic acid 3-fluorophenyl ester	3.42	3.12	−0.30
1554. $C_{13}H_{10}O_3NCl$	4-aminosalicylic acid 4-chlorophenyl ester	3.60	3.55	−0.05
1555. $C_{13}H_{10}O_3NCl$	4-aminosalicylic acid 2-chlorophenyl ester	3.72	3.55	−0.17
1556. $C_{13}H_{10}O_3NCl$	4-aminosalicylic acid 3-chlorophenyl ester	3.90	3.55	−0.35
1557. $C_{13}H_{10}O_3NBr$	4-aminosalicylic acid 4-bromophenyl ester	3.46	3.74	0.28
1558. $C_{13}H_{10}O_3NBr$	4-aminosalicylic acid 2-bromophenyl ester	3.74	3.74	0.00
1559. $C_{13}H_{10}O_3NBr$	4-aminosalicylic acid 3-bromophenyl ester	3.84	3.74	−0.10
1560. $C_{13}H_{11}N_3$	3,6-diaminoacridine	1.10	1.92	0.82
1561. $C_{13}H_{11}O_2N$	*N*-phenylanthranilic acid	4.36	3.59	−0.77
1562. $C_{13}H_{11}O_2N$	salicylanilide	3.27	2.96	−0.31
1563. $C_{13}H_{11}O_3N$	phenyl 4-aminosalicylate	3.15	2.90	−0.25
1564. $C_{13}H_{12}O_2$	(4,4′-dihydroxydiphenyl)methane	2.91	3.54	0.63
1565. $C_{13}H_{12}O_2$	*o*-phenoxyanisole	2.92	2.96	0.04
1566. $C_{13}H_{14}O_2N_2S$	*N*′-(4-methylphenyl)sulfanilamide	2.00	1.83	−0.17
1567. $C_{13}H_{14}O_3N_2S$	*N*′-(2-methoxyphenyl)sulfanilamide	1.56	1.43	−0.13
1568. $C_{13}H_{14}O_3N_2S$	*N*′-(4-methoxyphenyl)sulfanilamide	1.51	1.43	−0.08
1569. $C_{13}H_{19}O_4NS$	probenecid	3.21	2.77	−0.44
1570. $C_{13}H_{16}O_3$	benzylacetoacetic acid ethyl ester	2.52	2.74	0.22
1571. $C_{14}H_{16}O_3$	4-cyclopentylphenoxyacetic acid	3.41	2.63	−0.78
1572. $C_{13}H_{18}O_2$	ibuprofen	3.51	3.42	−0.09
1573. $C_{13}H_{19}O_2N$	2-*sec*-butylphenyl *N*,*N*-dimethylcarbamate	3.31	3.19	−0.12
1574. $C_{13}H_{19}O_2N$	3-methyl-4-*tert*-butylphenyl *N*-methylcarbamate	3.38	3.26	−0.12
1575. $C_{13}H_{19}O_2N$	3-methyl-5-*tert*-butylphenyl *N*-methylcarbamate	3.35	3.26	−0.09
1576. $C_{13}H_{19}O_2N$	3-methyl-6-*tert*-butylphenyl *N*-methylcarbamate	3.14	3.26	0.12
1577. $C_{13}H_{19}O_2N$	2-methyl-5-*tert*-butyl-4-hydroxyacetamide	2.67	2.53	−0.14
1578. $C_{13}H_{20}O_2N_2$	procaine	1.92	2.30	0.38
1579. $C_{13}H_{21}N$	*p*-octylpyridine	5.42	5.34	−0.08
1580. $C_{13}H_{21}ON_3$	procainamide	1.39	1.71	0.32
1581. $C_{13}H_{24}O_3N_4S$	timolol	1.91	1.44	−0.47
1582. $C_{14}H_8N_2S_2$	4,4′-diisothiocyanatobiphenyl	5.50	6.35	0.85
1583. $C_{14}H_9ONS$	4-isothiocyanobenzophenole	4.88	4.36	−0.52
1584. $C_{14}H_9O_2NS$	4-isothiocyanophenyl benzoate	4.90	4.44	−0.46
1585. $C_{14}H_{10}O_2$	benzil	3.38	2.37	−1.01
1586. $C_{14}H_{10}O_2NF_3$	*N*-(3-(trifluoromethyl)phenyl)anthranilic acid	5.62	4.69	−0.93
1587. $C_{14}H_{11}NS$	(4-isothiocyanophenyl)phenylmethane	4.40	5.26	0.86
1588. $C_{14}H_{12}O_3$	*m*-phenylphenoxyacetic acid	3.18	3.11	−0.07
1589. $C_{14}H_{12}O_3$	*o*-phenylphenoxyacetic acid	2.83	3.11	0.28
1590. $C_{14}H_{13}ON_3F_3Cl$	1-(2-(trifluoromethyl)-4-chlorophenylhydrazono)-1-cyano-3,3-dimethylacetone	5.67	5.77	0.10
1591. $C_{14}H_{13}ON_3F_3Cl$	1-(2-chloro-5-(trifluoromethyl)phenylhydrazono)-1-cyano-3,3-dimethylacetone	5.31	5.77	0.46
1592. $C_{14}H_{13}O_3N$	4-aminosalicylic acid 2-tolyl ester	3.14	3.31	0.17
1593. $C_{14}H_{13}O_3N$	4-aminosalicylic acid 4-tolyl ester	3.38	3.31	−0.07
1594. $C_{14}H_{13}O_3N$	4-aminosalicylic acid 3-tolyl ester	3.64	3.31	−0.33
1595. $C_{14}H_{13}O_4N$	4-aminosalicylic acid 2-methoxyphenyl ester	2.88	2.91	0.03
1596. $C_{14}H_{13}O_4N$	4-aminosalicylic acid 4-methoxyphenyl ester	3.07	2.91	−0.16
1597. $C_{14}H_{13}O_4N$	4-aminosalicylic acid 3-methoxyphenyl ester	3.25	2.91	−0.34
1598. $C_{14}H_{13}O_5N_3$	DA3832	2.03	2.00	−0.03
1599. $C_{14}H_{14}O_3$	naproxen	3.18	2.85	−0.33
1600. $C_{14}H_{16}ON_3Cl$	1-(2-methyl-4-chlorophenylhydrazono)-1-cyano-3,3-dimethylacetone	4.31	5.08	0.77
1601. $C_{14}H_{18}O_3$	4-cyclohexylphenoxyacetic acid	3.79	2.99	−0.80
1602. $C_{14}H_{18}O_3N_4$	trimethoprim(9624)	0.91	1.36	0.45
1603. $C_{14}H_{20}O_2N_2$	pindolol	1.92	1.77	−0.15
1604. $C_{14}H_{20}O_3$	*p*-hydroxybenzoic acid heptyl ester	4.83	4.77	−0.06
1605. $C_{14}H_{21}O_2N$	3,5-dipropyl-4-hydroxyacetanilide	3.16	2.97	−0.19
1606. $C_{14}H_{22}ON_2$	lidocaine	2.90	2.77	−0.13
1607. $C_{14}H_{22}O_3N_2$	practolol	0.79	1.07	0.28
1608. $C_{14}H_{22}O_3N_2$	atenolol	0.16	1.04	0.88
1609. $C_{15}H_9NS$	2-isothiocyanoanthrancene	5.70	5.11	−0.59
1610. $C_{15}H_{10}O_2$	2-phenylindanedione	2.90	2.83	−0.07
1611. $C_{15}H_{10}O_2N_2Cl_2$	lorazepam	2.38	3.03	0.65
1612. $C_{15}H_{11}N$	2-phenylquinoline	3.90	3.99	0.09
1613. $C_{15}H_{11}ON_2F$	1-methyl-4-phenyl-6-fluoroquinazolin-2-one	1.87	2.15	0.28
1614. $C_{15}H_{11}ON_2Cl$	1-methyl-4-phenyl-7-chloroquinazolin-2-one	2.36	2.59	0.23
1615. $C_{15}H_{11}ON_2Cl$	1-methyl-4-phenyl-6-chloroquinazolin-2-one	2.38	2.59	0.21
1616. $C_{15}H_{11}O_2N_2Cl$	oxazepam	2.17	2.37	0.20
1617. $C_{15}H_{11}O_3N_3$	nitrazepam	2.12	2.52	0.40

Table 4 (Continued)

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
	Multifunctional Compounds			
1618. $C_{15}H_{12}O_2$	9-carboxy-9,10-dihydroanthracene	2.67	3.05	0.38
1619. $C_{15}H_{12}ON_2$	1-methyl-4-phenylquinazolin-2-one	1.79	1.94	0.15
1620. $C_{15}H_{12}O_2N_2$	1-methyl-4-phenyl-6-hydroxyquinazolin-2-one	1.72	1.82	0.10
1621. $C_{15}H_{13}O_4N$	3-benzamidophenoxyacetic acid	1.99	2.11	0.12
1622. $C_{15}H_{15}O_3N$	2,6-dimethyl-4-aminosalicylic acid	3.38	3.72	0.34
1623. $C_{15}H_{16}ON_2$	1,1-diphenyl-3,3-dimethylurea	2.80	3.13	0.33
1624. $C_{15}H_{16}O_2$	bisphenol A(1311)	3.32	4.34	1.02
1625. $C_{15}H_{18}O_4$	helenalin(4542)	0.87	1.37	0.50
1626. $C_{15}H_{21}O_2N_3$	physostigmine	1.58	1.53	–0.05
1627. $C_{15}H_{23}O_2N$	alprenolol	3.10	2.70	–0.40
1628. $C_{15}H_{23}O_3N$	oxprenolol	2.37	2.30	–0.07
1629. $C_{15}H_{23}O_4N$	cycloheximide	0.55	1.30	0.75
1630. $C_{15}H_{25}O_3N$	metoprolol	2.34	2.27	–0.07
1631. $C_{16}H_{13}ON_2Cl$	diazepam	2.66	3.59	0.93
1632. $C_{16}H_{15}N_2Cl$	medazepam	4.05	4.21	0.16
1633. $C_{16}H_{17}ON_2Cl$	tetrazepam	2.76	3.51	0.75
1634. $C_{16}H_{18}O_4N_2S$	benzyl penicillin	1.83	1.70	–0.13
1635. $C_{16}H_{18}O_5N_2S$	phenoxymethyl penicillin	2.09	1.30	–0.79
1636. $C_{16}H_{18}O_5N_2S$	α-hydroxybenzyl penicillin	1.40	0.81	–0.59
1637. $C_{16}H_{21}O_2N$	propranolol	3.14	2.69	–0.45
1638. $C_{16}H_{21}O_3N$	atropine	1.76	1.77	0.01
1639. $C_{17}H_{13}N$	2,6-diphenylpyridine	4.82	4.75	–0.07
1640. $C_{17}H_{18}O_6N_2S$	carbenicillin	1.13	1.13	0.00
1641. $C_{17}H_{19}N_2SCl$	chlorpromazine	5.35	4.92	–0.43
1642. $C_{17}H_{20}O_5N_2S$	α-phenoxyethyl penicillin	2.28	1.65	–0.63
1643. $C_{17}H_{20}O_6N_2S$	methicillin	1.30	1.30	0.00
1644. $C_{17}H_{21}ON$	diphenhydramine	3.40	4.03	0.63
1645. $C_{17}H_{21}O_4N$	l-scopolamine	1.24	1.48	0.24
1646. $C_{17}H_{21}O_4N$	cocaine	2.09	2.29	0.20
1647. $C_{17}H_{23}ON_3$	mepyramine	2.85	3.67	0.82
1648. $C_{17}H_{23}O_3N$	atropine	1.79	2.13	0.34
1649. $C_{17}H_{25}O_3N$	levbunolol	2.40	2.51	0.11
1650. $C_{18}H_{22}N_2$	desipramine	4.90	3.74	–1.16
1651. $C_{18}H_{28}O_4N_2$	acebutolol	1.77	1.82	0.05
1652. $C_{18}H_{22}N_2S$	trimeprazine(9617)	3.44	4.62	1.18
1653. $C_{19}H_{17}ON_2Cl$	prazepam	3.72	4.17	0.45
1654. $C_{19}H_{24}N_2$	imipramine	4.62	4.17	–0.45
1655. $C_{19}H_{24}O_3N_2$	labetalol	2.51	3.42	0.91
1656. $C_{19}H_{31}O_2N$	fenbutolol	4.15	4.15	0.00
1657. $C_{19}H_{28}O_2$	testosterone(9109)	3.32	3.79	0.47
1658. $C_{20}H_{23}N$	amitriptyline(504)	4.92	5.23	0.31
1659. $C_{20}H_{25}N_3S$	perazine(7108)	2.90	3.93	1.03
1660. $C_{20}H_{27}O_4N$	bevantolol	3.00	3.53	0.53
1661. $C_{21}H_{30}O_2$	progesterone(7783)	3.87	4.53	0.66
1662. $C_{21}H_{30}O_2N_3F$	pipamperone	2.40	2.75	0.35
1663. $C_{23}H_{20}O_3N_2S$	sulfinpyrazone	2.30	2.43	0.13

[a] log P_e is the experimental value. [b] log P_c is the calculated value. [c] log P_r is the estimation error.

A cross-validation test was then used to evaluate the predictive ability of our final model. Approximately 5% of the compounds were randomly selected from the original database as a test set, while the other 95% remained as the training set. A log P calculation model was then developed on the basis of the training set, and a prediction was made for the compounds in the test set. The results of 15 such cross-validation tests are shown in Table 6. As can be seen, the r^2 value and standard deviation remained almost the same for each training set. The average predictive r^2 value and standard deviation of the 15 cross-validation tests are 0.926 and 0.404, respectively. This cross-validation test demonstrates the outstanding predictive power of our log P model.

It can be seen from Table 3 that the carbon fragment types, $-CH_3$, $-CH_2-$, and $-CH<$, are hydrophobic, while the $>C<$ atom is slightly hydrophilic. In our definition of basic group types, the hydrogen atom was not defined as one basic group, rather it was always expressed along with the heavy atom (C, N, O, S, P, etc.) to which it is directly attached. However, the contribution of the hydrogen atom can be estimated from those of the basic groups 1–15 in Table 3. The calculated value is found to be about 0.18, which is the same as that reported by Rekker,[8] but slightly less than that (0.23) reported by Leo.[9]

The presence of fluorine, chlorine, bromine, iodine, and sulfur increases the hydrophobicity (positive contribution to the log P) of compounds, while the presence of nitrogen and oxygen groups in general decreases hydrophobicity (negative contribution to the log P). The hydrophilic characteristics of the nitrogen and oxygen groups are probably due to the strong hydration effects of these groups. It is interesting to note that, as was also observed by Rekker,[9] some groups (–F, –OH, –COOH, $-NH_2$, etc.) become more hydrophobic when they are directly attached to aromatic ring systems.

A close examination of the correction fragments identified by the CASE program shows some analogy with the correction factors proposed by Leo[11] and Ghose et al.[16] Our correction fragments can be classified in several categories.

(a) Tautomerization Effects. Correction factors of this type (parameters 69, 87) have often been found in pyridine analogs. In the tautomeric equilibrium shown in Figure 5, solvation effects play an important role and subsequently determine the distribution ratio of the two tautomers. If the dominant form is not the entered structure for the calculation, the result will not be satisfactory. Some fragments related

Table 5. List of Compounds with Large Estimation log *P* Error

formula	name	log P_e[a]	log P_c[b]	log P_r[c]
179. $C_{13}H_8O$	9-fluorenone	3.58	2.66	−0.92
246. $C_6H_{13}N$	cyclohexylamine	1.49	0.44	−1.05
405. $C_{10}H_{13}O_4N_5$	Ado	−1.23	−2.13	−0.90
410. $C_{10}H_{13}O_5N_5$	Guo	−1.89	−3.09	−1.20
411. $C_{10}H_{13}O_4N_5$	dGuo	−1.30	−2.26	−0.96
414. $C_{10}H_{16}O_3N_6$	dDAPR	−0.52	−1.38	−0.86
441. $C_4H_4N_6$	adenine, 8Aza	−0.96	−0.11	0.85
450. $C_5H_4N_4$	purine	−0.37	0.53	0.90
479. C_2H_5OH	acetaldoxime	−0.12	0.82	0.94
480. C_2H_5OF	2-fluoroethanol	−0.92	−0.07	0.85
488. $C_2H_6O_2N_2$	1-methyl-1-hydroxyurea	−0.46	−1.29	−0.83
490. $C_3NH_2Br_3$	2,4,5-tribromoimidazole	1.96	2.79	0.83
495. C_3H_3NS	thiazole	0.44	1.25	0.81
518. $C_4H_4N_2$	pyrazine	−0.22	0.82	1.04
519. $C_4H_4N_2$	pyrimidine	−0.40	0.82	1.22
556. C_5NCl_5	2,3,4,5,6-pentachloropyridine	3.53	4.47	0.94
572. C_5H_5ON	pyridine 1-oxide	−1.30	−0.23	1.07
575. $C_5H_6N_2$	2-methylpyrazine	0.23	1.23	1.00
689. $C_6H_7NO_3$	6-aminonicotinamide	0.70	−0.50	−1.20
690. $C_6H_7ON_3$	isoniazid	−1.14	−0.01	1.13
697. $C_6H_8N_2$	γ-pyridylmethylamine	−0.38	0.47	0.85
699. $C_6H_8N_2$	4,6-dimethylpyrimidine	0.62	1.64	1.02
701. $C_6H_8O_2N_2S$	*m*-aminobenzenesulfonamide	−1.20	−0.10	1.10
742. $C_7H_5ON_2Cl$	zoxazolamide	2.46	1.56	−0.90
743. $C_7H_5OF_3$	trifluoromethoxybenzene	3.17	2.28	−0.89
756. $C_7H_5O_2F_3S$	phenyl-trifluoromethyl sulfone	2.68	1.86	−0.82
768. $C_7H_6N_2S$	*o*-phenylenethiourea	1.66	0.71	−0.95
818. $C_7H_7O_2FS$	*p*-(fluorosulfonyl)toluene	2.74	1.40	−1.34
855. $C_7H_9SCl_5$	1-(methylthio)pentachlorocyclohexane	3.75	4.63	0.88
856. C_7H_9ON	2-(α-pyridyl)ethanol	0.12	1.09	0.97
857. C_7H_9ON	2-(β-pyridiyl)ethanol	0.12	1.09	0.97
858. C_7H_9ON	2-(γ-pyridyl)ethanol	0.10	1.09	0.99
869. $C_7H_{10}N_2$	2-(α-pyridyl)ethylamine	0.08	0.88	0.80
870. $C_7H_{10}N_2$	2-(β-pyridyl)ethylamine	0.00	0.88	0.88
871. $C_7H_{10}N_2$	2-(γ-pyridyl)ethylamine	−0.01	0.88	0.89
886. $C_8HN_2F_3Cl_4$	4,5,6,7-tetrachloro-2-(trifluoromethyl)benzimidazole	3.97	5.01	1.04
887. $C_8NH_2F_3Br_4$	4,5,6,7-tetrabromo-2-(trifluoromethyl)benzimidazole	4.81	5.75	0.94
889. $C_8H_2N_2F_3Br_3$	4,5,6-tribromo-2-(trifluoromethyl)benzimidazole	4.08	4.91	0.83
890. $C_8H_3N_2F_3Cl_2$	4,7-dichloro-2-trifluoromethyl benzimidazole	2.87	3.70	0.83
905. $C_8H_5ONF_3Br$	*p*-trifluoroacetamide bromobenzene	3.34	2.51	−0.83
924. $C_8H_6O_2N_2$	quinazoline-2,3-dione	0.20	1.07	0.87
989. $C_8H_7O_4FS$	*p*-(fluorosulfonyl)phenoxyacetic acid	1.84	0.90	−0.94
1047. $C_8H_9O_2N$	*p*-aminophenylacetate	−0.16	0.92	1.08
1059. $C_8H_9O_2N$	*N*-phenylglycine	0.62	−0.35	−0.97
1160. $C_9H_8O_2N_2S$	8-sulfonamidoquinoline	0.36	1.19	0.83
1258. $C_{10}H_6NF_3$	8-trifluoromethylquinoline	2.50	3.32	0.82
1291. $C_{10}H_9ON$	*N*-methyl-4-quinolone	0.44	1.28	0.84
1319. $C_{10}H_{11}N$	1,2-dimethylindole	2.82	1.88	−0.94
1386. $C_{10}H_{14}ON_2$	γ-(α-pyridyl)pentamide	−0.01	0.84	0.85
1410. $C_{11}H_6O_2N_3F_3Cl_2$	1-(2,6-dichloro-4-(trifluoromethyl)phenylhydrazono)-1-cyanoacetic acid methyl ester	4.36	5.29	0.93
1427. $C_{11}H_8O_4N_3F_3S$	1-(4-[(trifluoromethyl)sulfonyl]phenylhydrazono)-1-cyanoacetic acid methyl ester	4.22	3.16	−1.06
1452. $C_{11}H_{13}O_2N_3$	1-(4-carboxybutyl)benzotriazole	0.93	1.77	0.84
1463. $C_{11}H_{14}O_3$	*p*-hydroxybenzoic acid butyl ester	3.57	2.70	−0.87
1489. $C_{12}H_8N_2$	4,7-phenanthroline	2.05	2.85	0.80
1491. $C_{12}H_9N$	carbazol	3.72	2.69	−1.03
1539. $C_{13}H_9ONS_2$	(4-isothiocyanophenyl) phenyl sulfoxide	4.40	3.53	−0.87
1546. $C_{13}H_{10}ON_2Cl_2$	1-(3,4-dichlorophenyl)-3-phenylurea	4.70	3.67	−1.03
1560. $C_{13}H_{11}N_3$	3,6-diaminoacridine	1.10	1.92	0.82
1582. $C_{14}H_8N_2S_2$	4,4′-diisothiocyanatebiphenyl	5.50	6.35	0.85
1585. $C_{14}H_{10}O_2$	benzil	3.38	2.37	−1.01
1586. $C_{14}H_{10}O_2NF_3$	*N*-(3-(trifluoromethyl)phenyl)anthranilic acid	5.62	4.69	−0.93
1587. $C_{14}H_{11}NS$	(4-isothiocyanophenyl)phenylmethane	4.40	5.26	0.86
1601. $C_{14}H_{18}O_3$	4-cyclohexylphenoxyacetic acid	3.79	2.99	−0.80
1608. $C_{14}H_{22}O_3N_2$	atenolol	0.16	1.04	0.88
1624. $C_{15}H_{16}O_2$	bisphenol A(1311)	3.32	4.34	1.02
1631. $C_{16}H_{13}ON_2Cl$	diazepam	2.66	3.59	0.93
1647. $C_{17}H_{23}ON_3$	mepyramine	2.85	3.67	0.82
1650. $C_{18}H_{22}N_2$	desipramine	4.90	3.74	−1.16
1652. $C_{18}H_{22}N_2S$	trimeprazine (9617)	3.44	4.62	1.18
1655. $C_{19}H_{24}O_3N_2$	labetalol	2.51	3.42	0.91
1659. $C_{20}H_{25}N_3S$	perazine (7108)	2.90	3.93	1.03

[a] log P_e is the experimental value. [b] log P_c is the calculated value. [c] log P_r is the estimation error.

to the tautomerization effect have been identified and are included in our log *P* calculation model.

(b) Dipolar Ion Effect (Zwitterion Effect). The log *P* values for compounds such as amino acids are largely underestimated by the model using group contribution alone. This is because a large fraction of these compounds in water is not in a neutral form, but rather exists in a dipolar ion form. This dipolar ion effect has been identified by the CASE program (parameters

Table 6. Cross-Validation Test Results for a Database of 1624 Compounds

	learning set			test set		
no.	no. of compds	r^2	SD	no. of compds	r^2	SD
1	1592	0.929	0.380	71	0.914	0.430
2	1585	0.929	0.382	78	0.927	0.406
3	1578	0.930	0.381	85	0.912	0.414
4	1590	0.929	0.391	73	0.924	0.419
5	1582	0.929	0.383	81	0.903	0.382
6	1575	0.929	0.383	88	0.919	0.381
7	1584	0.929	0.381	89	0.931	0.419
8	1590	0.928	0.384	71	0.946	0.350
9	1601	0.929	0.382	62	0.933	0.409
10	1580	0.929	0.383	83	0.928	0.374
11	1593	0.930	0.380	70	0.908	0.434
12	1595	0.929	0.382	68	0.906	0.412
13	1573	0.929	0.381	90	0.926	0.413
14	1598	0.929	0.382	65	0.925	0.399
15	1580	0.929	0.381	73	0.924	0.419
mean	1586	0.929	0.383	87	0.926	0.404

70, 81, and 90) and was included in our log P model.

(c) Proximity Effect. In aromatic systems, the interactions between two polar substituents ortho to each other were found to have a large effect on the log P values. For instance, in salicylic acid, the interaction between COOH and OH groups (the proximity effect) was found to be an important factor for the evaluation of its partition coefficient. Therefore, this effect should be included in an accurate log P model. Parameters 79 and 80 were identified by the CASE program to represent this effect. These parameters reflect the intramolecular hydrogen bonding between two polar ortho substituents. In aliphatic systems, compounds with structures such as X–CH_2–CH_2Y also show a proximity effect, when X and Y have strong intermolecular interaction. Parameter 85 has been identified to represent this effect.

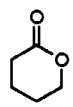
(d) Conjugated Multiheteroatomic Effect. The CASE program has identified some significant correction effects such as parameters 71, 78, 82, 83, 88, and 89 related to conjugated multi-heteroatomic interaction.

In our study, we found that a large systematic error for the hydrocarbon compounds arises when group contributions are used alone. This is probably due to the flexibility of the carbon chain in alkanes. We found, however, that the molecular weight (parameter 97) is a very effective correction factor for alkanes. Finally, an indicator parameter (parameter 98) was used to correct for the systematic error observed for the unsaturated hydrocarbons.

Using the group contribution alone, log P values were overestimated for compounds with structure such as CH_6-$(CH_2)_nX$ and pyridine–$(CH_2)_nX$, where X is a polar group (X = OH, NH_2, COOH, $CONH_2$, F, etc.) and $n \geq 2$. We found that this overestimation is probably caused by a folding effect;[13] i.e. when a molecule with this type of structure folds, the polar group at the end of the side chain interacts with the π cloud of the atomatic ring. A molecular dipole ($Ar^{\delta+}X^{\delta-}$) is developed which may reduce the lipophilicity of the molecule. Thus, we included parameters 94–96 in our log P estimation model to account for this folding effect.

Two examples are shown below to illustrate the calculation procedure. The log P values calculated by using CLOGP, developed by Leo et al.,[11] are also listed for comparison.

Example 1. δ-Valerolactone $C_5H_8O_2$



log P = 4(Pa.11) + (Pa.35) - 0.703
= −0.14

measured = -0.35; calculated by CLOGP = 0.66

Table 7. Experimental (LOGP) and Calculated log P Values Using Four Methods

no.	name	LOGP	KLOGP	ALOGP	CLOGP	BLOGP
1	Ado	−1.23	−2.13	−1.240	−2.941	0.182
2	dAdo	−0.54	−1.29	−0.630	−2.531	0.356
3	ddAdo	−0.21	−0.46	−0.190	−1.116	0.406
4	ddeAdo	−0.35	−0.42	0.040	−1.600	0.379
5	FddAdo	0.08	−0.23	−0.020	−1.273	0.522
6	Guo	−1.89	−3.09	−1.630	−3.923	−0.210
7	dGuo	−1.30	−2.26	−1.010	−3.338	−0.013
8	ddGuo	−1.00	−1.43	−0.580	−1.923	0.177
9	ddeGuo	−1.21	−1.39	−0.350	−2.407	0.115
10	dDAPR	−0.52	−1.38	−0.910	−2.592	−0.101
11	ddDAPR	−0.46	−0.55	−0.470	0.067	0.067
12	FddDAPR	0.05	−0.32	−0.300	−1.333	0.249
13	Urd	−1.71	−2.28	−1.590	−2.560	0.085
14	dUrd	−1.50	−1.44	−0.980	−2.090	0.456
15	ddUrd	−0.88	−0.61	−0.540	−0.675	0.667
16	ddeUrd	−1.07	−0.57	−0.320	−1.159	0.645
17	FddUrd	−0.48	−0.38	−0.370	−0.832	0.912
18	dThd	−1.17	−1.03	−0.820	−1.591	0.817
19	ddThd	−0.63	−0.20	−0.390	−0.176	1.042
20	ddeThd	−0.81	−0.16	−0.160	−0.660	0.999
21	FddThd	−0.27	0.03	−0.220	−0.333	1.269
22	Cyd	−2.51	−2.86	−1.420	−3.111	0.113
23	dCyd	−1.77	−2.03	−0.810	−2.549	0.478
24	ddCyd	−1.30	−1.20	−0.370	−1.133	0.619
25	ddeCyd	−1.42	−1.16	−0.140	−1.617	0.571
26	FddCyd	−0.91	−0.97	−0.200	−1.290	0.775
27	F6ddP	0.00	0.28	0.490	−0.906	0.247
28	F62AddP	−0.05	−0.11	0.210	−0.970	0.375
29	Br6ddP	0.35	0.81	1.080	−0.356	0.798
30	Br62AddP	0.33	0.42	0.800	−0.420	0.765
31	C16ddP	0.23	0.50	0.780	−0.386	0.489
32	Cl62AddP	0.21	0.11	0.500	−0.450	0.545
33	I6ddP	0.52	1.00	1.080	0.074	1.011
34	I62AddP	0.52	0.61	0.800	0.010	0.996
35	ddI	−1.24	−1.55	−0.950	−1.755	−0.335
36	uracil	−1.07	−0.86	−0.720	−1.060	−0.585
37	adenine, 8Aza	−0.96	−0.11	−0.670	−0.063	−0.034
38	guanine, 8Aza	−0.71	−1.14	−1.060	−1.004	−0.836
39	cytocine	−1.73	−1.45	−0.550	−1.846	−0.769
40	adenine	−0.09	0.23	−0.360	−0.426	0.036
41	thioguanine	−0.07	−0.37	−0.020	−1.824	0.308
42	adenine, 9Ppl	0.74	0.50	0.690	0.437	1.327
43	uracil, 6Aza	−0.59	−0.91	−0.490	−0.593	−1.013
44	guanine	−0.91	−1.17	−0.750	−1.264	−0.891
45	thymine	−0.62	−0.45	−0.560	−0.557	−0.130
46	hypoxanthine	−1.11	−0.89	−0.880	−1.260	−0.873
47	purine	−0.37	0.53	−0.280	−0.290	−0.139

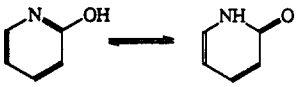
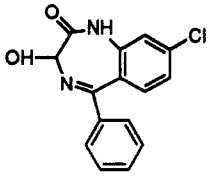


Figure 5. Equilibrium of tautomerization.

Example 2. Oxazepam $C_{15}H_{11}ClN_2O_2$



log P = (Pa.12) + 8(Pa.14) + 5(Pa.15) + (Pa.18) + (Pa.25) + (Pa.37) + (Pa.57) - 0.703
= 2.27

measured = 2.17; calculated by CLOGP = 3.33

(3) Comparison. Viswanadhan et al. have published a paper recently, in which they systematically evaluated three methods for their ability to accurately predict the log P for nucleosides.[29] The three methods used in their report are (1) the atomic constant approach of Viswanadhan and co-workers (ALOGP), (2) the molecular orbital approach of Bodor and co-workers (BLOGP), and (3) the fragmental constant approach of Leo and co-workers (CLOGP). A set of 47 nucleosides and nucleobases have been chosen for the comparison. It includes 35 nucleosides and analogs and 12 nucleobases and derivatives.

Table 8. Statistical Results Using ALOGP, BLOGP, CLOGP, and KLOGP Methods

	r (SD)[b]		
method[a]	all	nucleosides	bases
KLOGP	0.89 (0.46)	0.91 (0.47)	0.77 (0.46)
BLOGP	0.40 (1.20)	0.43 (1.37)	0.81 (0.53)
CLOGP	0.71 (0.93)	0.75 (1.02)	0.60 (0.63)
ALOGP	0.84 (0.51)	0.87 (0.55)	0.80 (0.42)

[a] The abbreviations used here are explained in the method. [b] r is the correlation coefficient; SD is the standard deviation.

In this study, we calculate the log P values for the same 47 compounds using our final model (KLOGP). Table 7 lists the experimental and calculated log P values using four different methods. As can be seen in Table 8, the overall correlation (r) of 0.89 with standard deviation (SD) of 0.46 calculated by KLOGP is the best among the four methods. For nucleosides only, it yields also the best correlation of 0.91 with SD = 0.47. However, for nucleobases, ALOGP has a better correlation of 0.80 with SD = 0.42 compared to KLOGP with a correlation of 0.77 and SD = 0.46. A close examination of these nucleobases reveals that the relatively large deviation calculated by using KLOGP was caused by only one compound, purine. This comparison shows that KLOGP is a better method than the other methods for this special class of compounds.

CONCLUSION

We have successfully combined the group contribution and the CASE methodology to develop a reliable and accurate log P estimation model ($n = 1663$, $r^2 = 0.93$, SD = 0.38). The CASE program has been shown to be a very useful tool in identifying the correction factors for log P calculations. The cross-validation experiments demonstrated that our model can give accurate log P predictions for complex compounds as well as for simple molecules. For nucleosides and nucleobases, our model has a better prediction ability than the other methods. In the future, by updating the learning database, the CASE program should be able to identify new correction factors to improve the predictive power of our log P estimation model even more.

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