Fuzzy ARTMAP and Back-Propagation Neural Networks Based Quantitative Structure−Property Relationships (QSPRs) for Octanol−Water Partition Coefficient of Organic Compounds

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Quantitative structure−property relationships (QSPRs) for estimating the logarithm octanol/water partition coefficients, logK_{ow}, at 25 °C were developed based on fuzzy ARTMAP and back-propagation neural networks using a heterogeneous set of 442 organic compounds. The set of molecular descriptors were derived from molecular connectivity indices and quantum chemical descriptors calculated from PM3 semiempirical MO-theory. Quantum chemical input descriptors include average polarizability, dipole moments, exchange energy, total electrostatic interaction energy, total two-center energy, and ionization potential. The fuzzy ARTMAP/QSPR performed, for a logK_{ow} range of −1.6 to 7.9, with average absolute errors of 0.03 and 0.14 logK_{ow} for the overall data and test sets, respectively. The optimal 12−11−1 back-propagation/QSPR model, for the same range of logK_{ow}, exhibited larger average absolute errors of 0.23 and 0.27 logK_{ow} for the test and validation data sets, respectively, over the same range of logK_{ow} values. The present results with the fuzzy ARTMAP-based QSPR are encouraging and suggest that high performance logK_{ow} QSPR that encompasses a wider range of chemical groups could be developed, following the present approach, by training with a larger heterogeneous data set.

INTRODUCTION

The octanol/water partition coefficient, K_{ow}, which is the ratio of a chemical's concentration in *n*-octanol to that in water in a two-phase system at equilibrium, is often used to quantify the lipophilic or hydrophobic nature of an organic compound. K_{ow} is an important physicochemical property in the environmental,[1−3] pharmaceutical,[4−6] biochemical, and toxicological sciences.[2] For example, K_{ow} is a key parameter required for estimates of the multimedia environmental mass distribution of organic compounds[1−3] including contaminant bioaccumulation in aquatic biota and plants. K_{ow} is also an important parameter utilized to predict potential interactions of drug molecules with receptor molecules. Although experimental K_{ow} values are available for a large data set of organic compounds, reliable experimental data are lacking for many chemical pollutants. Given the need to evaluate both present and potential future pollutants, there has been a steady increase in efforts to develop reliable K_{ow} estimation methods. Estimation approaches include group and atom contribution methods,[4−16] quantitative structure property relationships (QSPRs) derived from statistical regressions,[17−24] and neural networks-based QSPRs.[25−29] K_{ow} for organic compounds spans several orders of magnitude, from less than 10^{-4} to more than 10^{8}, and thus it is commonly reported as logK_{ow}.

Group and atom contribution models have typically been based on fragments, derived either from atoms or groups of atoms, which are assigned incremental logK_{ow} contributions[4,9,10] The standard deviation of predictions from group and atom contribution approaches for estimating logK_{ow} has generally been reported to vary from about 0.35−0.6 logK_{ow} units[7,8] for a logK_{ow} range of −3 to 6. The commercial CLOGP model is an example of a group contribution method that has been developed based on a large data set of about 8000 compounds.[5,10,11] In general, group contribution methods produce satisfactory results for simple compounds and various improvements to logK_{ow} group contribution methods have been developed to handle complex molecules through the introduction of corrections factors, refinements of fragments, and development of new fragments.[7,8] One advantage of atom contribution methods, relative to group contribution methods, is that ambiguity in the choice of fragments when dividing a molecule is eliminated. Both methods require a larger number of correction factors as the complexity of the molecule increases. Also, logK_{ow} can only be predicted for compounds consisting of fragments for which logK_{ow} contribution values are available. It has been reported that logK_{ow} estimation methods using fragmental contributions are generally comparable to those using atomic contributions[16] with both methods working well for simple structures.

Quantitative-structure−property-relations (QSPRs) have been developed as alternate methods of estimating logK_{ow}. The premise of QSPR for logK_{ow} is that physicochemical

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properties can be correlated with molecular structural characteristics (geometric and electronic) expressed in terms of appropriate molecular descriptors.[17] In general, high accuracy is obtained for QSPRs developed specifically for homologous series and data sets containing similar compound families.[18] QSPRs developed for heterogeneous data sets using topological descriptors[30−32] have performed with reported errors comparable to those of group contribution methods.[19,20] For example, the so-called VLOGP model[20] that utilizes a set of over 300 electrotopological-state[32] and kappa shape indices as chemical descriptors was developed using a training set of 6675 compounds ($-3.56 \leq \log K_{ow} \leq 7.73$) and performed with an average error of 0.201 $\log K_{ow}$ units.[20]

In recent years, improvements in $\log K_{ow}$ QSPRs have been proposed through the use of molecular descriptors derived from semiempirical Molecular Orbital theory (quantum mechanics) calculations.[21−25,33,34] For example, Bodor et al.,[21] using AM1 semiempirical MO theory, reported a standard deviation of 0.306 $\log K_{ow}$ for a 18 parameter linear correlation which was developed for estimating $\log K_{ow}$ for a heterogeneous data set 302 organic compounds ($-1.3 \leq \log K_{ow} \leq 6.6$). In later studies, Schüürmann[22,23] proposed linear correlations of $\log K_{ow}$ with a range of quantum chemical parameters based on data of 12 aromatic phosphorothionates[22] and 17 substituted benzenes.[23] A $\log K_{ow}$ correlation for 17 benzene derivatives over a range of approximately $4 \leq \log K_{ow} \leq 8$, based on the free energy of aqueous solvation and contact surface area, performed with a standard a deviation of 0.22 $\log K_{ow}$ units. In a more recent study, Eisfeld and Maurer[24] proposed a $\log K_{ow}$ correlation with dipole moment, polarizability, electrostatic potential, and molar volume as chemical descriptors, based on a heterogeneous set of 202 compounds ($-2 \leq \log K_{ow} \leq 5.7$) with a reported standard deviation and maximum absolute error of 0.287 and 1.004 $\log K_{ow}$ units, respectively. The introduction of indicator variables in the correlation, to account for the presence of nitrogen and oxygen atoms, lowered the standard deviation and maximum absolute error to 0.274 and 0.821 $\log K_{ow}$ units, respectively.[24]

The application of neural networks, as an alternative approach to developing QSPRs for $\log K_{ow}$, has been introduced in recent years. For example, Duprat et al.[25] developed neural network-based QSPR models of various back-propagation architectures for $\log K_{ow}$, for a set of 323 diverse organic compounds ($-1.3 \leq \log K_{ow} \leq 6.5$), with reported standard deviations ranging from 0.37 to 0.28 $\log K_{ow}$. The models of Duprat et al.[25] were based on a set of descriptors that included the number of carbon atoms, molecular surface, molecular weight, square root of the sum of the charges on oxygen, nitrogen, and sum of the absolute values of atomic charges on nitrogen and oxygen. More recently, Huuskonen et al.[26] proposed a 39−5−1 back-propagation neural network-based QSPR for $\log K_{ow}$, based on a diverse set of 1870 organic compounds ($-4.2 \leq \log K_{ow} \leq 5.9$), using atomic-type electrotopological-state (E-state)[32] indices as input descriptors, with a reported root-mean-square error of 0.41 $\log K_{ow}$ units.[26]

QSPRs for $\log K_{ow}$ based on neural networks (NN) with quantum mechanical descriptors have also been proposed in recent years.[27−29] For example, Breindl et al.[27] developed a NN/QSPR for $\log K_{ow}$ using two sets of 16 quantum chemical parameters that were calculated from AM1[33] and PM3[34] semiempirical Molecular Orbital theory. The QSPRs models for the AM1 and PM3 parameter sets were based on a 16−25−1 back-propagation network architecture developed with a data set of 1085 compounds ($-2.06 \leq \log K_{ow} \leq 7.41$).[27] Average absolute errors and standards deviations for the validation set (105 compounds) for AM1 and PM3 models were 0.45 (80%) and 0.30 (243.4%) $\log K_{ow}$ and 0.53 (86%) and 0.42 (227%) $\log K_{ow}$, respectively.[27] More recently, Beck et al.,[29] using the same chemical data set of Breindl et al.[27] and 16 quantum chemical descriptors (computed from AMI), developed a $\log K_{ow}$ QSPR based on a 16−10−1 back-propagation neural network architecture which performed with average and maximum errors for the cross-validation set of 0.56 and 2.1 $\log K_{ow}$, respectively.[29]

To date, published available NN/QSPRs for octanol/water partition coefficients have been based on back-propagation neural networks.[19,20,25−27,29] However, recent studies[35−37] suggests that it may be possible to develop NN-based QSPRs of greater accuracy by using the cognitive classifier fuzzy ARTMAP neural network classifier. The fuzzy ARTMAP neural networks approach, which was demonstrated for estimating boiling points of aliphatic hydrocarbons,[35] critical properties,[36] and aqueous solubility of organics,[37] has been shown to be superior to the back-propagation neural network approach as well as other regression-based statistical correlations reported in the literature. Fuzzy ARTMAP neural networks have several advantages owing to their capability to classify and analyze noisy information with fuzzy logic and to avoid the plasticity-stability dilemma of standard back-propagation architectures.

In the present study, we expand recent work to demonstrate that fuzzy ARTMAP-based QSPRs for $\log K_{ow}$ can be developed using a relatively small number of quantum chemical descriptors derived from PM3 semiempirical MO-theory. The present work presents a first demonstration of using the fuzzy ARTMAP approach to arrive at adequate $\log K_{ow}$ QSPR with a modest heterogeneous data set of 442 organics with the majority of compounds being of environmental interest. The performance of the fuzzy ARTMAP-based QSPR is compared to a back-propagation QSPR developed with the same set of input descriptors and to other published multiple linear regression (MLR) and back-propagation neural network (NN) based QSPR models.

II. METHODOLOGY

Data Set and Molecular Descriptors. The approach of developing the present neural network-based $\log K_{ow}$ QSPRs is summarized in Figure 1. Octanol/water partition coefficients at 25 °C for a diverse set of 442 organic compounds were compiled from the literature,[4,7,10,19,38] and these are listed in Tables 1 and 3 as $\log K_{ow}$. This heterogeneous set of compounds includes aromatic (polycyclic aromatic) and nonaromatic (normal, branched, cyclic) hydrocarbons, halogens, PCBs, mercaptans, sulfides, anilines, pyridines, alcohols, carboxylic acids, aldehydes, amines, ketones, and esters. Prior to model development, the input descriptors and octanol/water partition coefficient data were normalized from 0 to 1 as $X_n = X - X_{min}/(X_{max}-X_{min})$, where X and X_n are the actual and normalized $\log K_{ow}$ values, respectively, and X_{min} and X_{max} are the minimum and maximum $\log K_{ow}$ values in the data set, respectively.

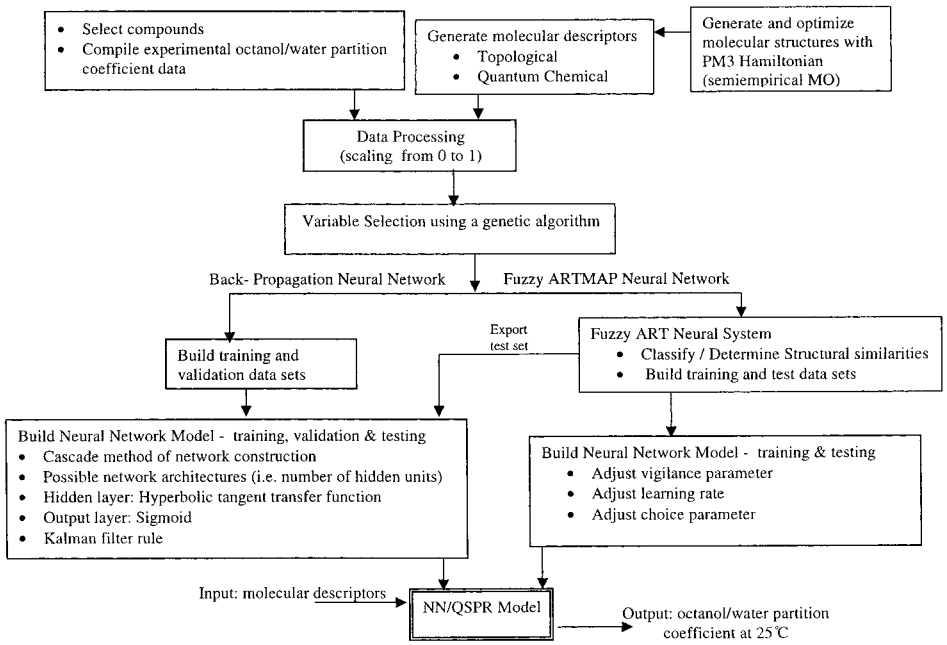

Figure 1. Process flow diagram for developing fuzzy ARTMAP and back-propagation QSPR/neural networks for predicating octanol/water partition coefficients.

The molecular descriptors for each compound were calculated from knowledge of the chemical structure. Molecular structures were drawn using Molecular Modeling Pro 3.01 (ChemSW Software Inc.)[39] and converted to three-dimensional structures using the CAChe Software (Oxford Molecular Ltd.).[40] The geometry of the three-dimensional structures were subsequently optimized using MOPAC[34,41], a semiempirical molecular orbital modeling program with the PM3 (parametric model 3) Hamiltonian[34] to arrive at the compounds' minimum energy conformations. In conjunction with the MOPAC energy minimization, quantum chemical descriptors, derived from the PM3 MO theory, were also calculated. The calculated descriptors included average polarizability, dipole moments, moments of inertia, ionization potential, number of number of doubly occupied (filled) MO levels, molecular weight, heat of formation, total energy, electronic energy, and nuclear−nuclear (core−core), and energy components partitioned into the individual one-center and two-center terms were calculated (see Table 2). The total energy, in terms of the PM3 MO, is the sum of the total one-center and two-center terms. The one-center energy terms include electron−electron repulsion and electron−nuclear attraction. The two-center energy terms include resonance energy, exchange energy, electron−electron repulsion, electron−nuclear attraction, and nuclear−nuclear repulsion. The total electrostatic (or Coulombic) interaction is equal to the sum of the following two-center energy terms: electron−electron repulsion, electron−nuclear attraction, and nuclear−nuclear repulsion energy. The resonance energy corresponds to the difference in delocalized pi electrons and pi electrons localized in a double bond.[42] The exchange energy involves two electrons where the energy of attraction is between the nuclei and the overlap charge in the bond.[42] Finally, molecular polarizability characterizes molecular bulk and dispersion interactions, and it has been shown to correlate with hydrophobicity as well as other biological activities.[43−45]

Molecular topological descriptors included the four valence molecular connectivity indices of orders 1, 2, 3, and 4 ($^1\chi^v$, $^2\chi^v$, $^3\chi^v$, $^4\chi^v$)[46,47] and the second Kappa shape index, $^2\kappa$.[48] The above molecular indices were generated from the two-dimensional molecular structure using Molecular Modeling Pro 3.01 software. Molecular connectivity indices are topological indices that encode two-dimensional structural information into numerical values or indexes. The molecular structure is expressed topologically by a hydrogen-suppressed graph. The carbons (and heteroatoms) are represented as vertices, and bonds connecting atoms are represented as edges. Briefly, the connectivity indices $^m\chi^v$ are valence-weighted counts of connected subgraphs. The first-order term $^1\chi^v$ is related to the degree of branching and size of the molecule expressed as the number of non-hydrogen atoms. The second-order term $^2\chi^v$ represents a dissection of the molecular skeleton into "two contiguous bond" fragments. The third-order term $^3\chi^v$ is a weighted count of four atoms (three-bond) fragments representing the potential for rotation around the central bond and is the smallest molecular structure necessary for conformational variability. The $^3\chi^v$ index also reflects the degree of branching at each of the four atoms in the fragment. The fourth-order term, $^4\chi^v$ represents path, cluster, path/cluster, and cyclic subgraphs of four edges. Structural information from the $^4\chi^v$ index is useful for compounds with at least five carbon atoms in a chain. Finally, the kappa 2 shape index,[19] $^2\kappa$, is included to characterize the level of branching among isomers.

A variable selection method, employing a nonlinear neural network-based genetic algorithm, was used to select the set of input descriptors.[49] The variable selection algorithm was performed on 15 separate neural networks establishing a frequency distribution of the selected descriptors for the different generated networks. The set of 12 descriptors that was selected, for all runs, at or above the 70th percentile was chosen as the final set of input descriptors for QSPR modeling. The set of 12 input parameter included in Table 1 and listed in Table 2 include the following: the first, second, and fourth-order valence molecular connectivity indices ($^1\chi^v$, $^2\chi^v$, $^4\chi^v$), dipole moment parameters (total point

Table 1. Molecular Descriptors and Experimental Octanol/Water Partition Coefficients

compound	MW[a]	D_P[b] [debye]	D_H[c] [debye]	D_S[d] [debye]	E2[e] [EV]	EX[f] [ev]	ELC[g] [ev]	IP[h] [kcal]	PO[i] [au]	VMC_1[j]	VMC_2[k]	VMC_4[l]	logK_{ow}
1,1,1-trichloroethane	133.41	0.78	0.60	1.38	612.86	−36.11	29.16	10.75	40.13	2.20	3.62	0.00	2.49
1,1,2,2-tetrachlorodifluoroethane	203.83	0.01	0.01	0.00	1392.95	−33.16	38.87	11.08	51.21	2.89	3.46	0.00	2.39
1,1,2-trichlorotrifluoroethane	187.38	2.25	0.71	1.56	1560.72	−33.60	43.16	11.34	41.28	2.52	2.70	0.00	3.16
1,1-dichloroethane	98.96	0.97	0.65	1.62	463.36	−37.15	28.15	10.58	30.76	1.88	2.05	0.00	1.79
1,1-dichloroethene	96.94	0.11	0.67	0.78	451.21	−31.18	25.06	9.74	31.89	1.49	1.44	0.00	2.13
1,1-difluoroethane	66.05	1.75	0.37	2.12	800.36	−37.89	36.22	12.82	15.34	1.01	0.52	0.00	0.75
1,1-difluoroethene	64.04	1.42	0.17	1.59	784.55	−31.67	32.96	10.76	16.88	0.73	0.34	0.00	1.24
1,2,3,5-tetramethylbenzene	134.22	0.30	0.05	0.26	713.21	−147.66	110.83	9.04	79.44	3.65	3.02	1.25	4.17
1,2,3-trimethylbenzene	120.19	0.55	0.03	0.52	640.82	−130.86	98.34	9.25	70.68	3.24	2.52	0.90	3.55
1,2,4,5-tetramethylbenzene	134.22	0.03	0.05	0.02	713.07	−147.68	110.88	8.95	79.74	3.65	3.02	1.10	4.00
1,2,4-trichlorobenzene	181.45	0.14	0.58	0.67	870.67	−77.98	65.54	9.24	76.04	3.44	2.81	1.00	4.02
1,2,4-trimethylbenzene	120.19	0.28	0.05	0.23	640.67	−130.91	98.41	9.08	71.24	3.24	2.59	0.89	3.65
1,2-dibromoethane	187.86	0.01	0.00	0.01	665.36	−36.03	25.08	11.22	40.17	3.27	1.96	0.00	1.96
1,2-dichlorobenzene	147.00	0.37	0.98	1.35	721.40	−78.84	64.02	9.29	64.47	2.96	2.23	0.71	3.38
1,2-dichloroethane	98.96	0.01	0.00	0.01	464.34	−37.04	27.93	10.67	30.35	2.10	1.13	0.00	1.48
1,2-dichlorotetrafluoroethane	170.92	1.72	0.43	1.33	1729.34	−34.26	48.04	11.43	33.23	2.14	2.23	0.00	2.82
1,2-difluorobenzene	114.09	2.56	0.18	2.74	1053.25	−79.19	71.38	9.98	48.42	2.21	1.41	0.44	3.60
1,3,5-heptatriene	92.14	0.34	0.04	0.38	495.12	−97.25	73.32	8.52	55.96	2.48	1.48	0.52	2.63
1,3,5-trichlorobenzene	181.45	0.00	0.00	0.00	871.70	−77.94	65.52	9.59	76.51	3.43	2.89	1.39	4.15
1,3,5-trimethylbenzene	120.19	0.01	0.00	0.00	640.46	−130.97	98.40	9.28	71.01	3.23	2.67	1.20	3.42
1,3-butadiene	54.09	0.00	0.00	0.00	292.12	−59.84	42.46	9.47	35.26	1.15	0.47	0.00	1.99
1,3-dibromopropane	201.89	1.59	0.23	1.82	740.18	−52.71	37.18	11.08	44.30	3.77	2.31	1.36	2.37
1,3-dichlorobenzene	147.00	0.34	0.54	0.88	722.53	−78.77	63.93	9.42	65.47	2.95	2.31	0.90	3.38
1,3-dichloropropane	112.99	0.84	0.66	1.50	538.91	−53.70	40.03	10.55	36.98	2.60	1.49	0.45	2.00
1,3-difluorobenzene	114.09	1.47	0.09	1.57	1055.63	−79.11	71.03	10.02	48.32	2.20	1.44	0.46	3.75
1,3-dimethylnaphthalene	156.23	0.35	0.01	0.36	837.74	−161.81	124.67	8.64	101.82	4.23	3.30	1.69	4.42
1,4,5-trimethylnaphthalene	170.25	0.32	0.03	0.30	911.18	−178.37	137.00	8.42	110.09	4.65	3.70	1.94	4.90
1,4-cyclohexadiene	80.13	0.00	0.00	0.00	430.74	−87.03	64.77	9.19	44.66	2.30	1.41	0.54	2.30
1,4-dichlorobenzene	147.00	0.00	0.00	0.00	722.59	−78.77	63.95	9.23	65.99	2.95	2.31	0.68	3.39
1,4-difluorobenzene	114.09	0.00	0.00	0.00	1055.51	−79.12	71.18	9.87	48.48	2.20	1.44	0.43	4.11
1,4-dimethylnaphthalene	156.23	0.02	0.01	0.01	837.77	−161.77	124.64	8.59	101.17	4.24	3.24	1.60	4.37
1,4-dioxane	88.11	0.01	0.00	0.01	673.45	−76.99	69.01	10.45	35.15	2.15	1.22	0.44	-0.27
1,4-pentadiene	68.12	0.08	0.00	0.08	366.89	−76.52	54.58	10.05	39.50	1.63	0.81	0.12	2.48
1,5-dimethylnaphthalene	156.23	0.01	0.00	0.01	837.89	−161.76	124.62	8.60	100.98	4.24	3.24	1.62	4.38
1,5-hexadiene	82.15	0.14	0.01	0.15	441.02	−93.18	66.68	10.10	46.40	2.13	1.15	0.24	2.45
1,6-heptadiene	96.17	0.08	0.00	0.08	515.20	−109.85	78.78	10.14	53.70	2.63	1.51	0.41	3.51
1-bromo-2-isoproplybenzene	199.09	0.93	0.15	1.04	891.37	−129.12	97.44	9.68	79.44	4.25	3.53	1.68	4.20
1-bromobutane	137.02	1.72	0.11	1.82	560.32	−71.17	50.12	10.93	40.18	3.09	1.83	0.69	2.75
1-bromoheptane	179.10	1.74	0.14	1.85	782.75	−121.16	86.40	10.93	61.58	4.59	2.89	1.09	4.36
1-bromohexane	165.07	1.75	0.11	1.84	708.62	−104.50	74.31	10.93	54.47	4.09	2.54	0.92	3.80
1-bromooctane	193.13	1.76	0.11	1.84	856.83	−137.82	98.45	10.93	68.70	5.09	3.25	1.27	4.89
1-bromopentane	151.05	1.73	0.14	1.84	634.50	−87.83	62.22	10.93	47.36	3.59	2.19	0.74	3.37
1-bromopropane	122.99	1.69	0.14	1.81	486.24	−54.50	38.03	10.93	32.94	2.59	1.48	0.00	2.10
1-butanethiol	89.18	1.24	1.14	2.38	404.67	−71.42	50.67	11.20	39.08	2.65	1.52	0.47	2.28
1-butene	56.11	0.23	0.03	0.21	298.46	−66.44	46.74	10.15	30.32	1.52	0.70	0.00	2.40
1-chloro-1,1-difluoroethane	100.50	1.74	0.41	2.02	949.66	−36.66	36.61	11.27	24.57	1.44	1.44	0.00	1.08
1-chlorobutane	92.57	1.07	0.50	1.56	459.04	−71.68	51.54	10.41	36.47	2.51	1.42	0.40	2.55
1-chlorohexane	120.62	1.09	0.49	1.58	607.34	−105.01	75.74	10.41	50.68	3.51	2.13	0.71	3.54
1-chloropentane	106.60	1.07	0.51	1.57	533.20	−88.35	63.64	10.41	43.60	3.01	1.77	0.53	2.73
1-choropropane	78.54	1.04	0.52	1.55	384.95	−55.02	39.45	10.41	29.32	2.01	1.07	0.00	2.04
1-ethylnaphthalene	156.23	0.34	0.04	0.31	839.69	−161.57	124.27	8.70	99.72	4.38	2.99	1.60	4.39
1-ethylpiperidine	113.20	0.07	1.21	1.16	621.47	−126.98	97.07	8.98	55.58	3.66	2.49	1.28	1.75
1-heptanol	116.20	0.89	0.65	1.41	720.58	−128.17	97.30	10.89	53.45	3.52	2.14	0.72	2.03
1-heptyne	96.17	0.55	0.18	0.37	512.60	−110.08	79.46	10.76	49.93	2.85	1.66	0.48	3.01
1-hexene	84.16	0.23	0.03	0.21	446.79	−99.77	70.92	10.15	44.67	2.52	1.43	0.35	3.99
1-hexyne	82.15	0.55	0.19	0.37	438.44	−93.41	67.35	10.76	42.78	2.35	1.31	0.28	2.73
1-methylnaphthalene	142.20	0.28	0.01	0.27	765.23	−145.00	112.18	8.71	92.33	3.82	2.80	1.39	3.87
1-methylcyclohexene	96.17	0.20	0.07	0.16	509.91	−110.35	81.16	9.33	51.61	3.05	2.30	1.00	3.51
1-nitropropane	89.09	3.73	0.53	4.21	724.91	−71.86	61.41	12.07	34.44	1.85	1.03	0.17	0.65
1-nonene	126.24	0.23	0.03	0.21	669.25	−149.77	107.22	10.15	65.97	4.02	2.49	0.89	5.15
1-octanol	130.23	0.91	0.62	1.40	794.73	−144.84	109.41	10.89	60.52	4.02	2.49	0.89	3.15
1-octene	112.21	0.23	0.03	0.21	595.10	−133.10	95.12	10.15	58.88	3.52	2.14	0.72	4.57
1-octyne	110.20	0.56	0.19	0.37	586.77	−126.74	91.55	10.77	57.03	3.35	2.01	0.65	3.50
1-pentanol	88.15	0.89	0.65	1.41	572.29	−94.85	73.15	10.89	39.32	2.52	1.43	0.36	1.40
1-pentyne	68.12	0.53	0.17	0.36	364.31	−76.75	55.26	10.76	35.61	1.85	0.95	0.14	1.98
1-propanol	60.10	0.89	0.64	1.43	424.01	−61.51	48.94	10.88	25.23	1.52	0.72	0.00	0.34
1-propene	42.08	0.23	0.00	0.23	224.52	−49.76	34.65	10.11	23.25	0.99	0.41	0.00	1.77
2,2′,3,3′,4,6′-hexachloro-1,1′-biphenyl	360.88	0.11	1.58	1.61	1726.06	−150.11	129.40	9.26	158.75	6.97	5.79	2.85	6.24
2,2′,3,4,4′,5′-hexachloro-1,1′-biphenyl	360.88	0.03	0.99	1.02	1726.50	−150.08	129.32	9.21	162.76	6.96	5.85	2.75	6.69
2,2′,4,4′,6,6′-hexachloro-1,1′-biphenyl	360.88	0.03	0.01	0.03	1728.50	−150.02	129.39	9.54	160.83	6.96	5.99	3.57	6.70
2,2′,4,5,5′-pentabromo-1,1′-biphenyl	548.69	0.45	0.17	0.61	2063.86	−147.36	118.77	9.53	167.20	8.55	7.70	3.80	5.96
2,2′,4,5,5′-pentachloro-1,1′-biphenyl	326.44	0.16	0.57	0.70	1579.62	−150.82	127.72	9.25	150.83	6.47	5.43	2.47	4.12
2,2′,5,6′-tetrachloro-1,1′-biphenyl	291.99	0.24	0.56	0.79	1431.05	−151.64	126.21	9.19	136.64	6.00	4.88	2.43	6.63
2,2′3,3′-tetrachloro-1,1′-biphenyl	291.99	0.39	1.37	1.76	1429.43	−151.72	126.22	9.31	135.97	6.00	4.77	2.23	6.67
2,2′4,4′,5,5′-hexachloro-1,1′-biphenyl	360.88	0.03	0.03	0.01	1727.52	−150.05	129.37	9.20	163.88	6.96	5.93	2.75	6.72

Table 1 (Continued)

compound	MW[a]	D_P[b] [debye]	D_H[c] [debye]	D_S[d] [debye]	E2[e] [EV]	EX[f] [ev]	ELC[g] [ev]	IP[h] [kcal]	PO[i] [au]	VMC_1[j]	VMC_2[k]	VMC_4[l]	logK_{ow}
2,2-dimethyl-1-propanol	88.15	0.76	0.65	1.35	571.04	−94.91	73.26	10.91	38.52	2.17	2.72	0.00	1.36
2,2-dimethylbutane	86.18	0.09	0.03	0.07	452.46	−106.32	75.26	11.48	42.24	2.56	2.91	0.00	3.88
2,2-dimethylpentane	100.20	0.11	0.05	0.06	526.54	−122.97	87.34	11.19	49.41	3.06	3.31	0.75	3.11
2,2-dimethylpropane	72.15	0.00	0.00	0.00	377.56	−89.78	63.20	12.06	35.06	2.00	3.00	0.00	3.11
2,3,6-trimethylnaphthalene	170.25	0.34	0.05	0.32	910.72	−178.50	137.11	8.55	110.16	4.65	3.68	1.77	4.73
2,3′-dichloro-1,1′-biphenyl	223.10	0.71	0.43	1.07	1134.18	−153.06	122.99	9.06	121.30	5.03	3.83	1.79	5.02
2,3-dimethyl-1-butene	84.16	0.37	0.02	0.36	445.48	−99.84	71.31	9.83	44.27	2.30	2.00	0.00	3.13
2,3-dimethylbutane	86.18	0.00	0.00	0.00	452.94	−106.27	75.17	11.30	42.63	2.64	2.49	0.00	3.85
2,3-dimethylnaphthalene	156.23	0.52	0.06	0.47	838.09	−161.74	124.68	8.64	101.55	4.23	3.28	1.47	4.40
2,3-dimethylpentane	100.20	0.04	0.02	0.04	527.44	−122.87	87.26	11.25	49.71	3.18	2.63	0.47	3.63
2,3-dimethylpyridine	107.16	0.76	1.33	1.91	595.49	−107.69	86.27	9.60	60.56	2.69	1.91	0.56	1.22
2,4-dibromotetrachlorocyclohexane	379.73	0.69	0.49	0.22	1559.01	−91.53	73.41	10.84	100.15	6.88	6.79	4.60	3.98
2,4′-dichloro-1,1′-biphenyl	223.10	0.56	0.94	1.49	1133.42	−153.31	123.10	9.15	119.08	5.03	3.83	1.69	5.10
2,4-dichloro-1,1′-biphenyl	223.10	0.21	0.69	0.83	1133.59	−153.11	123.06	8.92	124.28	5.03	3.83	1.86	5.15
2,4-dichloro-1-chloromethylbenzene	195.48	0.34	0.07	0.39	948.45	−94.27	77.07	9.44	82.00	4.02	2.98	1.40	3.82
2,4-dichlorotoluene	161.03	0.61	0.53	1.09	795.15	−95.58	76.49	9.26	74.02	3.37	2.74	0.97	4.24
2,4-dimethyl-2-pentanol	116.20	1.07	0.65	1.55	722.96	−127.95	96.74	11.19	53.04	3.14	3.41	1.00	2.13
2,4-dimethyl-3-pentanone	114.19	2.07	0.37	2.44	709.35	−121.77	93.06	10.35	52.44	3.09	2.71	0.67	1.86
2,4-dimethylpentane	100.20	0.11	0.08	0.03	526.84	−122.94	87.24	11.49	49.70	3.13	3.02	0.94	3.63
2,4-dimethylphenol	122.17	0.39	0.71	0.93	758.15	−119.72	96.91	8.85	68.05	2.96	2.29	0.81	2.30
2,5′-dichloro-1,1′-biphenyl	223.10	0.27	0.11	0.28	1133.62	−153.11	122.93	9.01	122.12	5.03	3.83	1.73	5.18
2,5-dimethylphenol	122.17	0.63	0.66	1.19	758.88	−119.63	96.77	8.96	67.78	2.96	2.29	0.72	2.33
2,6,dimethylnaphthalene	156.23	0.01	0.00	0.01	837.89	−161.76	124.62	8.60	100.98	4.24	3.24	1.62	4.31
2,6-dichloro-1,1′-biphenyl	223.10	0.74	0.29	1.03	1133.94	−152.96	122.96	9.00	120.66	5.04	3.78	1.99	5.30
2,6-dichlorotoluene	161.03	0.05	0.56	0.51	795.23	−95.58	76.46	9.38	73.10	3.38	2.66	0.98	4.29
2,6-dimethyl-phenol	122.17	0.49	0.70	1.18	758.30	−119.64	96.83	8.96	67.47	2.97	2.24	0.81	2.36
2-aminotoluene	107.16	0.76	1.19	1.33	594.97	−108.35	87.33	8.54	63.94	2.62	1.86	0.59	1.32
2-bromobutane	137.02	1.94	0.10	2.04	562.05	−71.16	50.28	10.87	41.01	2.82	2.75	0.00	2.58
2-bromophenol	173.01	0.74	0.59	0.61	860.36	−84.60	71.71	9.37	62.42	3.03	2.30	0.74	2.35
2-bromopropane	122.99	1.93	0.11	2.04	488.11	−54.51	38.22	10.86	33.96	2.29	2.84	0.00	2.14
2-bromotoluene	171.04	0.89	0.10	0.98	743.31	−95.84	73.36	9.64	65.59	3.31	2.60	0.84	2.92
2-butanone	72.11	2.24	0.47	2.70	488.50	−71.78	56.63	10.66	31.69	1.76	1.06	0.00	0.29
2-butene	56.11	0.00	0.01	0.00	297.76	−66.51	46.96	9.64	30.98	1.49	0.67	0.00	2.31
2-butyne	54.09	0.00	0.00	0.00	286.03	−60.33	44.18	10.34	30.95	1.25	0.50	0.00	1.46
2-chloro-1,1′-biphenyl	188.66	0.24	0.62	0.81	984.14	−153.98	121.47	8.95	110.88	4.55	3.25	1.56	4.54
2-chloro-1-ethylbenzene	140.61	0.46	0.53	0.84	719.69	−1144.93	87.02	9.28	70.55	3.45	2.35	1.05	2.95
2-chloro-2-methyl-butane	106.60	1.15	0.52	1.66	533.91	−88.36	63.70	10.36	43.58	2.63	3.09	0.00	2.52
2-chlorophenol	128.56	0.44	0.26	0.67	763.24	−85.19	73.37	9.21	59.63	2.62	1.86	0.59	2.15
2-chloropropane	78.54	1.16	0.51	1.66	385.68	−55.01	39.41	10.42	29.82	1.81	1.88	0.00	1.90
2-ethyl pyridine	107.16	0.38	1.39	1.67	596.77	−107.58	85.86	9.76	59.75	2.83	1.67	0.61	1.69
2-ethylnaphthalene	156.23	0.40	0.04	0.39	839.26	−161.68	124.34	8.75	100.87	4.38	3.04	1.46	4.38
2-ethylphenol	122.17	0.99	0.65	1.64	761.88	−119.35	96.38	8.99	66.91	3.11	1.98	0.81	2.47
2-ethylthiophene	112.19	1.10	1.67	0.76	531.79	−91.22	65.85	9.44	58.30	3.33	2.46	1.17	2.87
2-fluoro-3-bromotetrachlorocyclohexane	318.83	0.98	0.57	0.49	1627.22	−92.39	79.01	10.71	86.02	5.97	5.73	3.42	3.28
2-fluorochlorobenzene	130.55	1.56	0.63	2.04	887.61	−79.00	67.63	9.51	56.66	2.58	1.82	0.57	2.77
2-fluorophenol	112.10	1.28	0.58	0.94	929.44	−85.39	77.16	9.40	52.17	2.24	1.45	0.45	1.71
2-heptanone	114.19	2.16	0.51	2.66	711.13	−121.77	92.90	10.68	52.80	3.26	2.16	0.62	1.98
2-heptene	98.19	0.02	0.02	0.04	520.03	−116.48	83.27	9.70	53.55	3.03	1.71	0.49	3.56
2-hexanol	102.18	0.98	0.68	1.52	648.03	−111.40	84.96	11.00	46.34	2.95	1.99	0.50	1.76
2-hexanone	100.16	2.20	0.48	2.66	636.93	−105.10	80.80	10.68	45.76	2.76	1.81	0.43	1.38
2-iodophenol	220.01	0.47	0.69	0.68	818.82	−84.35	71.50	9.04	67.68	3.30	2.59	0.83	2.65
2-methoxynitrobenzene (2-nitroanisole)	153.14	5.03	0.80	5.83	1172.17	−118.45	105.82	9.94	74.08	2.99	1.90	0.76	1.73
2-methyl-1,3-butadiene	68.12	0.20	0.02	0.19	365.16	−76.61	54.90	9.36	39.36	1.55	1.05	0.00	2.42
2-methyl-1-pentene	84.16	0.33	0.06	0.37	445.54	−99.86	71.29	9.79	44.55	2.41	1.71	0.43	3.21
2-methyl-2-butene	70.13	0.19	0.05	0.22	370.23	−83.27	59.47	9.40	39.03	1.87	1.37	0.00	2.67
2-methyl-2-nitropropane	103.12	3.73	0.53	4.25	797.27	−88.59	73.69	11.81	40.96	2.00	2.28	0.00	1.01
2-methylbutane (isopentane)	72.15	0.06	0.03	0.04	378.59	−89.66	63.09	11.43	35.73	2.27	1.80	0.00	2.72
2-methyl-hexane	100.20	0.05	0.03	0.04	526.85	−122.99	87.29	11.18	49.86	3.27	2.54	0.61	3.71
2-methylnaphthalene	142.20	0.30	0.02	0.31	765.12	−145.03	112.23	8.76	93.38	3.82	2.85	1.31	3.86
2-methyl-pentane	86.18	0.06	0.05	0.02	452.44	−106.36	75.22	11.31	42.70	2.77	2.18	0.58	2.34
2-methylpyridine	93.13	0.48	1.34	1.75	523.14	−90.90	73.71	9.80	52.34	2.27	1.47	0.45	1.11
2-nitropropane	89.09	3.64	0.53	4.16	723.98	−71.92	61.60	11.92	34.20	1.74	1.32	0.00	0.93
2-nitrotoluene	137.14	4.37	0.63	5.00	989.28	−112.70	94.66	10.24	68.72	2.88	2.01	0.75	2.30
2-nonanone	142.24	2.15	0.48	2.62	859.44	−155.09	117.09	10.68	66.94	4.26	2.87	0.98	3.18
2-octanone	128.21	2.19	0.46	2.63	785.24	−138.43	104.98	10.68	59.90	3.76	2.51	0.80	2.76
2-pentanol	88.15	1.02	0.66	1.53	573.86	−94.74	72.87	11.00	39.28	2.45	1.64	0.42	1.19
2-pentanone	86.13	2.19	0.50	2.68	562.84	−88.44	68.69	10.67	38.71	2.26	1.45	0.35	0.91
2-pentene	70.13	0.04	0.02	0.04	371.86	−83.18	59.05	9.60	38.37	2.03	0.98	0.24	2.58
2-phenyl-1-ethanol	122.17	0.72	0.59	1.26	763.51	−119.15	95.54	9.46	65.10	3.08	1.96	0.77	1.36
2-phenylthiophene	160.23	1.10	1.70	0.63	796.00	−132.25	100.39	8.95	99.84	4.43	3.29	1.78	3.74
2-propanol	60.10	0.98	0.66	1.52	425.16	−61.48	48.72	11.04	25.03	1.41	1.09	0.00	0.05
2-propanone	58.08	2.33	0.46	2.78	415.03	−55.10	44.46	10.77	24.53	1.20	0.91	0.00	-0.24
2-pyrimidone	96.09	3.73	1.70	5.28	670.24	−74.30	73.06	9.41	49.93	1.89	1.09	0.31	-1.62
3,3,3-trifluoropropylbenzene	174.17	2.28	0.19	2.46	1606.76	−128.21	112.03	9.74	69.47	3.68	2.60	0.93	3.31
3,3′,4,4′-tetrachloro-1,1′-biphenyl	291.99	0.01	0.01	0.00	1430.61	−151.52	126.15	8.96	149.44	5.99	4.88	1.95	6.04

Table 1 (Continued)

compound	MW[a]	D_P[b] [debye]	D_H[c] [debye]	D_S[d] [debye]	E2[e] [EV]	EX[f] [ev]	ELC[g] [ev]	IP[h] [kcal]	PO[i] [au]	VMC_1[j]	VMC_2[k]	VMC_4[l]	logK_{ow}
3,3′,5,5′-tetrachloro-1,1′-biphenyl	291.99	0.02	0.02	0.00	1432.88	−151.40	126.02	9.36	145.45	5.98	5.06	2.49	6.85
3,3-dimethyl-2-butanol	102.18	0.87	0.68	1.46	647.12	−111.41	85.09	10.94	45.54	2.62	3.04	0.00	1.48
3,4-dichloro-1,1-biphenyl	223.10	0.62	0.96	1.57	1132.63	−153.21	123.04	8.92	124.94	5.03	3.81	1.60	5.51
3,4-dimethylchlorobenzene	140.61	0.93	0.54	1.45	718.15	−113.22	87.41	9.13	72.53	3.30	2.66	0.93	3.82
3,4-dimethylphenol	122.17	0.99	0.68	1.47	759.17	−119.63	96.79	8.87	67.93	2.96	2.27	0.73	2.23
3,5-dichloro-1,1′-biphenyl	223.10	0.70	0.51	1.21	1133.85	−153.14	122.95	9.16	123.54	5.03	3.90	1.88	5.37
3,5-dimethylphenol	122.17	0.73	0.70	1.24	759.30	−119.68	96.75	9.04	67.63	2.96	2.35	0.95	2.35
3-bromophenol	173.01	0.58	0.62	0.47	861.49	−84.59	71.75	9.41	63.16	3.03	2.39	0.86	2.63
3-chlorophenol	128.56	0.78	1.20	1.94	763.79	−85.22	73.40	9.28	60.70	2.61	1.92	0.66	2.52
3-ethylpentane	100.20	0.05	0.01	0.05	527.31	−122.85	87.19	11.00	50.12	3.35	2.09	0.87	2.40
3-ethylthiophene	112.19	0.68	1.65	1.00	532.25	−91.29	65.79	9.27	57.91	3.38	2.26	1.24	2.82
3-fluorophenol	112.10	0.98	0.62	0.71	930.66	−85.36	76.81	9.43	52.14	2.23	1.48	0.48	1.93
3-hexanol	102.18	1.02	0.67	1.60	647.94	−111.39	84.94	10.92	46.26	2.99	1.85	0.54	1.65
3-iodophenol	220.01	0.29	0.71	0.52	819.73	−84.35	71.49	9.05	68.89	3.29	2.71	0.99	2.93
3-methyl-1-butanol	88.15	0.95	0.60	1.44	572.44	−94.80	73.17	10.78	39.14	2.38	1.91	0.26	1.16
3-methyl-1-butene	70.13	0.18	0.04	0.16	372.15	−83.15	58.87	10.27	37.08	1.90	1.48	0.00	2.59
3-methyl-2-butanol	88.15	0.91	0.68	1.48	573.38	−94.76	72.89	11.01	39.03	2.32	1.98	0.00	1.28
3-methyl-2-butanone	86.13	2.18	0.43	2.60	561.98	−88.49	68.79	10.56	38.25	2.15	1.77	0.00	0.84
3-methylpentane	86.18	0.07	0.01	0.07	453.03	−106.28	75.21	11.44	42.74	2.81	1.92	0.29	3.60
3-methylpyridine	93.13	0.81	1.29	2.07	522.89	−90.89	73.87	9.80	52.21	2.26	1.53	0.45	1.20
3-methylthiophene	98.16	0.71	1.66	0.95	458.10	−74.63	53.67	9.31	50.77	2.82	2.08	1.00	2.34
3-nitrotoluene	137.14	4.97	0.49	5.46	987.54	−112.86	94.82	10.28	68.60	2.87	2.07	0.72	2.45
3-pentanol	88.15	1.04	0.68	1.61	573.66	−94.73	72.87	10.92	39.19	2.49	1.47	0.29	1.21
3-phenyl-1-chloropropane	154.64	0.87	0.55	1.41	798.40	−129.32	98.21	9.54	76.75	4.06	2.66	1.05	3.55
4,4′-dichloro-1,1′-biphenyl	223.10	0.01	0.00	0.01	1133.99	−153.14	123.02	8.85	128.40	5.03	3.88	1.54	5.58
4-bromophenol	173.01	0.95	0.71	1.52	861.29	−84.57	71.68	9.31	63.15	3.03	2.39	0.70	2.43
4-bromotoluene	171.04	1.41	0.09	1.49	743.31	−95.83	73.28	9.55	66.60	3.30	2.71	0.80	3.33
4-chloro-1,1′-biphenyl	188.66	0.54	0.52	1.06	984.18	−154.03	121.48	8.87	114.81	4.55	3.31	1.40	4.61
4-chlorophenol	128.56	0.49	0.93	1.39	763.66	−85.19	73.36	9.01	60.76	2.61	1.91	0.57	2.35
4-cyclopropyl-2-butanone	112.17	2.16	0.49	2.64	706.29	−115.16	90.49	10.67	52.21	3.28	2.68	1.31	1.50
4-ethenylcyclohexene	108.18	0.19	0.06	0.14	579.49	−120.33	88.72	9.59	59.27	3.21	2.28	1.03	3.34
4-ethylphenyl acetate	164.20	1.46	0.18	1.63	1090.27	−151.66	126.80	9.08	87.24	3.99	2.59	0.96	2.56
4-fluorophenol	112.10	1.33	0.71	1.84	930.15	−85.37	77.02	9.27	52.46	2.23	1.48	0.44	1.79
4-iodophenol	220.01	0.70	0.68	1.28	819.60	−84.34	71.41	8.84	68.86	3.29	2.70	0.79	2.91
4-methylpyridine	93.13	0.97	1.31	2.27	523.35	−90.87	73.87	10.06	51.97	2.26	1.52	0.43	1.20
4-methyl-1-pentene	84.16	0.27	0.05	0.25	446.89	−99.77	70.91	10.02	44.26	2.38	1.92	0.33	3.08
4-methyl-2-pentanone	100.16	2.11	0.52	2.62	636.88	−105.09	80.77	10.65	45.28	2.62	2.30	0.57	1.31
4-methylphenol	108.14	0.68	0.68	1.18	686.14	−102.90	84.36	8.95	59.63	2.54	1.84	0.54	1.94
4-*n*-propylphenol	136.19	0.78	0.64	1.23	834.43	−136.20	108.53	8.93	74.57	3.61	2.42	0.95	3.23
4-phenylbutyric acid	164.20	2.04	0.43	1.77	1100.35	−151.46	125.86	9.52	81.94	4.05	2.73	1.09	2.42
4-phenylphenol	170.21	0.46	0.69	1.11	1025.01	−160.47	130.89	8.64	109.40	4.21	2.91	1.28	3.20
4-pyrimidone	96.09	2.62	1.00	1.97	672.26	−74.15	72.92	9.56	49.49	1.88	1.10	0.30	-1.38
5-methyl-2-hexanone	114.19	2.21	0.47	2.67	711.10	−121.75	92.89	10.66	52.52	3.12	2.63	0.49	1.88
5-methyl-furfural(5-methylfuraldehyde)	110.11	2.70	0.42	3.08	793.52	−91.62	81.66	9.46	55.79	2.34	1.57	0.52	1.85
5-nonanone	142.24	2.05	0.49	2.54	858.82	−155.11	117.14	10.58	67.15	4.33	2.75	0.87	2.88
5-phenyl-2-pentanone	162.23	2.18	0.54	2.72	976.45	−162.72	127.39	9.45	85.90	4.32	3.04	1.19	2.42
9-fluorenone	180.21	2.39	0.46	2.85	1076.76	−164.53	135.51	9.22	113.17	4.61	3.42	1.98	3.58
9-methylanthracene	192.26	0.36	0.04	0.32	1035.21	−192.53	150.89	8.14	140.21	5.23	3.94	2.24	5.07
a,a,a-trichlorotoluene	195.48	1.27	0.57	1.84	949.79	−93.79	75.66	10.07	81.14	3.86	4.14	1.00	2.92
a,a,a-trifluorotoluene	146.11	2.87	0.24	3.11	1456.81	−94.96	87.53	10.34	54.18	2.73	1.86	0.63	2.79
a-bromotoluene	171.04	1.33	0.22	1.54	749.71	−95.52	72.56	9.73	64.88	3.65	2.18	0.94	2.92
acenaphthene	154.21	0.59	0.03	0.56	828.99	−155.50	122.02	8.59	98.45	4.45	3.43	2.19	3.92
acenaphthylene	152.20	0.22	0.07	0.30	821.33	−148.85	117.78	9.06	101.78	4.15	3.13	1.86	4.03
acetic acid	60.05	2.16	0.41	1.83	538.69	−43.86	42.98	11.44	20.52	0.93	0.52	0.00	-0.17
acetonitrile	41.05	2.29	0.91	3.21	239.64	−37.08	31.24	12.33	18.63	0.72	0.22	0.00	-0.34
acetophenone	120.15	2.36	0.44	2.79	753.10	−112.72	90.68	10.00	65.37	2.86	1.92	0.67	1.58
a-chlorotoluene	126.59	0.75	0.59	1.33	649.27	−96.02	73.97	9.66	61.49	3.06	1.89	0.74	2.30
acrylophenone	132.16	2.07	0.43	2.50	819.89	−122.77	98.28	9.96	75.98	3.06	1.93	0.72	1.88
allyl alcohol (2-propen-1-ol)	58.08	0.88	0.64	1.48	418.24	−54.92	44.63	10.07	26.12	1.13	0.47	0.00	-0.31
allyl bromide (3-bromo-1-propene)	120.98	1.52	0.18	1.69	479.66	−47.92	33.68	10.49	34.19	2.20	1.09	0.00	1.79
allylbenzene (2-propenyl)	118.18	0.09	0.06	0.15	638.20	−124.02	93.28	9.39	71.47	3.08	1.98	0.78	3.27
amylamine (pentyl)	87.16	0.19	1.44	1.32	480.21	−100.21	76.22	9.38	41.65	2.47	1.97	0.33	1.45
aniline	93.13	0.62	1.17	1.30	522.68	−91.57	74.83	8.61	55.86	2.20	1.41	0.45	0.90
anthracene	178.23	0.00	0.00	0.00	962.20	−175.83	138.45	8.25	131.41	4.81	3.55	1.88	4.54
benz[*a*]anthracene	228.29	0.04	0.02	0.02	1232.08	−223.51	177.31	8.33	173.21	6.22	4.71	2.70	5.61
benzaldehyde	106.12	2.27	0.42	2.69	677.51	−96.02	78.71	10.05	58.35	2.44	1.53	0.53	1.48
benzene	78.11	0.00	0.00	0.00	422.94	−80.55	60.89	9.75	45.60	2.00	1.15	0.38	2.13
benzoic acid	122.12	2.62	0.40	2.25	876.60	−101.54	89.18	10.13	61.38	2.59	1.67	0.58	1.81
benzoic acid methyl ester	136.15	2.12	0.06	2.08	943.00	−118.24	101.73	10.08	70.27	2.98	1.86	0.69	2.12
benzonitrile	103.12	2.75	0.86	3.61	577.42	−94.87	77.76	10.09	61.85	2.38	1.48	0.51	1.56
benzothiophene	134.20	0.57	1.63	1.09	653.98	−105.37	80.38	8.80	78.83	3.77	2.90	1.69	3.12
benzyl acetate	150.18	1.88	0.08	1.85	1018.71	−134.85	113.80	9.58	77.08	3.46	2.27	0.76	1.96
benzylamine	107.16	0.24	1.44	1.39	596.80	−107.94	86.63	9.29	60.22	2.67	1.69	0.61	1.09
benzylphenyl ether	184.24	0.50	0.41	0.92	1094.99	−177.04	142.60	9.13	110.20	4.67	3.09	1.26	3.79
beta-phenylethyl chloride (2-)	140.61	0.87	0.49	1.35	724.10	−112.65	86.03	9.62	70.24	3.56	2.30	0.97	2.95

Table 1 (Continued)

compound	MW[a]	D_P[b] [debye]	D_H[c] [debye]	D_S[d] [debye]	E2[e] [EV]	EX[f] [ev]	ELC[g] [ev]	IP[h] [kcal]	PO[i] [au]	VMC_1[j]	VMC_2[k]	VMC_4[l]	logK_{ow}
biphenyl	154.21	0.00	0.00	0.00	834.28	−154.92	119.94	8.92	102.00	4.07	2.73	1.26	4.09
bromobenzene	157.01	1.09	0.09	1.18	670.63	−79.03	60.77	9.80	57.59	2.89	2.21	0.72	2.99
bromochloromethane	129.38	1.21	0.62	1.51	487.57	−20.12	14.93	10.56	26.20	2.19	1.57	0.00	1.41
bromocyclohexane	163.06	2.01	0.06	2.05	701.50	−98.24	71.94	10.86	54.27	3.95	3.53	1.70	3.20
bromoethane	108.97	1.71	0.14	1.85	412.50	−37.82	25.94	10.91	25.99	2.09	1.39	0.00	1.61
bromomethane	94.94	1.36	0.19	1.55	336.32	−21.19	13.72	11.01	17.07	1.96	0.00	0.00	1.19
bromotrifluoromethane	148.91	0.87	0.03	0.90	1285.01	−19.25	29.58	12.23	20.17	1.55	1.33	0.00	1.86
butanol	74.12	0.92	0.62	1.42	498.13	−78.18	61.03	10.89	32.28	2.02	1.08	0.16	0.88
butylamine	73.14	0.19	1.45	1.34	405.93	−83.60	64.18	9.38	34.76	2.12	1.14	0.20	0.81
butyl benzene	134.22	0.36	0.04	0.34	717.90	−147.33	109.69	9.41	76.07	3.97	2.59	1.03	4.26
butyl ethyl ether	102.18	0.75	0.37	1.12	640.19	−111.48	85.25	10.48	47.83	2.99	1.55	0.39	2.03
butyldimethylamine	101.19	0.16	1.20	1.10	554.27	−116.65	87.75	9.06	50.01	2.92	2.16	0.47	1.70
butylmethylamine	87.16	0.18	1.32	1.21	480.41	−100.17	76.12	9.19	42.51	2.56	1.46	0.35	1.33
butyraldehyde	72.11	2.21	0.35	2.54	488.07	−71.68	56.55	10.62	31.72	1.85	0.96	0.12	0.88
butyric acid	88.11	2.16	0.46	1.81	686.86	−77.16	67.11	11.36	34.78	1.99	1.14	0.21	0.79
butyronitrile	69.11	2.44	0.87	3.30	387.92	−70.40	55.34	11.89	33.12	1.78	0.91	0.11	0.53
chlorobenzene	112.56	0.39	0.54	0.93	572.87	−79.66	62.43	9.38	55.14	2.48	1.73	0.56	2.84
chlorodifluoromethane	86.47	1.26	0.43	1.52	874.14	−20.02	25.07	11.36	17.11	1.09	0.58	0.00	1.08
chloroethane	64.51	1.02	0.53	1.55	310.94	−38.34	27.35	10.41	22.24	1.51	0.80	0.00	1.43
chloromethane	50.49	0.81	0.57	1.38	235.97	−21.72	15.34	10.48	14.02	1.13	0.00	0.00	0.91
chlorotrifluoromethane	104.46	1.32	0.27	1.04	1189.55	−19.49	30.28	11.88	17.01	1.13	0.86	0.00	1.65
cis-1−2-dimethylcyclohexane	112.21	0.00	0.01	0.01	591.74	−133.40	96.93	10.96	55.26	3.80	3.24	1.50	4.01
crotonic acid (2-butenoic acid)	86.09	2.54	0.40	2.16	679.73	−70.66	62.79	10.61	37.99	1.63	0.84	0.14	0.72
cycloheptane	98.19	0.06	0.05	0.02	517.72	−116.69	84.78	11.03	48.56	3.50	2.47	1.24	4.00
cycloheptene	96.17	0.26	0.05	0.21	511.25	−110.20	80.77	9.76	49.67	3.15	2.11	0.94	3.45
cyclohexane	84.16	0.00	0.00	0.00	444.05	−100.10	72.66	11.29	41.86	3.00	2.12	1.06	3.44
cyclohexanol	100.16	1.02	0.67	1.50	639.06	−105.19	82.44	10.89	45.08	3.07	2.29	1.08	1.23
cyclohexanone	98.14	2.46	0.37	2.81	628.36	−98.83	78.24	10.48	44.80	2.91	2.10	0.95	0.81
cyclohexene	82.15	0.16	0.01	0.17	436.51	−93.60	68.95	9.52	43.64	2.65	1.76	0.76	2.86
cyclooctane	112.21	0.00	0.01	0.00	592.36	−133.26	96.75	11.06	55.09	4.00	2.83	1.41	4.45
cyclopentane	70.13	0.03	0.02	0.01	369.99	−83.45	60.35	11.09	33.86	2.50	1.77	0.88	3.00
cyclopentanone	84.12	2.39	0.32	2.71	554.83	−82.18	66.03	10.60	37.02	2.41	1.75	0.77	0.63
cyclopentene	68.12	0.16	0.01	0.15	364.25	−76.79	56.15	9.52	35.87	2.15	1.40	0.59	2.47
cyclopropane	42.08	0.00	0.00	0.00	226.29	−49.72	36.35	11.77	20.85	1.50	1.06	0.53	1.72
decachlorobiphenyl	498.66	0.05	0.00	0.05	2314.97	−146.63	134.64	8.89	220.38	8.91	7.66	4.30	7.92
decanoic acid	172.27	2.16	0.48	1.79	1131.74	−177.16	139.71	11.35	77.18	4.99	3.27	1.23	4.09
di(*n*-propyl) ether	102.18	0.70	0.41	1.11	640.17	−111.48	85.27	10.48	47.83	2.99	1.61	0.39	2.03
diallylamine	97.16	0.29	1.31	1.10	543.23	−103.67	79.62	9.28	53.48	2.34	1.24	0.29	1.11
dibromomethane	173.84	1.13	0.32	1.45	584.96	−19.60	13.17	10.59	27.97	2.77	2.72	0.00	1.57
dichlorodifluoromethane	120.91	1.18	0.39	0.80	1020.93	−18.89	25.59	11.33	26.94	1.51	1.57	0.00	2.16
dichlorofluoromethane	102.92	0.98	0.56	1.25	705.44	−19.60	20.78	10.99	25.13	1.53	1.23	0.00	1.55
dichloromomethane	84.93	0.68	0.68	1.36	388.12	−20.50	16.11	10.58	22.36	1.60	0.91	0.00	1.25
diethyl sulfide	90.18	0.37	1.57	1.94	408.85	−76.44	52.60	8.86	43.08	3.14	2.34	0.61	1.95
diethylamine	73.14	0.18	1.31	1.18	406.28	−83.49	63.88	9.15	35.68	2.12	0.96	0.25	0.57
diethyl ether	74.12	0.78	0.37	1.15	491.95	−78.15	61.09	10.48	33.58	1.99	0.78	0.20	0.89
difluoromethane	52.02	1.46	0.36	1.81	724.24	−21.30	24.80	12.86	8.19	0.53	0.10	0.00	0.20
dimethyl ether	46.07	0.85	0.40	1.26	343.01	−44.89	37.52	10.69	18.64	0.82	0.41	0.00	0.10
dimethyl sulfide	62.13	0.36	1.60	1.96	261.81	−43.13	28.15	8.88	26.75	2.44	1.22	0.00	0.92
dimethyl sulfoxide	78.13	4.89	2.11	4.49	468.70	−48.47	28.10	9.35	35.55	2.09	1.58	0.00	-1.35
di-*n*-butylamine	129.25	0.22	1.34	1.15	702.87	−150.15	112.27	9.19	64.01	4.12	2.46	0.73	2.68
di-*n*-propyl-amine	101.19	0.21	1.35	1.16	554.58	−116.81	88.03	9.18	49.82	3.12	1.75	0.48	1.73
di-*n*-propyl-amine	101.19	0.21	1.35	1.16	554.58	−116.81	88.03	9.18	49.82	3.12	1.75	0.48	1.67
diphenylacetic acid	212.25	2.17	0.58	1.67	1363.07	−192.52	160.33	9.55	124.17	5.12	3.59	1.77	3.05
diphenylmethane	168.24	0.18	0.02	0.17	908.69	−171.66	132.00	9.42	102.60	4.98	3.54	1.68	4.14
diphenylsulfide	186.27	1.01	1.76	0.75	935.91	−158.63	121.52	7.91	129.00	5.04	3.87	1.97	4.41
ethane	30.07	0.00	0.00	0.00	155.85	−39.70	26.79	11.98	14.95	1.00	0.00	0.00	1.87
ethanol	46.07	0.93	0.62	1.45	349.87	−44.85	36.86	10.90	18.20	1.02	0.32	0.00	0.10
ethene	28.05	0.00	0.00	0.00	150.98	−33.05	22.31	10.64	15.01	0.50	0.00	0.00	1.13
ethoxybenzene	122.17	0.79	0.36	1.12	756.42	−119.36	96.02	9.07	67.95	3.11	1.75	0.68	2.51
ethyl acetate	88.11	1.90	0.05	1.92	680.12	−77.18	67.27	11.25	36.43	1.90	0.92	0.20	0.73
ethyl benzene	106.17	0.35	0.03	0.33	569.59	−114.00	85.50	9.40	61.53	2.97	1.84	0.71	3.15
ethyl benzoate	150.18	2.09	0.04	2.09	1017.96	−134.86	113.44	10.06	78.21	3.56	2.09	0.79	2.63
ethyl mercaptan	61.12	1.17	1.16	2.33	256.26	−38.10	26.51	11.21	24.64	1.65	0.95	0.00	1.21
ethyl propionate (C5H10O2)	102.13	1.81	0.11	1.83	753.89	−93.83	79.35	11.15	43.77	2.46	1.16	0.26	1.21
ethylallylamine	85.15	0.29	1.29	1.22	474.85	−93.57	71.70	9.18	44.22	2.23	1.10	0.25	0.81
ethyldiisopropylamine	129.25	0.19	1.19	1.04	703.67	−149.72	111.07	8.96	64.18	3.85	3.02	1.33	2.68
ethyldimethylamine	73.14	0.14	1.20	1.12	405.97	−83.32	63.58	9.05	35.79	1.92	1.40	0.00	0.70
ethylene oxide (oxirane)	44.05	1.88	0.10	1.78	338.59	−37.99	33.65	11.34	17.18	1.08	0.61	0.22	-0.30
ethylvinyl ether	72.11	1.27	0.36	1.60	485.82	−71.77	57.27	9.46	36.12	1.64	0.62	0.12	1.04
ethynylbenzene	102.14	0.34	0.17	0.17	554.38	−101.18	77.67	9.39	66.19	2.45	1.51	0.53	2.53
fluorene	166.22	0.36	0.01	0.37	896.37	−165.66	130.28	8.84	108.81	4.61	3.49	2.08	4.18
fluorobenzene	96.10	1.49	0.11	1.60	739.66	−79.81	65.97	9.80	46.96	2.10	1.30	0.41	2.27
fluoromethane	34.03	1.14	0.30	1.44	402.89	−22.13	19.84	12.92	7.92	0.38	0.00	0.00	0.51
fluoropentachlorocyclohexane	274.38	0.85	0.31	0.55	1527.97	−92.82	80.37	10.37	78.31	5.49	5.18	2.88	3.19
formaldehyde	30.03	1.83	0.34	2.16	262.53	−21.73	20.53	10.63	9.92	0.29	0.00	0.00	0.35

Table 1 (Continued)

compound	MW[a]	D_P[b] [debye]	D_H[c] [debye]	D_S[d] [debye]	E2[e] [EV]	EX[f] [ev]	ELC[g] [ev]	IP[h] [kcal]	PO[i] [au]	VMC_1[j]	VMC_2[k]	VMC_4[l]	logK_{ow}
formic acid	46.03	3.02	0.91	3.94	460.17	−27.35	31.55	11.29	13.66	0.49	0.11	0.00	-0.54
furan	68.08	0.07	0.15	0.22	468.69	−59.25	51.36	9.38	32.09	1.47	0.79	0.23	1.34
hexachlorobenzene	284.78	0.00	0.00	0.00	1312.02	−75.76	70.32	9.31	108.70	4.90	4.15	2.00	5.23
hexachlorocyclopentadiene	272.77	0.74	0.05	0.78	1248.22	−65.12	60.78	9.04	97.73	4.65	4.66	2.13	5.04
hexafluorobenzene	186.06	0.00	0.00	0.00	2298.86	−77.08	93.50	10.85	54.96	2.63	1.88	0.58	2.22
hexafluroethane	138.01	0.01	0.00	0.01	2064.12	−35.43	57.55	14.47	16.67	1.38	1.00	0.00	2.00
hexamethylbenzene	162.27	0.01	0.00	0.01	859.01	−181.00	135.63	8.87	96.21	4.50	3.75	1.69	4.31
hexanal	100.16	2.26	0.34	2.58	636.30	−105.01	80.74	10.63	45.94	2.85	1.66	0.48	1.78
hexane	86.18	0.00	0.00	0.00	452.51	−106.37	75.19	11.28	43.01	2.91	1.71	0.50	4.11
hexanenitrile	97.16	2.51	0.85	3.35	536.18	−103.72	79.51	11.70	47.36	2.78	1.62	0.45	1.66
hexanoic acid	116.16	2.15	0.47	1.80	835.15	−110.50	91.35	11.36	48.86	2.99	1.85	0.53	1.88
hydroquinone	110.11	0.86	1.36	2.22	804.33	−91.63	82.88	8.76	56.33	2.27	1.52	0.45	0.59
indane	118.18	0.47	0.02	0.45	633.52	−124.56	95.34	9.22	67.86	3.53	2.62	1.51	3.23
indene	116.16	0.51	0.02	0.52	627.56	−117.85	91.09	8.97	71.47	3.21	2.31	1.20	2.92
iodobenzene	204.01	0.82	0.03	0.79	628.92	−78.79	60.51	9.04	63.21	3.16	2.52	0.82	3.25
iodoethane	155.97	1.77	0.06	1.83	369.10	−37.65	25.98	9.44	29.61	2.47	1.77	0.00	2.00
iodomethane	141.94	1.32	0.12	1.44	293.26	−21.02	13.66	9.47	19.95	2.50	0.00	0.00	1.51
isobutane	58.12	0.05	0.04	0.01	304.03	−73.06	51.03	11.59	28.61	1.73	1.73	0.00	2.76
isobutanol	74.12	0.82	0.65	1.39	497.82	−78.19	61.06	10.92	31.98	1.88	1.58	0.00	0.65
isobutyl acetate	116.16	1.96	0.06	1.94	828.00	−110.52	91.46	11.24	50.42	2.76	2.20	0.28	1.78
isobutylamine	73.14	0.24	1.53	1.36	406.50	−83.58	64.06	9.43	34.54	2.03	1.39	0.00	0.88
isobutyronitrile	69.11	2.43	0.86	3.29	387.78	−70.43	55.31	12.07	32.70	1.67	1.28	0.00	0.46
isopentanol	88.15	0.94	0.60	1.44	572.39	−94.80	73.15	10.80	39.14	2.38	1.91	0.26	1.42
isopropylamine	59.11	0.20	1.43	1.32	331.70	−66.94	51.97	9.38	27.54	1.49	1.24	0.00	-0.03
isopropylbenzene	120.19	0.23	0.04	0.21	643.18	−130.70	97.60	9.53	67.96	3.35	2.57	0.84	3.66
m-chlorotoluene	126.59	0.63	0.52	1.12	645.62	−96.45	74.92	9.32	63.78	2.89	2.23	0.85	3.42
m-cresol (3-hydroxytoluene)	108.14	0.49	0.69	0.96	686.62	−102.88	84.31	9.11	59.21	2.54	1.84	0.63	1.96
methanol	32.04	0.93	0.62	1.49	275.22	−28.21	25.06	11.14	10.94	0.45	0.00	0.00	-0.66
methoxybenzene(anisole)	108.14	0.72	0.37	1.08	681.78	−102.73	84.25	9.11	59.74	2.52	1.52	0.56	2.11
methycyclopentane	84.16	0.03	0.02	0.04	443.91	−100.13	72.50	11.11	40.70	2.89	2.39	1.13	3.37
methyl acetate	74.08	1.84	0.07	1.83	605.17	−60.55	55.49	11.27	28.71	1.32	0.70	0.00	0.18
methylamine	31.06	0.08	1.45	1.40	183.41	−33.62	28.06	9.40	13.55	0.58	0.00	0.00	-0.57
methyl butyl ether	88.15	0.80	0.39	1.18	565.72	−94.85	73.49	10.58	40.32	2.40	1.35	0.29	1.66
methyl mercaptan	47.10	1.00	1.24	2.23	182.06	−21.46	14.37	11.26	18.55	1.34	0.00	0.00	0.78
methyl propanoate	88.11	1.78	0.12	1.76	678.96	−77.22	67.61	11.17	36.00	1.88	0.93	0.14	1.96
methyl propyl ether	60.10	0.82	0.39	1.21	417.48	−61.52	49.30	10.57	26.13	1.40	0.58	0.00	1.21
methylbenzylamine	107.16	0.72	1.07	1.27	597.34	−108.09	86.71	8.55	64.05	2.66	1.62	0.60	1.52
methylcyclohexane	98.19	0.00	0.02	0.02	517.80	−116.77	84.84	11.06	48.58	3.39	2.74	1.31	3.61
methylethylamine	59.11	0.15	1.32	1.23	332.12	−-66.85	51.98	9.18	28.38	1.56	0.71	0.00	0.15
methylthiobenzene	124.20	0.35	1.62	1.63	598.71	−100.95	74.88	8.56	69.94	3.74	2.39	0.98	2.74
m-methyl styrene	118.18	0.24	0.03	0.25	635.87	−124.19	93.67	9.07	74.90	3.02	2.12	0.80	3.44
m-methylbenzyl alcohol	122.17	0.53	0.66	1.18	761.28	−119.32	95.92	9.29	66.21	2.99	2.15	0.81	1.60
m-phenylphenol	170.21	0.48	0.68	1.05	1025.37	−160.44	130.76	8.91	107.38	4.21	2.92	1.32	3.23
m-xylene	106.17	0.25	0.02	0.26	567.94	−114.16	85.90	9.31	62.57	2.82	2.16	0.81	3.13
naphthalene	128.17	0.00	0.00	0.00	692.59	−128.23	99.73	8.84	83.80	3.40	2.35	1.13	3.35
n-benzylaniline	183.25	0.71	1.04	1.23	1010.58	−182.35	145.36	8.55	115.05	4.78	3.21	1.36	3.13
n-butane	58.12	0.00	0.00	0.00	304.20	−73.04	50.99	11.35	28.95	1.91	1.00	0.00	2.89
n-ethylaniline	121.18	0.81	1.08	1.27	671.75	−124.70	98.64	8.54	72.04	3.22	1.90	0.76	2.16
n-heptylamine	115.22	0.21	1.47	1.33	628.33	−133.58	100.38	9.40	55.97	3.62	2.20	0.75	2.57
n-hexylamine	101.19	0.21	1.45	1.33	554.23	−116.92	88.31	9.39	48.88	3.12	1.85	0.57	2.06
nitrobenzene	123.11	4.76	0.48	5.24	914.88	−96.06	82.30	10.60	59.94	2.46	1.56	0.54	1.85
nitroethane	75.07	3.53	0.55	4.06	650.39	−55.25	49.48	12.08	27.19	1.35	0.61	0.00	0.18
nitromethane	61.04	3.40	0.59	3.99	577.26	−38.57	37.24	12.17	19.98	0.76	0.42	0.00	0.08
N-methylaniline	107.16	0.73	1.06	1.28	597.38	−108.11	86.79	8.55	64.04	2.66	1.62	0.60	1.82
N-methy-*N*-benzylaniline	183.25	0.43	0.85	0.83	1010.53	−182.34	144.83	8.34	117.68	4.72	3.23	1.45	4.22
N,*N*-dimethyl acetamide	87.12	2.81	0.81	3.18	591.97	−82.51	69.79	9.50	39.89	1.82	1.41	0.00	-0.77
N,*N*-dimethylaniline	121.18	0.76	0.94	1.21	671.61	−124.53	98.32	8.44	72.30	3.03	2.23	0.73	2.31
n-propylamine	59.11	0.19	1.46	1.34	331.79	−66.94	52.09	9.39	27.71	1.62	0.79	0.00	0.48
n-propylaniline	135.21	0.84	1.09	1.26	745.87	−141.37	110.73	8.53	79.45	3.72	2.29	0.83	2.45
n-propylbenzene	120.19	0.35	0.06	0.34	643.75	−130.66	97.59	9.40	68.88	3.47	2.24	0.93	3.68
n-propylpropionate	116.16	1.83	0.10	1.83	827.88	−110.51	91.45	11.16	50.96	2.96	1.57	0.32	1.85
o-cresol (2-hydroxytoluene)	108.14	0.77	0.67	1.40	686.28	−102.83	84.31	9.06	58.99	2.55	1.79	0.56	1.95
octafluorocyclobutane	200.03	0.01	0.00	0.01	2826.00	−60.60	88.72	13.19	33.49	2.51	2.30	0.66	2.29
octane	114.23	0.00	0.00	0.00	600.81	−139.69	99.35	11.27	57.13	3.91	2.41	0.85	5.18
o-ethyltoluene	120.19	0.48	0.03	0.45	642.30	−130.73	97.96	9.32	69.38	3.39	2.28	1.01	3.53
o-isobutylphenol	150.22	0.23	0.73	0.87	908.51	−152.81	120.61	9.03	80.81	3.97	3.23	1.12	3.31
o-methylbenzaldehyde	120.15	2.37	0.42	2.79	750.49	−112.78	91.14	9.76	66.76	2.85	1.97	0.72	2.26
o-methylbenzyl alcohol	122.17	0.81	0.59	1.39	761.65	−119.20	96.10	9.23	66.60	3.00	2.08	0.79	1.58
o-phenylphenol	170.21	0.74	0.65	1.38	1025.18	−160.37	130.97	8.69	107.90	4.21	2.88	1.34	3.09
o-*sec*-butylphenol	150.22	0.23	0.72	0.88	908.51	−152.83	120.66	9.03	80.79	3.97	3.23	1.12	3.27
o-xylene	106.17	0.45	0.01	0.46	567.95	−114.13	85.89	9.30	62.31	2.83	2.08	0.66	3.12
pentachlorobenzene	250.34	0.18	0.61	0.43	1165.34	−76.48	68.74	9.25	97.46	4.41	3.73	1.65	5.17
pentafluoroethylbenzene	196.12	2.25	0.07	2.25	2137.11	−110.90	112.19	10.43	69.62	3.51	2.40	0.96	3.36
pentanal	86.13	2.21	0.36	2.56	561.88	−88.36	68.69	10.63	38.88	2.35	1.31	0.29	1.31
pentane	72.15	0.03	0.03	0.00	378.35	−89.70	63.08	11.30	35.97	2.41	1.35	0.35	3.62

Table 1 (Continued)

compound	MW[a]	D_P[b] [debye]	D_H[c] [debye]	D_S[d] [debye]	E2[e] [EV]	EX[f] [ev]	ELC[g] [ev]	IP[h] [kcal]	PO[i] [au]	VMC_1[j]	VMC_2[k]	VMC_4[l]	logK_{ow}
pentanenitrile	83.13	2.49	0.84	3.33	462.04	−87.06	67.44	11.80	40.24	2.28	1.26	0.26	1.12
pentanoic acid	102.13	2.17	0.48	1.80	760.96	−93.84	79.24	11.36	41.82	2.49	1.50	0.33	3.00
p-ethyltoluene	120.19	0.07	0.03	0.04	642.11	−130.77	97.98	9.18	70.30	3.38	2.34	0.82	3.63
phenanthrene	178.23	0.05	0.02	0.03	962.48	−175.88	138.56	8.74	123.59	4.82	3.51	1.95	4.57
phenol	94.11	0.53	0.69	1.14	613.91	−86.08	71.81	9.18	50.76	2.13	1.34	0.43	1.46
phenyl benzoate	198.22	2.16	0.13	2.27	1281.58	−175.87	148.37	9.31	114.95	4.68	3.07	1.23	3.59
phenyl formate	122.12	3.11	0.47	3.53	866.28	−101.70	90.44	9.61	64.58	2.59	1.53	0.55	1.26
phenylacetaldehyde	120.15	2.13	0.35	2.45	753.21	−112.62	91.16	9.73	64.84	2.91	1.86	0.71	1.78
phenylacetic acid	136.15	1.69	0.32	1.54	952.51	−118.02	101.60	9.60	67.36	3.05	2.06	0.77	1.41
phenylacetic acid ethyl ester	164.20	1.61	0.16	1.76	1093.92	−151.33	125.85	9.54	84.47	4.02	2.47	0.97	2.42
phenylacetic acid methyl ester	150.18	1.49	0.13	1.63	1018.96	−134.72	114.16	9.56	76.36	3.43	2.24	0.83	1.96
phenylacetonitrile	117.15	2.32	0.90	3.20	652.51	−111.40	89.85	9.85	65.84	2.84	1.82	0.69	1.56
phenylacetylene	102.14	0.34	0.17	0.17	554.39	−101.18	77.66	9.40	66.17	2.45	1.51	0.53	2.40
phenylethyl sulfide	138.23	0.59	1.61	1.64	672.31	−117.61	87.12	8.55	78.69	4.09	3.08	1.36	3.20
phenylpropyl ether	136.19	0.80	0.37	1.12	830.47	−136.02	108.07	9.08	75.28	3.61	2.16	0.74	3.18
p-isobutylphenol	150.22	0.76	0.62	1.25	908.55	−152.81	120.59	8.94	81.43	3.96	3.26	1.10	2.94
p-methyl styrene	118.18	0.30	0.02	0.30	635.79	−124.19	93.69	8.94	75.94	3.02	2.11	0.70	3.35
p-methylacetophenone	134.18	2.60	0.43	3.02	825.86	−129.52	103.19	9.72	74.73	3.28	2.42	0.79	2.28
p-methylbenzyl alcohol	122.17	0.69	0.66	1.29	761.20	−119.32	95.94	9.18	66.61	2.99	2.14	0.69	1.59
propane	44.10	0.03	0.03	0.00	230.04	−56.37	38.89	11.51	21.93	1.41	0.71	0.00	2.36
propanenitrile	55.08	2.38	0.87	3.25	313.72	−53.74	43.26	12.01	25.81	1.28	0.51	0.00	0.16
propionaldehyde	58.08	2.15	0.36	2.51	413.93	−55.01	44.45	10.62	24.59	1.35	0.57	0.00	0.59
propionicacid	74.08	2.16	0.46	1.80	612.56	−60.52	55.08	11.35	27.69	1.49	0.75	0.00	0.33
propiophenone	134.18	2.23	0.46	2.69	826.59	−129.40	102.88	10.00	72.87	3.43	2.14	0.83	2.19
propyl formate	88.11	3.33	0.61	3.90	676.96	−77.27	67.65	11.16	36.95	1.97	0.97	0.17	0.82
propylallylamine	99.18	0.32	1.31	1.18	549.01	−110.23	83.79	9.20	51.42	2.73	1.49	0.38	1.33
propylbutylamine	115.22	0.22	1.35	1.16	628.72	−133.48	100.16	9.18	56.90	3.62	2.10	0.60	2.12
propylisobutylamine	115.22	0.24	1.38	1.14	628.81	−133.47	100.19	9.13	56.57	3.48	2.60	0.57	2.07
propyl-*sec*-butylamine	115.22	0.33	1.35	1.12	629.23	−133.36	99.94	9.17	56.81	3.54	2.26	0.54	1.91
propyne	40.07	0.51	0.15	0.36	216.17	−43.40	31.12	10.89	20.97	0.79	0.29	0.00	0.94
p-xylene	106.17	0.02	0.03	0.05	567.85	−114.17	85.92	9.18	62.95	2.82	2.15	0.64	3.20
pyrazine	80.09	0.00	0.00	0.00	477.16	−67.65	61.85	10.16	41.91	1.70	0.89	0.25	-0.22
pyrazine-2-one	96.09	2.89	1.44	3.47	670.20	−74.37	73.11	9.27	50.29	1.88	1.10	0.31	-1.49
pyridine	79.10	0.62	1.31	1.93	450.57	−74.07	61.32	10.10	43.62	1.85	1.02	0.31	0.64
pyrrole	67.09	1.89	0.29	2.18	387.11	−65.44	53.72	8.93	35.76	1.58	0.88	0.28	0.75
pyrrolidine	71.12	0.22	1.37	1.46	399.05	−77.19	61.07	9.27	32.80	2.21	1.46	0.63	0.46
sec-butyl alcohol	74.12	0.91	0.69	1.48	498.97	−78.14	60.82	11.04	32.14	1.95	1.26	0.00	0.61
sec-butylamine	73.14	0.23	1.52	1.37	406.50	−83.57	64.05	9.43	34.55	2.03	1.39	0.00	0.74
sec-butylbenzene	134.22	0.30	0.04	0.27	717.97	−147.27	109.68	9.52	75.50	3.89	2.72	1.02	4.57
styrene	104.15	0.02	0.01	0.02	563.31	−107.39	81.22	9.13	66.26	2.61	1.61	0.59	3.16
tert-butylbenzene	134.22	0.30	0.02	0.30	717.41	−147.28	109.67	9.50	74.90	3.66	3.62	0.94	4.11
tert-butyl alcohol	74.12	0.98	0.70	1.54	499.47	−78.18	60.69	11.28	31.58	1.72	2.17	0.00	0.37
tert-butyl amine	73.14	0.28	1.52	1.36	406.10	−83.62	63.95	9.47	34.08	1.79	2.37	0.00	0.40
tetrachlorocyclohexane	221.94	0.02	0.01	0.03	1059.93	−94.83	74.99	10.17	70.95	4.91	4.77	2.38	3.72
tetrachloroethene	165.83	0.00	0.00	0.00	746.46	−29.58	27.77	9.22	52.79	2.51	2.41	0.00	3.40
tetrachloromethane	153.82	0.01	0.00	0.01	685.86	−18.39	17.85	10.99	42.79	2.26	3.85	0.00	2.83
tetrafluoromethane	88.01	0.00	0.00	0.00	1357.35	−20.33	35.55	16.79	8.02	0.76	0.43	0.00	1.18
tetrahydrofuran	72.11	1.29	0.38	1.67	485.09	−71.84	58.31	10.26	30.42	2.08	1.32	0.51	0.46
tetrahydropyran	86.13	0.98	0.40	1.38	559.13	−88.54	70.76	10.57	38.59	2.58	1.67	0.69	0.95
thiophene	84.14	1.01	1.68	0.67	386.08	−57.80	41.05	9.54	42.24	2.41	1.61	0.68	1.81
thiophenol	100.14	0.60	2.28	1.69	573.99	−63.29	52.39	9.27	47.46	2.50	1.87	0.72	2.52
toluene	92.14	0.25	0.02	0.26	495.45	−97.35	73.38	9.44	45.60	2.41	1.65	0.53	2.69
trans-1,2-diphenylethene	180.25	0.00	0.00	0.00	975.15	−181.73	140.11	8.63	131.69	4.73	3.15	1.32	4.81
tribromomethane	252.73	0.60	0.35	0.95	828.40	−18.26	13.15	10.84	39.97	3.40	6.66	0.00	3.20
trichloroethene	131.39	0.14	0.63	0.49	600.09	−30.32	26.40	9.38	42.05	2.07	1.62	0.00	2.42
trichlorofluoromethane	137.37	0.98	0.42	0.56	852.90	−18.53	21.45	11.16	35.44	1.89	2.57	0.00	2.53
trichloromethane	119.38	0.41	0.60	1.02	538.25	−19.39	16.95	10.84	32.20	1.96	2.22	0.00	1.97
triethylamine	101.19	0.14	1.16	1.06	554.45	−116.52	87.36	9.04	50.43	3.07	1.62	0.67	1.44
trifluorobenzene	132.09	0.00	0.00	0.00	1370.93	−78.46	76.08	10.37	49.65	2.30	1.59	0.52	2.52
trifluoromethane	70.01	1.56	0.33	1.89	1044.43	−20.61	29.75	14.36	8.27	0.65	0.25	0.00	0.64
trifluoromethylbenzene	146.11	2.87	0.24	3.11	1456.81	−94.96	87.53	10.34	54.18	2.73	1.86	0.63	3.01
triiodomethane	393.73	0.43	0.18	0.61	704.29	−17.72	12.93	8.98	64.07	4.33	10.83	0.00	2.00
trimethylamine	59.11	0.05	1.20	1.15	331.52	−66.75	51.72	9.07	28.46	1.34	1.34	0.00	0.27
tripropylamine	143.27	0.26	1.24	1.00	777.06	−166.50	123.62	9.07	71.93	4.57	2.84	1.28	2.79
vinyl bromide	106.95	1.18	0.15	1.33	402.44	−31.31	21.76	10.44	25.86	1.54	0.80	0.00	1.57

[a] MW = molecular weight. [b] D_P = dipole moment_total point-charge [debye]. [c] D_H = dipole moment_total hybrid [debye]. [d] D_S = dipole moment_total sum [debye]. [e] E2 = total two-center energy [ev]. [f] EX = exchange energy (two-center term) [ev]. [g] ELC = total electrostatic interaction (two-center term) [ev]. [h] IP = ionization potential [kcal]. [i] PO = average polarizability [au]. [j] VMC_1 = first-order valence molecular connectivity index. [k] VMC_2 = second-order valence molecular connectivity index. [l] VMC_4 = fourth-order valence molecular connectivity index.

charge component, total hybridization component, and total sum = point charge + hybrid), molecular weight, first-order average polarizability, ionization potential, exchange energy, total two-center energy, and total electrostatic interaction energy (two-center). We note that, in all 15 runs, the following descriptors were selected: dipole moment-total

Table 2. Molecular Descriptors Generated for NN/QSPRs

type of molecular descriptors generated	units	variables selected for NN/QSPR
molecular weight		X
Quantum Chemical Descriptors		
number of filled molecular orbital levels		
ionization potential	kcal	X
average molecular polarizability dipole moments	au	X
total dipole (point charge)	debye	X
total dipole (hybridization)	debye	X
total dipole (sum = point charge + hybridization)	debye	X
principal moments of inertia		
moment of inertia, A direction	cm^{-1}	
moment of inertia, B direction	cm^{-1}	
moment of inertia, C direction	cm^{-1}	
heat of formation	ev	
total energy[a]	ev	
total one-center energy[b]	ev	
electron−electron repulsion (one-center term)	ev	
electron−nuclear attraction (one-center term)	ev	
total two-center energy[c]	ev	X
resonance energy (two-center term)	ev	
exchange energy (two-center term)	ev	X
resonance energy + exchange energy (two-center term)	ev	
total electrostatic inaction energy (two-center term)[d]	ev	X
electron−electron repulsion (two-center term)	ev	
electron−nuclear attraction (two-center term)	ev	
nuclear−nuclear repulsion (two-center term)	ev	
Topological Indices		
first-order valence molecular connectivity index		X
second-order valence molecular connectivity index		X
third-order valence molecular connectivity index		
fourth-order valence molecular connectivity index		X
second-order kappa shape index		

[a] Total energy = total one-center energy + total two-center energy. [b] Total one-center energy = electron−electron repulsion + electron−nuclear attraction. [c] Total two-center energy = resonance energy + exchange energy + total electrostatic inaction energy. [d] Total electrostatic inaction energy = electron−electron repulsion (two-center term) + electron−nuclear attraction (two-center term) + nuclear−nuclear repulsion (two-center term).

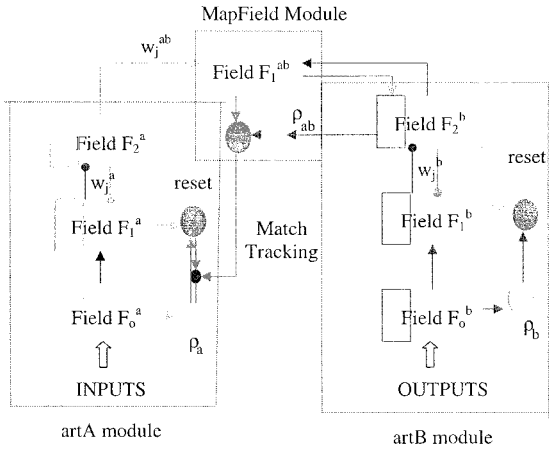

Figure 2. Block diagram of the fuzzy ARTMAP neural network.

hybridization component, dipole moment-total sum, and total electrostatic interaction energy. The average polarizability and first-order valence molecular connectivity index were ranked at the 93rd and 86th percentile range, respectively. The remaining descriptors listed in Tables 1 and 2 were ranked at or above the 73rd percentile range.

Fuzzy ARTMAP Neural Network Systems. The present study focused on the development of logK_{ow} QSPRS derived based on a fuzzy ARTMAP and back-propagation neural networks. The fuzzy ARTMAP neural network system used in the present study was recently introduced for developing QSPRs for boiling temperatures,[35] critical properties,[36] and aqueous solubilities.[37] The current fuzzy ARTMAP system is the modification introduced by Giralt et al.[50,51] to the original model of Carpenter et al.[52−56] Briefly, the basic learning mechanism of the fuzzy ARTMAP neural system consists of creating new categories (equivalent to hidden units in back-propagation) when dissimilar molecular descriptors and different values of the physical property are encountered. The modified network consists of two fuzzy ART modules, *artA* and *artB*, that are linked together via an inter-ART module (Figure 2). Each ART system includes a field, F_o, of nodes that represent a current input vector and a field F_1 that receives both bottom-up input from F_o and top-down input from a field F_2 that represents the active code or category. The *artA* module categorizes the input patterns (molecular descriptors), while *artB* module develops categories of the target patterns (physical property) during supervised learning (training). During supervised learning, the *artA* module receives the molecular descriptors, and the *artB* module receives the correct physical property prediction of the input pattern presented to F_o^a. The *artA* module attempts the prediction through the *map field* of the category to which the current target belongs. The inter-ART module, called a *map field*, is an associative learning network that forms an internal controller designed to create a minimal number of *artA* recognition categories, or "hidden units", by following the *match tracking rule.* The fuzzy ARTMAP dynamics are determined by vigilance ρ_a, ρ_b, $\rho_{ab} \in [0,1]$, learning rates β_a, $\beta_b \in [0,1]$, and choice $\alpha > 0$, parameters. The vigilance parameters calibrate how well an input pattern must match the learned prototype or cluster of input features that the category deems to be relevant, for a category to be accepted. The learning rate parameter determines how the map field weights change through the learning process. Finally, the choice parameter controls the fuzzy subsethood of the category choice function and accounts for the noise in the activation of the F_1 layer. Additional information about fuzzy ART and fuzzy ARTMAP systems can be found elsewhere.[57−61]

The fuzzy ARTMAP-based QSPR for logK_{ow} was developed following the methodology described in Figure 1. About 85% (371) of compounds in the complete data set were selected for training by the fuzzy ART classifier to ensure that adequate information was provided to the system. Training of the fuzzy ARTMAP consisted of presenting the molecular descriptors and target properties of the training set to modules *artA* and *artB* (see Figure 2), respectively, to establish input and output categories and relate them through the *map field* (F_1^{ab}). After training with a data set of 371 compounds, the hypothesis components of the *artB* module (F_o^b and F_1^b) were disconnected and an output in its category layer F_2^b was implemented.[35] Therefore, through the map field module F_1^{ab}, a prediction for the target physical property is obtained for any input of descriptors presented to module *artA*. The model was then evaluated with a test a set containing 71 compounds.

Table 3. Experimental and Predicted Octanol/Water Partition Coefficients Using Fuzzy ARTMAP and Back-Propagation QSPRs

	data set[a]		logK_{ow}			absolute error, logK_{ow}		absolute percent error, %[b]	
compounds	fuzzy ARTMAP	back-propagation	reported logK_{ow}	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation
1,1,1-trichloroethane	tr	tr/v	2.49	2.47	2.52	0.02	0.03	0.80	1.40
1,1,2,2,-tetrachlorodifluoroethane	tr	tr/v	2.39	2.39	2.84	0.00	0.45	0.00	18.69
1,1,2-trichlorotrifluoroethane	tr	tr/v	3.16	3.15	2.90	0.01	0.26	0.32	8.28
1,1-dichloroethane	tr	tr/v	1.79	1.76	1.91	0.03	0.12	1.68	6.90
1,1-dichloroethene	tr	tr/v	2.13	2.10	1.76	0.03	0.37	1.41	17.14
1,1-difluoroethane	tr	tr/v	0.75	0.72	0.43	0.03	0.32	4.00	42.87
1,1-difluoroethene	tr	v	1.24	1.22	1.56	0.02	0.32	1.61	25.51
1,2,3,5-tetramethylbenzene	ts	ts	4.17	3.98	3.68	0.19	0.49	4.56	11.86
1,2,3-trimethylbenzene	tr	tr/v	3.55	3.55	3.26	0.00	0.29	0.00	8.14
1,2,4,5-tetramethylbenzene	tr	tr/v	4	3.98	3.95	0.02	0.05	0.50	1.30
1,2,4-trichlorobenzene	tr	tr/v	4.02	4.01	3.86	0.01	0.16	0.25	3.87
1,2,4-trimethylbenzene	tr	tr/v	3.65	3.63	3.49	0.02	0.16	0.55	4.49
1,2-dibromoethane	tr	tr/v	1.96	1.94	1.94	0.02	0.02	1.02	0.78
1,2-dichlorobenzene	tr	tr/v	3.38	3.36	3.44	0.02	0.06	0.59	1.91
1,2-dichloroethane	tr	tr/v	1.48	1.48	2.23	0.00	0.75	0.00	50.73
1,2-dichlorotetrafluoroethane	tr	tr/v	2.82	2.82	2.60	0.00	0.22	0.00	7.83
1,2-difluorobenzene	tr	tr/v	3.6	3.59	3.15	0.01	0.45	0.28	12.38
1,3,5-heptatriene	tr	tr/v	2.63	2.63	2.58	0.00	0.05	0.00	2.07
1,3,5-trichlorobenzene	tr	tr/v	4.15	4.15	3.98	0.00	0.17	0.00	4.21
1,3,5-trimethylbenzene	ts	ts	3.42	3.63	3.75	0.21	0.33	6.14	9.74
1,3-butadiene	tr	v	1.99	1.98	1.61	0.01	0.38	0.50	19.24
1,3-dibromopropane	tr	v	2.37	2.35	2.07	0.02	0.30	0.84	12.81
1,3-dichlorobenzene	ts	ts	3.38	3.42	3.32	0.04	0.06	1.18	1.74
1,3-dichloropropane	tr	v	2	1.98	2.14	0.02	0.14	1.00	6.99
1,3-difluorobenzene	tr	v	3.75	3.72	3.34	0.03	0.41	0.80	10.81
1,3-dimethylnaphthalene	ts	ts	4.42	4.36	4.11	0.06	0.31	1.36	6.95
1,4,5-trimethylnaphthalene	tr	tr/v	4.9	4.89	4.29	0.01	0.61	0.20	12.44
1,4-cyclohexadiene	tr	v	2.3	2.29	2.65	0.01	0.35	0.43	15.21
1,4-dichlorobenzene	ts	ts	3.39	3.15	3.68	0.24	0.29	7.08	8.64
1,4-difluorobenzene	tr	tr/v	4.11	4.09	2.80	0.02	1.31	0.49	31.92
1,4-dimethylnaphthalene	tr	tr/v	4.37	4.36	4.38	0.01	0.01	0.23	0.22
1,4-dioxane	tr	v	-0.27	-0.30	1.96	0.03	2.23	11.11	827.10
1,4-pentadiene	tr	tr/v	2.48	2.47	2.25	0.01	0.23	0.40	9.34
1,5-dimethylnaphthalene	ts	ts	4.38	4.36	4.39	0.02	0.01	0.46	0.12
1,5-hexadiene	tr	tr/v	2.45	2.43	2.85	0.02	0.40	0.82	16.33
1,6-heptadiene	tr	tr/v	3.51	3.51	3.50	0.00	0.01	0.00	0.20
1-bromo-2-isoproplybenzene	tr	tr/v	4.2	4.18	4.14	0.02	0.06	0.48	1.49
1-bromobutane	tr	tr/v	2.75	2.72	2.45	0.03	0.30	1.09	10.75
1-bromoheptane	tr	v	4.36	4.36	4.11	0.00	0.25	0.00	5.78
1-bromohexane	tr	tr/v	3.8	3.79	3.64	0.01	0.16	0.26	4.17
1-bromooctane	tr	tr/v	4.89	4.89	4.51	0.00	0.38	0.00	7.71
1-bromopentane	tr	tr/v	3.37	3.36	3.04	0.01	0.33	0.30	9.90
1-bromopropane	tr	tr/v	2.1	2.10	1.96	0.00	0.14	0.00	6.43
1-butanethiol	tr	tr/v	2.28	2.26	2.04	0.02	0.24	0.88	10.59
1-butene	tr	tr/v	2.4	2.39	1.83	0.01	0.57	0.42	23.78
1-chloro-1,1-difluoroethane	tr	tr/v	1.08	1.08	1.56	0.00	0.48	0.00	44.80
1-chlorobutane	tr	v	2.55	2.55	2.05	0.00	0.50	0.00	19.66
1-chlorohexane	tr	v	3.54	3.51	3.12	0.03	0.42	0.85	11.92
1-chloropentane	tr	tr/v	2.73	2.72	2.60	0.01	0.13	0.37	4.66
1-choropropane	tr	v	2.04	2.03	1.60	0.01	0.44	0.49	21.45
1-ethylnaphthalene	ts	ts	4.39	4.36	4.14	0.03	0.25	0.68	5.68
1-ethylpiperidine	tr	tr/v	1.75	1.75	2.20	0.00	0.45	0.00	25.46
1-heptanol	tr	tr/v	2.03	2.03	2.43	0.00	0.40	0.00	19.87
1-heptyne	tr	tr/v	3.01	2.99	3.24	0.02	0.23	0.66	7.53
1-hexene	tr	v	3.99	3.98	3.10	0.01	0.89	0.25	22.34
1-hexyne	tr	v	2.73	2.72	2.63	0.01	0.10	0.37	3.70
1-methylnaphthalene	ts	ts	3.87	3.86	3.94	0.01	0.07	0.26	1.81
1-methylcyclohexene	tr	tr/v	3.51	3.51	3.24	0.00	0.27	0.00	7.78
1-nitropropane	tr	tr/v	0.65	0.65	0.93	0.00	0.28	0.00	42.62
1-nonene	tr	v	5.15	5.15	4.43	0.00	0.72	0.00	14.04
1-octanol	tr	v	3.15	3.15	2.86	0.00	0.29	0.00	9.28
1-octene	tr	tr/v	4.57	4.54	4.08	0.03	0.49	0.66	10.78
1-octyne	tr	v	3.5	3.50	3.70	0.00	0.20	0.00	5.82
1-pentanol	tr	v	1.4	1.38	1.49	0.02	0.09	1.43	6.74
1-pentyne	tr	tr/v	1.98	1.98	2.00	0.00	0.02	0.00	1.21
1-propanol	tr	tr/v	0.34	0.33	0.51	0.01	0.17	2.94	49.89
1-propene	tr	tr/v	1.77	1.76	1.15	0.01	0.62	0.56	34.83
2,2′,3,3′,4,6′-hexachloro-1,1′-biphenyl	tr	v	6.24	6.24	5.80	0.00	0.44	0.00	7.13
2,2′,3,4,4′,5′-hexachloro-1,1′-biphenyl	ts	ts	6.69	6.24	6.92	0.45	0.23	6.73	3.47
2,2′,4,4′,6,6′-hexachloro-1,1′-biphenyl	ts	ts	6.7	6.85	6.87	0.15	0.17	2.24	2.61

Table 3 (Continued)

compounds	data set[a]		logK_{ow}			absolute error, logK_{ow}		absolute percent error, %[b]	
	fuzzy ARTMAP	back-propagation	reported logK_{ow}	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation
2,2′,4,5,5′-pentabromo-1,1′-biphenyl	tr	tr/v	5.96	5.96	6.30	0.00	0.34	0.00	5.64
2,2′,4,5,5′-pentachloro-1,1′-biphenyl	tr	tr/v	4.12	4.09	3.77	0.03	0.35	0.73	8.44
2,2′,5,6′-tetrachloro-1,1′-biphenyl	tr	tr/v	6.63	6.63	6.55	0.00	0.08	0.00	1.26
2,2′3,3′-tetrachloro-1,1′-biphenyl	tr	tr/v	6.67	6.67	6.60	0.00	0.07	0.00	1.12
2,2′4,4′,5,5′-hexachloro-1,1′-biphenyl	ts	ts	6.72	6.85	6.93	0.13	0.21	1.93	3.17
2,2-dimethyl-1-propanol	tr	tr/v	1.36	1.33	1.26	0.03	0.10	2.21	7.52
2,2-dimethylbutane	tr	tr/v	3.88	3.86	3.34	0.02	0.54	0.52	13.97
2,2-dimethylpentane	tr	v	3.11	3.11	3.79	0.00	0.68	0.00	21.77
2,2-dimethylpropane	tr	tr/v	3.11	3.11	3.05	0.00	0.06	0.00	1.94
2,3,6-trimethylnaphthalene	tr	tr/v	4.73	4.73	4.32	0.00	0.41	0.00	8.60
2,3′-dichloro-1,1′-biphenyl	ts	ts	5.02	5.30	4.99	0.28	0.03	5.58	0.54
2,3-dimethyl-1-butene	tr	tr/v	3.13	3.11	2.69	0.02	0.44	0.64	13.99
2,3-dimethylbutane	tr	tr/v	3.85	3.82	3.52	0.03	0.33	0.78	8.55
2,3-dimethylnaphthalene	ts	ts	4.4	4.36	3.98	0.04	0.42	0.91	9.46
2,3-dimethylpentane	tr	tr/v	3.63	3.63	4.10	0.00	0.47	0.00	13.01
2,3-dimethylpyridine	tr	tr/v	1.22	1.22	1.44	0.00	0.22	0.00	17.86
2,4-dibromotetrachlorocyclohexane	tr	tr/v	3.98	3.98	3.96	0.00	0.02	0.00	0.60
2,4′-dichloro-1,1′-biphenyl	ts	ts	5.1	5.30	4.91	0.20	0.19	3.92	3.70
2,4-dichloro-1,1′-biphenyl	ts	ts	5.15	5.30	5.07	0.15	0.08	2.91	1.50
2,4-dichloro-1-chloromethylbenzene	tr	tr/v	3.82	3.82	4.49	0.00	0.67	0.00	17.51
2,4-dichlorotoluene	tr	v	4.24	4.24	3.85	0.00	0.39	0.00	9.15
2,4-dimethyl-2-pentanol	ts	ts	2.13	2.03	2.12	0.10	0.01	4.69	0.66
2,4-dimethyl-3-pentanone	tr	tr/v	1.86	1.85	1.86	0.01	0.00	0.54	0.01
2,4-dimethylpentane	tr	tr/v	3.63	3.63	3.88	0.00	0.25	0.00	7.00
2,4-dimethyl-phenol	tr	tr/v	2.3	2.29	2.18	0.01	0.12	0.43	5.28
2,5′-dichloro-1,1′-biphenyl	tr	v	5.18	5.15	5.34	0.03	0.16	0.58	3.15
2,5-dimethylphenol	tr	tr/v	2.33	2.31	2.16	0.02	0.17	0.86	7.34
2,6,dimethylnaphthalene	ts	ts	4.31	4.36	4.39	0.05	0.08	1.16	1.75
2,6-dichloro-1,1′-biphenyl	tr	tr/v	5.3	5.30	4.95	0.00	0.35	0.00	6.69
2,6-dichlorotoluene	ts	ts	4.29	4.24	3.70	0.05	0.59	1.17	13.79
2,6-dimethyl-phenol	tr	tr/v	2.36	2.35	2.12	0.01	0.24	0.42	10.24
2-aminotoluene	tr	tr/v	1.32	1.31	1.33	0.01	0.01	0.76	1.03
2-bromobutane	ts	ts	2.58	2.72	2.26	0.14	0.32	5.43	12.47
2-bromophenol	tr	tr/v	2.35	2.35	2.85	0.00	0.50	0.00	21.45
2-bromopropane	ts	ts	2.14	2.10	1.88	0.04	0.26	1.87	11.97
2-bromotoluene	ts	ts	2.92	3.33	3.46	0.41	0.54	14.04	18.42
2-butanone	tr	tr/v	0.29	0.27	0.27	0.02	0.02	6.90	6.18
2-butene	tr	tr/v	2.31	2.31	1.80	0.00	0.51	0.00	21.98
2-butyne	tr	tr/v	1.46	1.43	1.72	0.03	0.26	2.05	17.53
2-chloro-1,1′-biphenyl	tr	tr/v	4.54	4.54	4.28	0.00	0.26	0.00	5.70
2-chloro-1-ethylbenzene	tr	tr/v	2.95	2.95	3.69	0.00	0.74	0.00	24.97
2-chloro-2-methylbutane	ts	ts	2.52	2.72	2.28	0.20	0.24	7.94	9.65
2-chlorophenol	tr	tr/v	2.15	2.15	2.73	0.00	0.58	0.00	27.03
2-chloropropane	tr	v	1.9	1.90	1.47	0.00	0.43	0.00	22.56
2-ethyl pyridine	tr	v	1.69	1.69	1.65	0.00	0.04	0.00	2.20
2-ethylnaphthalene	tr	tr/v	4.38	4.36	4.20	0.02	0.18	0.46	4.18
2-ethylphenol	tr	tr/v	2.47	2.47	2.08	0.00	0.39	0.00	15.67
2-ethylthiophene	tr	tr/v	2.87	2.86	2.74	0.01	0.13	0.35	4.55
2-fluoro-3-bromotetrachlorocyclohexane	tr	v	3.28	3.28	3.58	0.00	0.30	0.00	9.28
2-fluorochlorobenzene	tr	tr/v	2.77	2.76	2.73	0.01	0.04	0.36	1.54
2-fluorophenol	tr	tr/v	1.71	1.70	1.78	0.01	0.07	0.59	4.29
2-heptanone	tr	tr/v	1.98	1.98	1.91	0.00	0.07	0.00	3.76
2-heptene	ts	ts	3.56	3.51	3.69	0.05	0.13	1.40	3.73
2-hexanol	ts	ts	1.76	1.76	1.91	0.00	0.15	0.00	8.39
2-hexanone	tr	tr/v	1.38	1.38	1.54	0.00	0.16	0.00	11.33
2-iodophenol	ts	ts	2.65	2.91	2.68	0.26	0.03	9.81	1.24
2-methoxynitrobenzene (2-nitroanisole)	tr	tr/v	1.73	1.70	1.68	0.03	0.05	1.73	2.95
2-methyl-1,3-butadiene	ts	ts	2.42	2.47	2.16	0.05	0.26	2.07	10.82
2-methyl-1-pentene	ts	ts	3.21	3.05	2.65	0.16	0.56	4.98	17.58
2-methyl-2-butene	ts	ts	2.67	2.58	2.08	0.09	0.59	3.37	21.94
2-methyl-2-nitropropane	tr	tr/v	1.01	1.01	1.25	0.00	0.24	0.00	23.80
2-methylbutane (isopentane)	tr	tr/v	2.72	2.72	2.98	0.00	0.26	0.00	9.47
2-methylhexane	tr	tr/v	3.71	3.71	4.15	0.00	0.44	0.00	11.92
2-methylnaphthalene	tr	v	3.86	3.86	4.00	0.00	0.14	0.00	3.67
2-methylpentane	tr	tr/v	2.34	2.31	3.51	0.03	1.17	1.28	49.98
2-methylpyridine	tr	tr/v	1.11	1.11	1.17	0.00	0.06	0.00	5.19
2-nitropropane	tr	tr/v	0.93	0.92	0.91	0.01	0.02	1.08	2.16
2-nitrotoluene	tr	tr/v	2.3	2.29	2.04	0.01	0.26	0.43	11.50
2-nonanone	tr	tr/v	3.18	3.18	2.65	0.00	0.53	0.00	16.76
2-octanone	ts	ts	2.76	3.18	2.28	0.42	0.48	15.22	17.44
2-pentanol	tr	tr/v	1.19	1.18	1.37	0.01	0.18	0.84	15.20
2-pentanone	ts	ts	0.91	0.81	1.07	0.10	0.16	10.99	17.56
2-pentene	tr	tr/v	2.58	2.58	2.42	0.00	0.16	0.00	6.12
2-phenyl-1-ethanol	tr	v	1.36	1.33	2.12	0.03	0.76	2.21	55.60

Table 3 (Continued)

compounds	data set[a]		logK_{ow}			absolute error, logK_{ow}		absolute percent error, %[b]	
	fuzzy ARTMAP	back-propagation	reported logK_{ow}	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation
2-phenylthiophene	tr	tr/v	3.74	3.72	3.94	0.02	0.20	0.53	5.46
2-propanol	tr	tr/v	0.05	0.05	0.14	0.00	0.09	0.01	179.44
2-propanone	tr	tr/v	−0.24	−0.24	−0.14	0.00	0.10	0.00	40.93
2-pyrimidone	tr	tr/v	−1.62	−1.62	−1.05	0.00	0.57	0.00	35.08
3,3,3-trifluoropropylbenzene	tr	tr/v	3.31	3.28	3.67	0.03	0.36	0.91	11.01
3,3′,4,4′-tetrachloro-1,1′-biphenyl	tr	tr/v	6.04	6.04	5.92	0.00	0.12	0.00	1.93
3,3′,5,5′-tetrachloro-1,1′-biphenyl	tr	v	6.85	6.85	6.81	0.00	0.04	0.00	0.57
3,3-dimethyl-2-butanol	tr	tr/v	1.48	1.48	1.78	0.00	0.30	0.00	20.18
3,4-dichloro-1,1-biphenyl	ts	ts	5.51	5.30	5.05	0.21	0.46	3.81	8.40
3,4-dimethylchlorobenzene	tr	v	3.82	3.82	3.09	0.00	0.73	0.00	19.00
3,4-dimethylphenol	tr	tr/v	2.23	2.22	2.05	0.01	0.18	0.45	8.04
3,5-dichloro-1,1′-biphenyl	ts	ts	5.37	5.30	4.99	0.07	0.38	1.30	6.99
3,5-dimethylphenol	tr	tr/v	2.35	2.35	1.98	0.00	0.37	0.00	15.82
3-bromophenol	ts	ts	2.63	2.35	2.78	0.28	0.15	10.65	5.86
3-chlorophenol	tr	v	2.52	2.51	2.02	0.01	0.50	0.40	19.75
3-ethylpentane	tr	tr/v	2.4	2.39	2.19	0.01	0.21	0.42	8.62
3-ethylthiophene	tr	v	2.82	2.82	2.88	0.00	0.06	0.00	2.18
3-fluorophenol	tr	tr/v	1.93	1.90	1.86	0.03	0.07	1.55	3.86
3-hexanol	tr	v	1.65	1.65	1.88	0.00	0.23	0.00	13.91
3-iodophenol	ts	ts	2.93	2.91	2.63	0.02	0.30	0.68	10.13
3-methyl-1-butanol	ts	ts	1.16	1.38	1.40	0.22	0.24	18.97	20.80
3-methyl-1-butene	tr	tr/v	2.59	2.58	2.38	0.01	0.21	0.39	8.16
3-methyl-2-butanol	tr	tr/v	1.28	1.26	1.42	0.02	0.14	1.56	10.88
3-methyl-2-butanone	tr	v	0.84	0.81	1.16	0.03	0.32	3.57	37.71
3-methylpentane	tr	tr/v	3.6	3.59	3.67	0.01	0.07	0.28	1.98
3-methylpyridine	ts	ts	1.2	1.18	1.07	0.02	0.13	1.67	10.95
3-methylthiophene	tr	v	2.34	2.31	2.28	0.03	0.06	1.28	2.56
3-nitrotoluene	tr	tr/v	2.45	2.43	2.18	0.02	0.27	0.82	11.08
3-pentanol	tr	tr/v	1.21	1.18	1.41	0.03	0.20	2.48	16.92
3-phenyl-1-chloropropane	tr	tr/v	3.55	3.55	3.70	0.00	0.15	0.00	4.31
4,4′-dichloro-1,1′-biphenyl	tr	v	5.58	5.58	5.60	0.00	0.02	0.00	0.32
4-bromophenol	tr	v	2.43	2.43	3.15	0.00	0.72	0.00	29.52
4-bromotoluene	tr	tr/v	3.33	3.33	3.49	0.00	0.16	0.00	4.88
4-chloro-1,1′-biphenyl	tr	tr/v	4.61	4.61	4.36	0.00	0.25	0.00	5.47
4-chlorophenol	tr	v	2.35	2.35	2.59	0.00	0.24	0.00	10.15
4-cyclopropyl-2-butanone	tr	v	1.5	1.48	1.78	0.02	0.28	1.33	18.52
4-ethenylcyclohexene	tr	tr/v	3.34	3.33	3.60	0.01	0.26	0.30	7.77
4-ethylphenyl acetate	ts	ts	2.56	2.39	2.73	0.17	0.17	6.64	6.58
4-fluorophenol	tr	tr/v	1.79	1.76	1.80	0.03	0.01	1.68	0.33
4-iodophenol	tr	tr/v	2.91	2.91	3.05	0.00	0.14	0.00	4.81
4-methyl pyridine	tr	tr/v	1.2	1.18	1.06	0.02	0.14	1.67	11.86
4-methyl-1-pentene	tr	tr/v	3.08	3.05	2.81	0.03	0.27	0.97	8.62
4-methyl-2-pentanone	tr	v	1.31	1.31	1.39	0.00	0.08	0.00	5.89
4-methylphenol	tr	tr/v	1.94	1.94	1.86	0.00	0.08	0.00	4.34
4-*n*-propylphenol	tr	tr/tv	3.23	3.23	2.49	0.00	0.74	0.00	22.91
4-phenylbutyric acid	tr	tr/v	2.42	2.39	2.43	0.03	0.01	1.24	0.60
4-phenylphenol	ts	ts	3.2	3.23	3.33	0.03	0.13	0.94	3.97
4-pyrimidone	tr	tr/v	−1.38	−1.38	−1.19	0.00	0.19	0.00	13.56
5-methyl-2-hexanone	ts	ts	1.88	1.98	1.96	0.10	0.08	5.32	3.99
5-methyl-furfural(5-methylfuraldehyde)	tr	v	1.85	1.85	1.45	0.00	0.40	0.00	21.83
5-nonanone	tr	v	2.88	2.86	2.74	0.02	0.14	0.69	4.95
5-phenyl-2-pentanone	tr	tr/v	2.42	2.39	2.87	0.03	0.45	1.24	18.55
9-fluorenone	tr	v	3.58	3.55	3.41	0.03	0.17	0.84	4.69
9-methylanthracene	tr	tr/v	5.07	5.07	4.81	0.00	0.26	0.00	5.05
a,a,a-trichlorotoluene	tr	tr/v	2.92	2.91	4.01	0.01	1.09	0.34	37.36
a,a,a-trifluorotoluene	tr	tr/v	2.79	2.76	2.86	0.03	0.07	1.08	2.65
a-bromotoluene	ts	ts	2.92	3.33	3.18	0.41	0.26	14.04	8.85
acenaphthene	tr	tr/v	3.92	3.92	4.03	0.00	0.11	0.00	2.75
acenaphthylene	tr	tr/v	4.03	4.01	4.31	0.02	0.28	0.50	7.05
acetic acid	tr	v	−0.17	−0.17	−0.22	0.00	0.05	0.00	27.40
acetonitrile	tr	v	−0.34	−0.34	−0.45	0.00	0.11	0.00	32.27
acetophenone	tr	tr/v	1.58	1.58	1.87	0.00	0.29	0.00	18.17
a-chlorotoluene	tr	tr/v	2.3	2.29	2.99	0.01	0.69	0.43	30.05
acrylophenone	tr	tr/v	1.88	1.85	2.09	0.03	0.21	1.60	10.92
allyl alcohol (2-propen-1-ol)	tr	tr/v	−0.31	−0.34	−0.21	0.03	0.10	9.68	30.97
allyl bromide (3-bromo-1-propene)	tr	v	1.79	1.76	1.90	0.03	0.11	1.68	6.30
allylbenzene (2-propenyl)	tr	tr/v	3.27	3.25	3.61	0.02	0.34	0.61	10.32
amylamine (pentyl)	ts	ts	1.45	1.33	1.11	0.12	0.34	8.28	23.65
aniline	tr	tr/v	0.9	0.88	1.06	0.02	0.16	2.22	17.77
anthracene	ts	ts	4.54	4.54	4.97	0.00	0.43	0.00	9.39
benz[*a*]anthracene	tr	tr/v	5.61	5.58	5.98	0.03	0.37	0.53	6.64
benzaldehyde	tr	v	1.48	1.48	1.58	0.00	0.10	0.00	6.49
benzene	tr	v	2.13	2.10	2.59	0.03	0.46	1.41	21.79
benzoic acid	tr	tr/v	1.81	1.81	1.46	0.00	0.35	0.00	19.57

Table 3 (Continued)

	data set[a]		logK_{ow}			absolute error, logK_{ow}		absolute percent error, %[b]	
compounds	fuzzy ARTMAP	back-propagation	reported logK_{ow}	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation
benzoic acid methyl ester	tr	v	2.12	2.10	1.87	0.02	0.25	0.94	11.92
benzonitrile	tr	v	1.56	1.55	1.31	0.01	0.25	0.64	16.23
benzothiophene	ts	ts	3.12	3.18	3.44	0.06	0.32	1.92	10.11
benzyl acetate	ts	ts	1.96	1.94	2.29	0.02	0.33	1.02	16.61
benzylamine	tr	tr/v	1.09	1.08	1.34	0.01	0.25	0.92	22.73
benzylphenyl ether	tr	tr/v	3.79	3.79	3.57	0.00	0.22	0.00	5.81
beta-phenylethyl chloride (2-)	tr	v	2.95	2.95	3.42	0.00	0.47	0.00	15.87
biphenyl	tr	tr/v	4.09	4.09	4.46	0.00	0.37	0.00	8.94
bromobenzene	tr	tr/v	2.99	2.99	2.94	0.00	0.05	0.00	1.61
bromochloromethane	tr	tr/v	1.41	1.38	1.93	0.03	0.52	2.13	37.15
bromocyclohexane	tr	v	3.2	3.18	3.25	0.02	0.05	0.62	1.59
bromoethane	tr	tr/v	1.61	1.58	1.61	0.03	0.00	1.86	0.26
bromomethane	tr	tr/v	1.19	1.18	1.29	0.01	0.10	0.84	8.62
bromotrifluoromethane	tr	tr/v	1.86	1.85	1.30	0.01	0.56	0.54	30.02
butanol	tr	tr/v	0.88	0.88	1.01	0.00	0.13	0.00	14.42
butylamine	tr	tr/v	0.81	0.81	0.67	0.00	0.14	0.00	17.25
butyl benzene	tr	tr/v	4.26	4.24	4.04	0.02	0.22	0.47	5.25
butyl ethyl ether	tr	tr/v	2.03	2.03	2.33	0.00	0.30	0.00	14.81
butyldimethylamine	tr	tr/v	1.7	1.70	1.68	0.00	0.02	0.00	0.96
butylmethylamine	tr	v	1.33	1.33	1.19	0.00	0.14	0.00	10.18
butyraldehyde	tr	tr/v	0.88	0.88	0.76	0.00	0.12	0.00	13.31
butyric acid	ts	ts	0.79	0.78	0.67	0.01	0.12	1.27	15.01
butyronitrile	tr	tr/v	0.53	0.51	0.52	0.02	0.01	3.77	1.56
chlorobenzene	tr	v	2.84	2.82	2.56	0.02	0.28	0.70	9.78
chlorodifluoromethane	tr	v	1.08	1.08	1.20	0.00	0.12	0.00	11.11
chloroethane	tr	tr/v	1.43	1.43	1.12	0.00	0.31	0.00	21.43
chloromethane	tr	tr/v	0.91	0.88	0.72	0.03	0.19	3.30	21.39
chlorotrifluoromethane	tr	tr/v	1.65	1.65	1.31	0.00	0.34	0.00	20.89
cis-1−2-dimethylcyclohexane	tr	v	4.01	4.01	4.45	0.00	0.44	0.00	11.02
crotonic acid (2-butenoic acid)	tr	tr/v	0.72	0.72	0.50	0.00	0.22	0.00	30.17
cycloheptane	tr	tr/v	4	3.98	4.07	0.02	0.07	0.50	1.87
cycloheptene	tr	tr/v	3.45	3.42	3.45	0.03	0.00	0.87	0.13
cyclohexane	tr	tr/v	3.44	3.42	3.62	0.02	0.18	0.58	5.31
cyclohexanol	tr	tr/v	1.23	1.22	1.88	0.01	0.65	0.81	52.87
cyclohexanone	tr	tr/v	0.81	0.81	1.55	0.00	0.74	0.00	90.79
cyclohexene	tr	tr/v	2.86	2.86	2.92	0.00	0.06	0.00	1.97
cyclooctane	tr	v	4.45	4.45	4.66	0.00	0.21	0.00	4.65
cyclopentane	tr	tr/v	3	2.99	2.89	0.01	0.11	0.33	3.51
cyclopentanone	tr	tr/v	0.63	0.61	1.10	0.02	0.47	3.17	74.50
cyclopentene	ts	ts	2.47	2.58	2.30	0.11	0.17	4.45	6.89
cyclopropane	tr	v	1.72	1.70	2.04	0.02	0.32	1.16	18.41
decachlorobiphenyl	tr	tr/v	7.92	7.92	6.92	0.00	1.00	0.00	12.67
decanoic acid	tr	v	4.09	4.09	3.19	0.00	0.90	0.00	22.08
di(*n*-propyl) ether	ts	ts	2.03	2.03	2.32	0.00	0.29	0.00	14.37
diallylamine	tr	v	1.11	1.11	1.12	0.00	0.01	0.00	1.29
dibromomethane	tr	tr/v	1.57	1.55	2.08	0.02	0.51	1.27	32.71
dichlorodifluoromethane	tr	tr/v	2.16	2.15	1.83	0.01	0.33	0.46	15.45
dichlorofluoromethane	tr	tr/v	1.55	1.55	1.71	0.00	0.16	0.00	10.56
dichloromomethane	tr	tr/v	1.25	1.22	1.56	0.03	0.31	2.40	24.85
diethyl sulfide	tr	v	1.95	1.94	2.06	0.01	0.11	0.51	5.60
diethylamine	tr	tr/v	0.57	0.57	0.76	0.00	0.19	0.00	33.66
diethyl ether	tr	v	0.89	0.88	1.18	0.01	0.29	1.12	32.38
difluoromethane	tr	tr/v	0.2	0.18	0.17	0.02	0.03	10.00	13.33
dimethyl ether	tr	v	0.1	0.08	0.10	0.02	0.00	20.00	0.71
dimethyl sulfide	tr	v	0.92	0.92	1.07	0.00	0.15	0.00	15.84
dimethyl sulfoxide	tr	tr/v	−1.35	−1.38	−1.55	0.03	0.20	2.22	15.04
di-*n*-butylamine	tr	tr/v	2.68	2.68	2.50	0.00	0.18	0.00	6.58
di-*n*-propylamine	tr	tr/v	1.73	1.70	1.70	0.03	0.03	1.73	1.81
di-*n*-propylamine	ts	ts	1.67	1.70	1.70	0.03	0.03	1.80	1.72
diphenylacetic acid	tr	tr/v	3.05	3.05	3.84	0.00	0.79	0.00	25.83
diphenylmethane	ts	ts	4.14	4.36	4.55	0.22	0.41	5.31	9.86
diphenylsulfide	tr	tr/v	4.41	4.41	4.47	0.00	0.06	0.00	1.34
ethane	tr	v	1.87	1.85	1.68	0.02	0.19	1.07	10.37
ethanol	ts	ts	0.1	0.08	0.20	0.02	0.10	20.00	96.40
ethene	tr	tr/v	1.13	1.11	0.93	0.02	0.20	1.77	17.48
ethoxybenzene	tr	v	2.51	2.51	2.26	0.00	0.25	0.00	9.83
ethyl acetate	tr	v	0.73	0.72	0.97	0.01	0.24	1.37	33.29
ethyl benzene	tr	tr/v	3.15	3.15	3.28	0.00	0.13	0.00	4.05
ethyl benzoate	tr	v	2.63	2.63	2.34	0.00	0.29	0.00	10.95
ethyl mercaptan	tr	v	1.21	1.18	1.08	0.03	0.13	2.48	10.81
ethyl propionate (C5H10O2)	tr	tr/v	1.21	1.18	1.55	0.03	0.34	2.48	28.45
ethylallylamine	tr	v	0.81	0.81	0.96	0.00	0.15	0.00	18.11
ethyldiisopropylamine	v	v	2.68	2.68	2.17	0.00	0.51	0.00	19.11
ethyldimethylamine	tr	tr/v	0.7	0.70	0.82	0.00	0.12	0.00	17.02

Table 3 (Continued)

compounds	data set[a]		logK_{ow}			absolute error, logK_{ow}		absolute percent error, %[b]	
	fuzzy ARTMAP	back-propagation	reported logK_{ow}	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation
ethylene oxide (oxirane)	tr	tr/v	−0.3	−0.30	−0.15	0.00	0.15	0.00	49.77
ethylvinyl ether	tr	tr/v	1.04	1.01	0.82	0.03	0.22	2.88	20.99
ethynylbenzene	tr	tr/v	2.53	2.51	2.91	0.02	0.38	0.79	14.99
fluorene	tr	v	4.18	4.18	4.45	0.00	0.27	0.00	6.44
fluorobenzene	tr	v	2.27	2.26	1.85	0.01	0.42	0.44	18.53
fluoromethane	tr	v	0.51	0.51	0.71	0.00	0.20	0.00	40.03
fluoropentachlorocyclohexane	tr	v	3.19	3.18	3.83	0.01	0.64	0.31	20.14
formaldehyde	tr	v	0.35	0.33	0.63	0.02	0.28	5.72	80.50
formic acid	tr	tr/v	−0.54	−0.57	−0.81	0.03	0.27	5.56	49.95
furan	tr	tr/v	1.34	1.33	1.10	0.01	0.24	0.75	18.28
hexachlorobenzene	tr	tr/v	5.23	5.23	5.09	0.00	0.14	0.00	2.68
hexachlorocyclopentadiene	ts	ts	5.04	5.23	4.89	0.19	0.15	3.77	3.00
hexafluorobenzene	tr	tr/v	2.22	2.22	2.68	0.00	0.46	0.00	20.66
hexafluroethane	tr	tr/v	2	1.98	2.00	0.02	0.00	1.00	0.04
hexamethylbenzene	tr	tr/v	4.31	4.31	4.40	0.00	0.09	0.00	2.04
hexanal	tr	v	1.78	1.76	1.59	0.02	0.19	1.12	10.70
hexane	tr	tr/v	4.11	4.09	3.81	0.02	0.30	0.49	7.23
hexanenitrile	tr	tr/v	1.66	1.65	1.39	0.01	0.27	0.60	16.34
hexanoic acid	tr	tr/v	1.88	1.85	1.62	0.03	0.26	1.60	13.96
hydroquinone	tr	v	0.59	0.57	0.63	0.02	0.04	3.39	7.45
indane	tr	tr/v	3.23	3.23	3.54	0.00	0.31	0.00	9.48
indene	tr	v	2.92	2.91	3.30	0.01	0.38	0.34	13.17
iodobenzene	tr	tr/v	3.25	3.25	2.84	0.00	0.41	0.00	12.62
iodoethane	ts	ts	2	1.58	1.86	0.42	0.14	21.00	6.93
iodomethane	tr	tr/v	1.51	1.48	1.62	0.03	0.11	1.99	7.51
isobutane	tr	v	2.76	2.76	2.41	0.00	0.35	0.00	12.77
isobutanol	tr	v	0.65	0.65	0.92	0.00	0.27	0.00	42.08
isobutyl acetate	tr	tr/v	1.78	1.76	1.99	0.02	0.21	1.12	11.59
isobutylamine	tr	tr/v	0.88	0.88	0.61	0.00	0.27	0.00	30.27
isobutyronitrile	ts	ts	0.46	0.51	0.45	0.05	0.01	10.87	1.29
isopentanol	ts	ts	1.42	1.38	1.41	0.04	0.01	2.82	1.03
isopropylamine	tr	tr/v	−0.03	−0.03	−0.12	0.00	0.09	0.01	290.82
isopropylbenzene	tr	v	3.66	3.63	3.81	0.03	0.15	0.82	4.18
m-chlorotoluene	tr	v	3.42	3.42	2.86	0.00	0.56	0.00	16.31
m-cresol (3-hydroxytoluene)	tr	tr/v	1.96	1.94	1.83	0.02	0.13	1.02	6.65
methanol	tr	tr/v	−0.66	−0.66	−0.45	0.00	0.21	0.00	31.26
methoxybenzene (anisole)	ts	ts	2.11	1.94	1.82	0.17	0.29	8.06	13.87
methycyclopentane	tr	v	3.37	3.36	3.35	0.01	0.02	0.30	0.52
methyl acetate	tr	v	0.18	0.18	0.36	0.00	0.18	0.00	99.33
methylamine	tr	tr/v	−0.57	−0.57	−0.79	0.00	0.22	0.00	38.33
methyl butyl ether	tr	tr/v	1.66	1.65	1.62	0.01	0.04	0.60	2.33
methyl mercaptan	tr	v	0.78	0.78	0.75	0.00	0.03	0.00	4.04
methyl propanoate	tr	tr/v	1.96	1.94	0.90	0.02	1.06	1.02	54.29
methyl propyl ether	tr	v	1.21	1.18	0.52	0.03	0.69	2.48	57.21
methylbenzylamine	tr	tr/v	1.52	1.52	1.46	0.00	0.06	0.00	4.01
methylcyclohexane	tr	v	3.61	3.59	4.01	0.02	0.40	0.55	11.10
methylethylamine	tr	tr/v	0.15	0.15	0.20	0.00	0.05	0.00	36.60
methylthiobenzene	tr	tr/v	2.74	2.72	3.36	0.02	0.62	0.73	22.59
m-methyl styrene	tr	tr/v	3.44	3.42	3.46	0.02	0.02	0.58	0.52
m-methylbenzyl alcohol	tr	tr/v	1.6	1.58	2.11	0.02	0.51	1.25	31.85
m-phenylphenol	tr	v	3.23	3.23	3.24	0.00	0.01	0.00	0.29
m-xylene	tr	v	3.13	3.11	3.21	0.02	0.08	0.64	2.55
naphthalene	tr	v	3.35	3.33	4.01	0.02	0.66	0.60	19.83
n-benzylaniline	tr	tr/v	3.13	3.11	3.27	0.02	0.14	0.64	4.62
n-butane	tr	tr/v	2.89	2.86	2.59	0.03	0.30	1.04	10.49
n-ethylaniline	tr	v	2.16	2.15	1.84	0.01	0.32	0.46	14.82
n-heptylamine	tr	tr/v	2.57	2.55	1.98	0.02	0.59	0.78	22.78
n-hexylamine	tr	tr/v	2.06	2.03	1.59	0.03	0.47	1.46	22.85
nitrobenzene	tr	tr/v	1.85	1.85	1.83	0.00	0.02	0.00	0.92
nitroethane	tr	tr/v	0.18	0.18	0.31	0.00	0.13	0.00	74.85
nitromethane	tr	tr/v	0.08	0.08	0.14	0.00	0.06	0.00	76.13
N-methylaniline	tr	tr/v	1.82	1.81	1.45	0.01	0.37	0.55	20.08
N-methyl-*N*-benzylaniline	tr	tr/v	4.22	4.22	3.33	0.00	0.89	0.00	21.03
N,*N*-dimethyl acetamide	tr	v	-0.77	-0.77	-0.45	0.00	0.32	0.00	41.00
N,*N*-dimethylaniline	tr	v	2.31	2.31	1.92	0.00	0.39	0.00	17.01
n-propylamine	tr	tr/v	0.48	0.46	0.18	0.02	0.30	4.17	62.99
n-propylaniline	tr	v	2.45	2.43	2.27	0.02	0.18	0.82	7.40
n-propylbenzene	ts	ts	3.68	3.63	3.65	0.05	0.03	1.36	0.86
n-propylpropionate	ts	ts	1.85	1.76	2.11	0.09	0.26	4.86	13.92
o-cresol (2-hydroxytoluene)	tr	tr/v	1.95	1.94	1.80	0.01	0.15	0.51	7.86
octafluorocyclobutane	tr	v	2.29	2.29	1.31	0.00	0.98	0.00	42.59
octane	tr	tr/v	5.18	5.15	4.85	0.03	0.33	0.58	6.38
o-ethyl-toluene	ts	ts	3.53	3.55	3.39	0.02	0.14	0.57	3.89
o-isobutylphenol	ts	ts	3.31	2.91	3.01	0.40	0.30	12.08	9.08
o-methylbenzaldehyde	tr	tr/v	2.26	2.26	1.89	0.00	0.37	0.00	16.51
o-methylbenzyl alcohol	tr	tr/v	1.58	1.58	2.03	0.00	0.45	0.00	28.69

Table 3 (Continued)

compounds	data set[a]		logK_{ow}			absolute error, logK_{ow}		absolute percent error, %[b]	
	fuzzy ARTMAP	back-propagation	reported logK_{ow}	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation
o-phenylphenol	ts	ts	3.09	3.23	3.19	0.14	0.10	4.53	3.25
o-*sec*-butylphenol	ts	ts	3.27	2.91	3.01	0.36	0.26	11.01	8.08
o-xylene	ts	ts	3.12	3.11	3.06	0.01	0.06	0.32	1.89
pentachlorobenzene	tr	tr/v	5.17	5.15	4.64	0.02	0.53	0.39	10.21
pentafluoroethylbenzene	tr	tr/v	3.36	3.36	4.07	0.00	0.71	0.00	21.21
pentanal	tr	tr/v	1.31	1.31	1.20	0.00	0.11	0.00	8.67
pentane	tr	tr/v	3.62	3.59	3.12	0.03	0.50	0.83	13.86
pentanenitrile	tr	tr/v	1.12	1.11	0.98	0.01	0.14	0.89	12.52
pentanoic acid	tr	v	3	2.99	3.15	0.01	0.15	0.33	5.14
p-ethyltoluene	tr	v	3.63	3.63	3.85	0.00	0.22	0.00	6.14
phenanthrene	tr	v	4.57	4.54	4.86	0.03	0.29	0.66	6.44
phenol	tr	tr/v	1.46	1.43	1.50	0.03	0.04	2.05	2.56
phenyl benzoate	tr	tr/v	3.59	3.59	3.34	0.00	0.25	0.00	6.91
phenyl formate	tr	tr/v	1.26	1.26	1.61	0.00	0.35	0.00	27.55
phenylacetaldehyde	tr	tr/v	1.78	1.76	1.84	0.02	0.06	1.12	3.51
phenylacetic acid	tr	tr/v	1.41	1.38	1.92	0.03	0.51	2.13	35.83
phenylacetic acid ethyl ester	ts	ts	2.42	2.39	2.63	0.03	0.21	1.24	8.68
phenylacetic acid methyl ester	tr	v	1.96	1.94	2.25	0.02	0.29	1.02	14.79
phenylacetonitrile	tr	tr/v	1.56	1.55	1.54	0.01	0.02	0.64	1.38
phenylacetylene	tr	v	2.4	2.39	2.91	0.01	0.51	0.42	21.21
phenylethyl sulfide	tr	tr/v	3.2	3.18	3.51	0.02	0.31	0.62	9.82
phenylpropyl ether	ts	ts	3.18	3.23	2.66	0.05	0.52	1.57	16.20
p-isobutylphenol	tr	tr/v	2.94	2.91	2.89	0.03	0.05	1.02	1.83
p-methyl styrene	ts	ts	3.35	3.25	3.44	0.10	0.09	2.99	2.72
p-methylacetophenone	tr	tr/v	2.28	2.26	2.28	0.02	0.00	0.88	0.07
p-methylbenzyl alcohol	tr	v	1.59	1.58	2.01	0.01	0.42	0.63	26.65
propane	tr	tr/v	2.36	2.35	2.00	0.01	0.36	0.42	15.26
propanenitrile	tr	tr/v	0.16	0.15	0.05	0.01	0.11	6.25	69.13
propionaldehyde	tr	tr/v	0.59	0.57	0.49	0.02	0.10	3.39	16.31
propionicacid	tr	tr/v	0.33	0.33	0.23	0.00	0.10	0.00	31.49
propiophenone	ts	ts	2.19	1.85	2.21	0.34	0.02	15.52	0.94
propyl formate	tr	tr/v	0.82	0.81	0.81	0.01	0.01	1.22	1.62
propylallylamine	tr	tr/v	1.33	1.33	1.38	0.00	0.05	0.00	3.79
propylbutylamine	tr	tr/v	2.12	2.10	2.11	0.02	0.01	0.94	0.28
propylisobutylamine	tr	tr/v	2.07	2.07	2.11	0.00	0.04	0.00	1.78
propyl-*sec*-butylamine	tr	tr/v	1.91	1.90	2.07	0.01	0.16	0.52	8.63
propyne	tr	tr/v	0.94	0.92	0.79	0.02	0.15	2.13	16.45
p-xylene	ts	ts	3.2	3.11	3.41	0.09	0.21	2.81	6.67
pyrazine	tr	tr/v	-0.22	-0.24	-0.70	0.02	0.48	9.09	220.17
pyrazine-2-one	tr	v	-1.49	-1.49	-1.59	0.00	0.10	0.00	6.83
pyridine	tr	tr/v	0.64	0.61	0.73	0.03	0.09	4.69	14.43
pyrrole	tr	tr/v	0.75	0.72	0.70	0.03	0.05	4.00	6.47
pyrrolidine	tr	v	0.46	0.46	0.69	0.00	0.23	0.00	49.38
sec-butyl alcohol	tr	tr/v	0.61	0.61	0.70	0.00	0.09	0.00	14.22
sec-butylamine	tr	tr/v	0.74	0.72	0.62	0.02	0.12	2.70	15.98
sec-butylbenzene	ts	ts	4.57	4.24	4.08	0.33	0.49	7.22	10.65
styrene	tr	tr/v	3.16	3.15	3.37	0.01	0.21	0.32	6.57
tert-butylbenzene	tr	v	4.11	4.09	4.15	0.02	0.04	0.49	0.98
tert-butyl alcohol	tr	tr/v	0.37	0.37	0.72	0.00	0.35	0.00	93.32
tert-butyl amine	tr	tr/v	0.4	0.37	0.45	0.03	0.05	7.50	13.00
tetrachlorocyclohexane	tr	tr/v	3.72	3.72	3.89	0.00	0.17	0.00	4.56
tetrachloroethene	tr	tr/v	3.4	3.40	2.98	0.00	0.42	0.00	12.42
tetrachloromethane	tr	tr/v	2.83	2.82	2.62	0.01	0.21	0.35	7.38
tetrafluoromethane	tr	v	1.18	1.18	1.46	0.00	0.28	0.00	23.83
tetrahydrofuran	tr	tr/v	0.46	0.46	0.59	0.00	0.13	0.00	28.70
tetrahydropyran	tr	v	0.95	0.92	1.62	0.03	0.67	3.16	70.44
thiophene	tr	v	1.81	1.81	1.76	0.00	0.05	0.00	2.55
thiophenol	tr	tr/v	2.52	2.51	1.47	0.01	1.05	0.40	41.61
toluene	tr	v	2.69	2.68	2.41	0.01	0.28	0.37	10.24
trans-1,2-diphenylethene	tr	v	4.81	4.81	4.96	0.00	0.15	0.00	3.20
tribromomethane	tr	tr/v	3.2	3.18	2.74	0.02	0.46	0.62	14.33
trichloroethene	ts	ts	2.42	2.10	2.49	0.32	0.07	13.22	2.84
trichlorofluoromethane	tr	tr/v	2.53	2.51	2.17	0.02	0.36	0.79	14.34
trichloromethane	tr	tr/v	1.97	1.94	2.04	0.03	0.07	1.52	3.47
triethylamine	tr	v	1.44	1.43	1.64	0.01	0.20	0.69	13.58
trifluorobenzene	tr	tr/v	2.52	2.51	2.87	0.01	0.35	0.40	14.08
trifluoromethane	tr	v	0.64	0.61	0.41	0.03	0.23	4.69	36.48
trifluoromethylbenzene	ts	ts	3.01	2.76	2.86	0.25	0.15	8.31	4.84
triiodomethane	tr	tr/v	2	1.98	2.15	0.02	0.15	1.00	7.71
trimethylamine	tr	v	0.27	0.27	0.21	0.00	0.06	0.00	23.31
tripropylamine	tr	tr/v	2.79	2.76	2.63	0.03	0.16	1.08	5.70
vinyl bromide	tr	v	1.57	1.55	1.26	0.02	0.31	1.27	19.48

[a] ts = test set, tr = training set, v = validation set; tr/v designate the training compounds added to the validation set to form a cross-validation set. [b] Absolute percent error % = $(|(\log K_{ow})_{EXP} - (\log K_{ow})_{PRE}|*100)/(|(\log K_{ow})_{EXP}|)$ where subsripts EXP and PRE designate the experimental and predicted values, respectively.

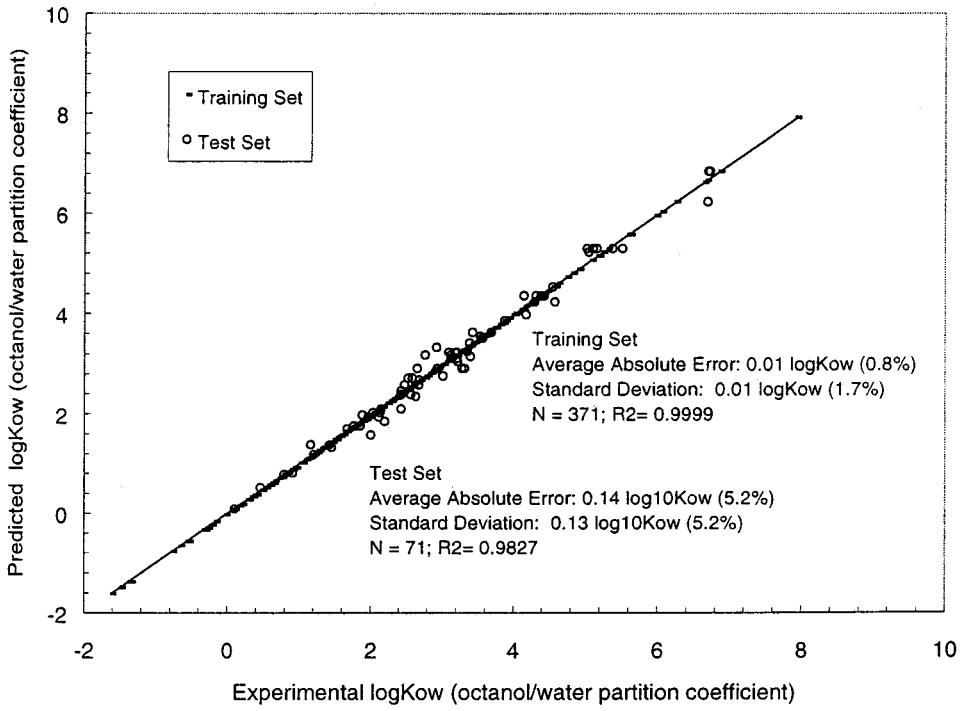

Figure 3. Octanol/water partition coefficient results for the fuzzy ARTMAP QSPR.

Back-Propagation Neural Network System. The normalized logK_{ow} data and molecular descriptors, normalized from 0 to 1, were divided into training, validation, and test data sets. The test data set of 71 compounds (about15% of the complete data set) was identical to the fuzzy ARTMAP test set to enable direct comparison of the QSPRs derived from two different networks. A random selection of 259 compounds of the remaining 371 compounds (about 58% of the total data set) made up the training set. However, to maintain an adequate validation set, the training (259 compounds) and nontraining data sets (112 compounds) were combined.

Model building with the back-propagation neural network proceeded with the same 12 input descriptors and logK_{ow} data set used for the fuzzy ARTMAP model. The architecture of the neural network was developed using a cascade method of network construction, together with a Kalman filtering learning rule.[62] In the above approach, hidden nodes are added one or two at a time with new hidden units having connections from both the input buffer and previously established hidden nodes. Construction is stopped when the validation set shows no further performance improvement. The optimal back-propagation neural network/QSPR for logK_{ow} had a 12−11−1 architecture in which the hyperbolic tangent transfer functions were chosen to correlate weighted inputs and outputs of the hidden layer. The optimal neural network architecture was then validated and tested using two separate data subsets as described above.

III. RESULTS AND DISCUSSION

The optimal fuzzy ARTMAP/QSPR for logK_{ow} was obtained (i.e. training phase) for vigilance parameters ρ_a = 0, ρ_b = 0.996, ρ_{ab} = 0.996, learning rate parameters β_a =1, β_b = 1, and choice parameter α = 0.0001. The performances of the above model and the logK_{ow} QSPR resulting from the 12−11−1 back-propagation neural network are described in Table 3 and Figures 3 and 4, with a summary of the error analysis provided in Tables 4 and 5.

The performance of the fuzzy ARTMAP logK_{ow} QSPR for the complete data set of 442 compounds was with average absolute and maximum errors of 0.03 and 0.45 logK_{ow} units, respectively, and a corresponding standard deviation of 0.07 logK_{ow} units (see Table 4). The fuzzy ARTMAP/QSPR performance for the test data set was evaluated with a relaxed vigilance parameter setting of ρ_a = 0.9, resulting in average and maximum absolute errors and standard deviation of 0.14, 0.45, and 0.13 logK_{ow} units, respectively. Although the performance of the logK_{ow} fuzzy ARTMAP/QSPR was excellent for the relatively heterogeneous compound data set, there were several compounds which were misclassified, thereby resulting in elevated logK_{ow} errors. It appears that while chemical input descriptors parameters can be similar for some chemicals (e.g., structural isomers), there may be a relatively large difference in their logK_{ow} values. For example, 2,2′,3,4,4′,5-hexachloro-1,1′-biphenyl (2,2′3,4,4′5-PCB) with a logK_{ow} = 6.69 was matched to the recognition category represented by 2,2′3,3′4,6-PCB with a logK_{ow} = 6.24, resulting in an absolute error of 0.45 logK_{ow} units. Another example of misclassification is the placing of 3-methyl-1-butanol into a recognition category generated for 1-pentanol; both compounds are primary alcohols with molecular formula of $C_5H_{12}O$ but with logK_{ow} values of 1.16 and 1.4, respectively. There were two cases for iodoethane and 2-octanone where high errors were observed since a suitable recognition category was not available. Iodoethane (logK_{ow} = 2) was classified with bromoethane (logK_{ow} = 1.6), and 2-octanone (logK_{ow} = 2.76) was matched with 2-nonanone (logK_{ow}= 3.18), resulting in absolute errors of 0.4 and 0.42 logK_{ow} units, respectively. The above examples clearly suggest that further improvements of the accuracy of the logK_{ow} QSPR would require a data set that contains

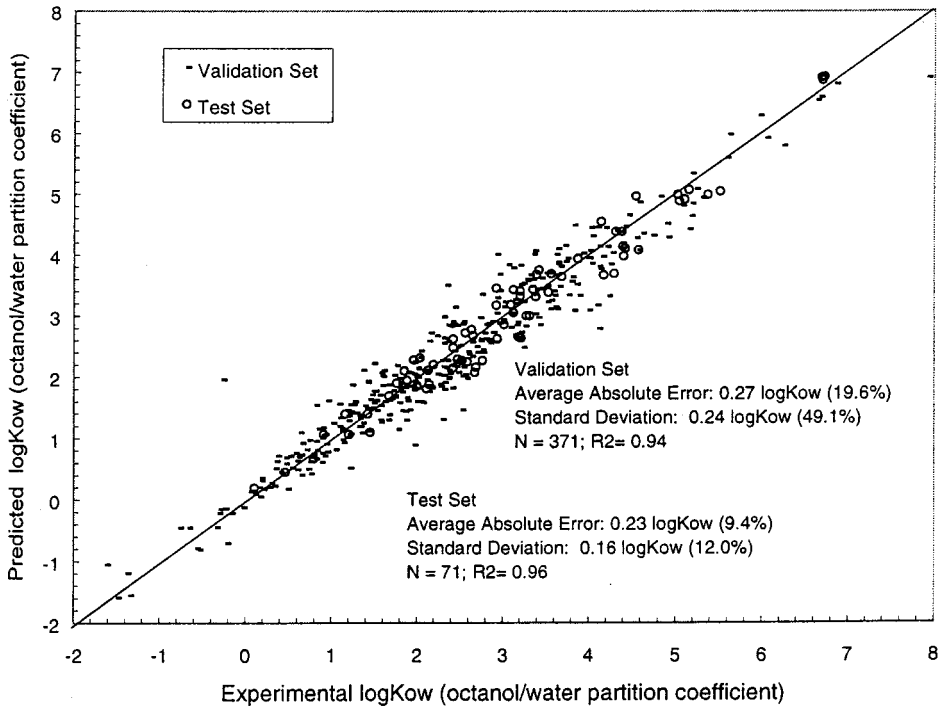

Figure 4. Octanol/water partition coefficient results for back-propagation QSPR.

Table 4. QSPR Performance for Octanol/Water Partition Coefficients ($\log K_{ow}$): Fuzzy ARTMAP and Back-Propagation Neural Networks based Models[a]

data set	no. of data points	av absolute error		max. absolute error		SD	
		$\log K_{ow}$	%	$\log K_{ow}$	%	$\log K_{ow}$	%
Fuzzy ARTMAP							
all data	442	0.03	1.55	0.45	21	0.07	3.1
training	371	0.01	0.84	0.03	20	0.01	1.7
test	71	0.14	5.24	0.45	21	0.13	5.2
Back-Propagation							
all data	442	0.27	18.0	2.2	827	0.23	45
training	259	0.26	17.6	1.3	291	0.22	28
validation	371	0.27	19.5	2.2	827	0.24	49.1
test	71	0.23	9.4	0.59	96.4	0.16	12.0

[a] Errors are expressed as $\log K_{ow}$ estimation errors.

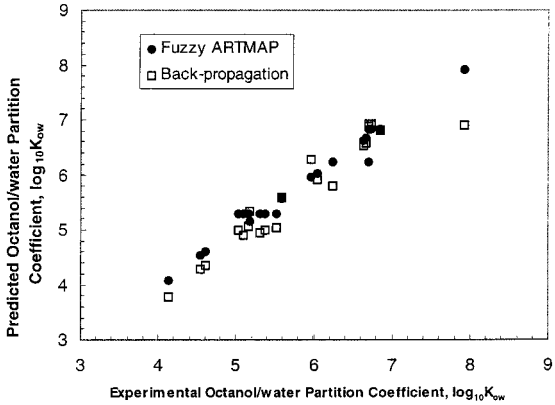

Figure 5. Octanol/water partition coefficient estimates for PCBs at 298 K.

a larger number of compounds per class and a refined set of molecular descriptors to allow greater ability to differentiate among complex or apparently very similar structures.

The performance of the optimal 11−12−1 back-propagation/QSPR was inferior, relative to the fuzzy ARTMAP based model, with average and maximum errors and standard deviation for the training set of 0.26 $\log K_{ow}$ units (17.6%), 1.3 $\log K_{ow}$ units (290.9%), and 0.22 $\log K_{ow}$ units (28%), respectively. Performance of the back-propagation/QSPR for the validation set was with with average and maximum errors and standard deviation of 0.27 $\log K_{ow}$ units (19.5%), 2.2 $\log K_{ow}$ units (827%), and 0.24 $\log K_{ow}$ units (49%), respectively. Performance of the back-propagation/QSPR was also lower relative to the fuzzy ARTMAP, for the same test set, with average and maximum absolute errors and standard deviation of 0.23 $\log K_{ow}$ units (9.4%), 0.59 $\log K_{ow}$ units (96.4%), and 0.16 $\log K_{ow}$ units (12.0%), respectively. We note, however, that the average absolute error and standard deviation for both the present fuzzy ARTMAP and back-propagation QSPRs are lower than those reported for experimental octanol/water partition data, which are generally of the order of about 0.4 $\log K_{ow}$ units.[4,5]

The highest error was encounter for 1,4-dioxan (2.2 $\log K_{ow}$ or 827%), which was classified as an outlier for the back-propagation/QSPR model. Three other outliers for the above model include isopropylamine, pyrazine, and 2-propanol ($\log K_{ow}$ of −0.03, −0.22, and 0.05, respectively) with corresponding $\log K_{ow}$ errors of 0.08 (or 291%), 0.48 (or 220%), and 0.08 (or 179%), respectively. The above four outliers were among the 15 compounds in the data set (representing 3% of the total data set) with $|\log K_{ow}|$ values ranging from 0.03 to 0.27. It should also be noted that absolute percent errors were generally higher for compounds with $|\log K_{ow}| < 0.3$.

The $\log K_{ow}$ estimation performance of the present QSPR models for a broad spectrum of compounds was further evaluated by inspecting chemical group-specific errors as given in Table 5 and Figures 5−8. Although absolute $\log K_{ow}$ errors are commonly reported in the literature, such errors can be misleading since the actual percent error can be

Table 5. Error Analysis Based on Chemical Class and Functional Group[a]

chemical class and functional group	no. of compds	av absolute error		percent absolute error	
		fuzzy ARTMAP	back-propagation	fuzzy ARTMAP	back-propagation
alkanes	27	0.01	0.35	0.42	11.23
alkenes	24	0.03	0.33	1.04	12.45
alkynes	6	0.01	0.16	0.87	8.71
aromatics	23	0.05	0.23	1.26	7.29
carboxcyclic acids	12	0.01	0.31	1.01	23.09
aldehydes	8	0.01	0.17	1.42	19.50
ketones	22	0.06	0.25	3.23	21.55
alcohols	23	0.02	0.20	2.98	32.88
ethers	9	0.01	0.24	3.01	22.04
amines	29	0.01	0.16	1.09	25.77
PCBs, PBrBs[b]	21	0.08	0.25	1.42	4.31
halogenated nonaromatic	59	0.03	0.27	1.82	15.36
halogenated aromatics	41	0.04	0.38	1.38	11.59
nitriles	8	0.01	0.12	2.96	18.84
nitro	9	0.01	0.15	0.45	27.34
esters	15	0.03	0.30	1.53	23.10
PAHs[c]	25	0.03	0.27	0.67	6.63
phenols	25	0.05	0.27	2.10	12.93
heterocyclic ring-nitrogen (e.g. pyridines)	11	0.01	0.24	1.92	37.46
mercaptans (sulfure containing)	16	0.02	0.23	0.75	10.29
furan (heterocyclic ring − oxygen)[d]	3	0.00	0.26	0.25	22.93
halogenate phenols	12	0.05	0.28	2.11	11.53
aromatic amines	11	0.01	0.26	0.58	12.06

[a] Errors are reported as logK_{ow} estimation errors averaged for each listed chemical group. [b] PBrBs are polybromobiphenyls. [c] Group contains some halogenated PAHs. [d] 1,4-Dioxan was declared an outliner and therefore was not included in this analysis.

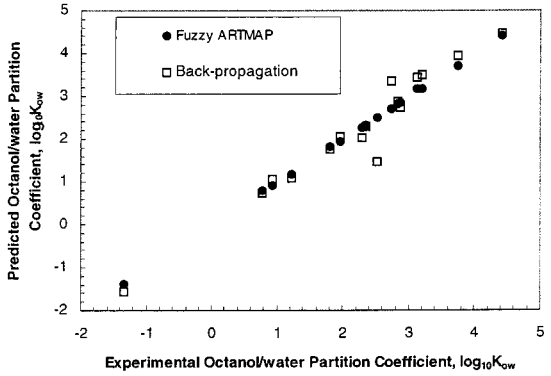

Figure 6. Octanol/water partition coefficient estimates for thiols at 298 K.

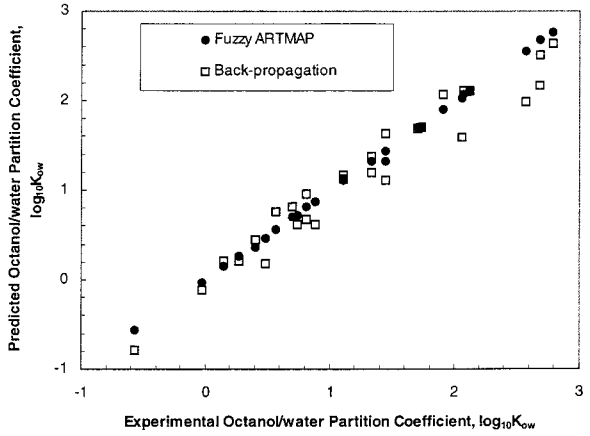

Figure 7. Octanol/water partition coefficient estimates for amines at 298 K.

significant even for a seemingly low absolute logK_{ow} error if, for example, the logK_{ow} values for such compounds are small. Conversely, a reported high absolute logK_{ow} error can

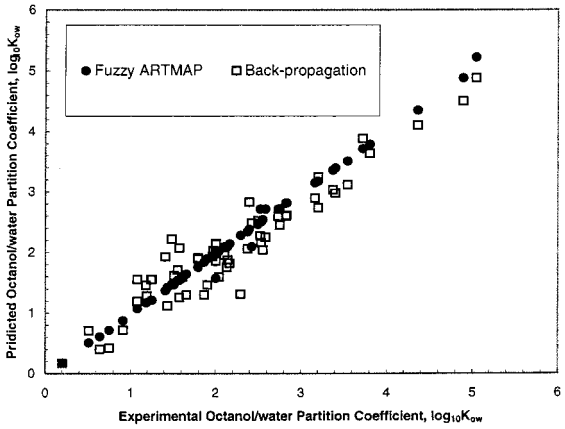

Figure 8. Octanol/water partition coefficient estimates for halogens at 298 K.

also be misleading if it pertains to a range of high logK_{ow} values. Therefore, to present a more balanced evaluation of the model performance for the 24 chemical groups in the complete data set, both the average |logK_{ow}| error along with the absolute percent logK_{ow} error are presented in Table 5.

For the present QSPR models, the absolute average and percent logK_{ow} errors for the different chemical groups varied by factors ranging from about 3.1−5 and 8.7−12%, respectively. The ranges for the average absolute and percent logK_{ow} errors for the fuzzy ARTMAP/QSPR were 0.0−0.8 logK_{ow} units and 0.25−3.23%, respectively. The average absolute and percent logK_{ow} errors for the back-propagation QSPR, for the different chemical groups, ranged from 0.12 to 0.38 logK_{ow} units and 4.31 to 37.46%, respectively. Inspection of Table 5 confirms that errors for the different chemical groups are of similar order for each respective model. Superior performance (in terms of absolute percent logK_{ow} error) of the back-propagation model was obtained for PCBs, PAHs, aromatics, and alkynes, relative to the other

Table 6. Comparison of the Present QSPRS with Other Published QSPRs

						comparison with present study			
						fuzzy ARTMAP		back-propagation	
study	approach	no. of compds in study	no. of common data points[a]	av absolute error[b]	absolute SD[b]	av absolute error[b]	absolute SD	av absolute error[b]	absolute SD
Klopmann et al. (1994)	group contribution	1663	274	0.18 (14.05)	0.21 (34.58)	0.027 (1.52)	0.03 (1.23)	0.25 (17.86)	0.2 (28)
Basak et al. (1996)	linear regression QSPR	219	205	0.31 (18.71)	0.39 (66.35)	0.03 (1.23)	0.06 (2.35)	0.25 (15.67)	0.19 (28.33)
Gombar and Enslein (1996)	multiple linear regression QSPR	6675	111	0.29 (31.53)	0.53 (66.3)	0.03 (1.31)	0.06 (2.58)	0.25 (19.85)	0.19 (37.08)
Eisfeld and Maurer (1999)	linear regression QSPR	202	91	0.18 (25.54)	0.13 (58.28)	0.02 (1.7)	0.04 (3.65)	0.25 (22.25)	0.19 (27.4)
Sblijic et al. (1993)	linear regression QSPR	31	15	0.19 (3.52)	0.21 (3.19)	0.04 (1.05)	0.07 (1.82)	0.30 (6.97)	0.23 (5.35)
Kamlet et al. (1988)	linear regression QSPR	102	22	0.17 (3.21)	0.23 (3.18)	0.021 (0.41)	0.03 (0.58)	0.28 (5.86)	0.22 (4.44)
Huuskonen et al. (2000)	neural network QSPR	1870	12	0.37 (23.9)	0.29 (22.3)	0.019 (1.01)	0.024 (1.26)	0.29 (20.9)	0.22 (19.9)

[a] Number of compounds common with the present study. [b] Absolute errors and standard deviation are given in terms of logK_{ow} units. The corresponding percent absolute logK_{ow} error and standard deviation are enclosed in parentheses.

groups (<10%). The highest error for the fuzzy ARTMAP model was obtained for the ketones group (3.23%), while errors of less than 2% were encountered for 18 of the 24 chemical groups.

Error analysis for the different chemical groups was also carried out for the back-propagation model (see Table 5). Average group percent errors of less than the overall average percent error for the back-propagation/QSPR test set (9.4%) were exhibited by alkynes, aromatics, PAHs, and PCBs (see Table 5). Average absolute errors of less than 0.23 logK_{ow} (i.e., average error for back-propagation/QSPR test set) were found for compounds that belong to the chemical groups containing alkynes, aldehydes, amines, nitriles, and nitro compounds. Average absolute and percent errors for the majority of the individual chemical groups were below the overall average errors for the validation and training sets of the back-propagation/QSPR model. However, six of the chemical groups (alkanes, alkenes, carboxcyclic acids, halogenated aromatics, esters, and halogenated phenols), representing 33% of the data set exhibited average absolute errors above 0.27 logK_{ow} (i.e., the average absolute logK_{ow} error for the back-propagation/QSPR based on the validation and overall data sets). Moreover, logK_{ow} estimation for nine of the chemical groups, representing 30% of the data set, were with average absolute logK_{ow} percent errors above 19.5% (the error observed by the back-propagation/QSPR based on the validation set). Carboxcyclic acids and esters were the only two functional groups with both average absolute and average percent errors above the average errors exhibited by the back-propagation/QSPR. For the back-propagation/QSPR, aromatic compounds (including PAHs, aromatic amines, aromatic halogens, and phenol) generally exhibited lower average percent errors relative to aliphatic compounds. It is also noted that the higher average percent errors were observed from compounds with an oxygen atom. Also, it is interesting to note that nitro compounds and alcohols, for which relatively low average absolute error ($\leq$0.2 logK_{ow}) were obtained, had a relatively higher average percent error (27−33%).

The performance of the fuzzy ARTMAP/QSPR and back-propagation/QSPR models suggest that the quantum chemical descriptors were suitable for characterizing the structural information of 442 organic compounds, which represented about 24 different chemical groups in the data set. The performance of the fuzzy ARTMAP and back-propagation/QSPR models for a number of specific chemical classes (PCBs, thiols (sulfur groups), amines, and halogens) is shown in Figures 5−8. The majority of the deviations is attributed to those chemical groups whose logK_{ow} data sets were either too sparse or too concentrated in a particular region. Clearly improved correlations would require the use of a uniformly distributed data set for training various chemical groups as well as for the overall data set.

The present fuzzy ARTMAP and back-propagation QSPRs were compared to previously reported neural network/QSPR and multiple linear regression/QSPR logK_{ow} models. We note that the range of average estimation errors for published models for predicting octanol/water partition coefficients for heterogeneous data sets[19,20,22,24−27,29] are 0.22−0.67 logK_{ow}. Average estimation logK_{ow} errors ranging from 0.22 to 0.45 logK_{ow} have been reported for multiple linear regression/QSPR models relative to 0.28−0.67 logK_{ow} errors typically reported for neural network/QSPRs. The performance of the fuzzy ARTMAP model, for the test set, with average absolute error and standard deviation of 0.14 and 0.13 logK_{ow}, respectively, was superior relative to both previous models as well as the present back-propagation neural network/QSPR. The performance of the present back-propagation/QSPR, with absolute error and standard deviation of 0.23 and 0.16 logK_{ow}, respectively, was well within the performance range or with greater accuracy than previously published back-propagation neural network/QSPR models. For example, Duprat et al.[25] developed several 6−7−1 and 7−6−1 neural network/QSPRs for estimating logK_{ow} for a set of 321 compounds and reported standard errors of 0.37−0.28 logK_{ow}. In a more recent study, Huuskonen et al.[26] developed a 39−5−1 neural network/QSPR derived from atomic-type electrotopological-state indices, for a diverse set of 1870 organic compounds[26] ($-4.2 \leq \log K_{ow} \leq 5.9$) and reported a root-mean-square error of 0.41 logK_{ow}.[26] Breindl et al.[27] developed two 16−25−1 back-propagation/QSPRs with descriptors derived from AM1 and PM3 Molecular

Orbital theory, based on a set of 1085 compounds ($-2.06 \leq \log K_{ow} \leq 7.41$). The latter two QSPRs was proposed of Breindl et al.,[27] which were validated based on a set of 105 compounds, performed with average absolute errors and standards deviations of 0.45 (80%) and 0.30 (243%) $\log K_{ow}$ and 0.53 (86%) and 0.42 (227%) $\log K_{ow}$ units, respectively. Recently, Beck et al.,[29] using the same compounds and 16 parameters (computed from AM1) as Breindl et al.,[27] proposed a 16−10−1 neural network/QSPR model which was tested with a set of 41 nucleosides and with a reported standard and maximum absolute error in predictions of $\log K_{ow}$ to be 0.39 and 1.05 $\log K_{ow}$, respectively.

The present back-propagation/QSPR was well within the performance range or with greater accuracy than previously published multiple linear regression/QSPR models. For example, Basak et al.[19] reported a standard error of 0.45 $\log K_{ow}$ for two multiple linear regression-based $\log K_{ow}$ QSPRs derived from topological and geometrical parameters ($0.2 \leq \log K_{ow} \leq 5.5$) of a heterogeneous set of 219 compounds. Gomber and Enslein[20] developed the VLOGP QSPR which makes use of a 363 chemical descriptors based on a set of 6675 chemicals ($-3.6 \leq \log K_{ow} \leq 7.7$). Performance of the VLOGP model, for a test set of 113 compounds, was reported as the average deviations for "best fit" and "worst fit" which corresponded to 0.27 and 0.44 $\log K_{ow}$ units. More recently, Eisfeld and Maurer[24] proposed a linear regression $\log K_{ow}$ QSPR, derived using quantum chemical descriptors and a set of 202 compounds ($-2 \leq \log K_{ow} \leq 5.7$), with a reported standard deviation and maximum absolute error to 0.274 and 0.821 $\log K_{ow}$ units, respectively. A more specific performance comparison of the present QSPRs for compounds that are common between the above studies and the present study is presented in Table 6. In all cases the fuzzy ARTMAP QSPR displayed lower errors and standard deviation. The performance of the back-propagation QSPR was mixed with lower errors, for the same set of compounds, compared with the QSPRs of Gombar and Enslein (1996) and Basak et al. (1996) but slightly higher average absolute error for compounds common with the studies of Klopmann et al. (1994), Esifeld and Maurer (1999), Sblijic et al. (1993), and Kamlet et al. (1988). However, it is emphasized that the percent error was lower for the present back-propagation QSPR when compared with the predictions of the QSPRs of Eisfeld and Maurer (1999) and with a lower standard deviation compared to the QSPRs of Klopmann et al. (1994) and Eisfeld and Maurer (1999). The lower errors for the Sblijic et al. (1993) and Kamlet et al. (1988) results are not surprising since these studies focused on relatively homogeneous chemical data sets. Better performance of the present back-propagation $\log K_{ow}$ QSPR model, compared to QSPRs developed from much larger data set, could also be, in part, due to the more heterogeneous character of these larger data sets.

CONCLUSIONS

The applicability of fuzzy ARTMAP networks for developing a $\log K_{ow}$ was demonstrated using a set of molecular descriptor calculated from PM3 semiempirical MO-theory. The set of descriptors obtained from PM3 semiempirical MO-theory calculations represented different forms of three-dimensional information for characterizing the various atoms and functional groups for a set of heterogeneous organic compounds. The fuzzy ARTMAP-based $\log K_{ow}$ QSPR, developed from a heterogeneous data set of 442 compounds ($-1.6 \leq \log K_{ow} \leq 7.0$), performed with average absolute errors of 0.03 and 0.14 $\log K_{ow}$ units for the overall and test sets, respectively. In contrast, the 12−11−1 back-propagation based $\log K_{ow}$ QSPR performed with average absolute errors for the test and validation data sets of 0.23 and 0.27 $\log K_{ow}$ units, respectively. The fuzzy ARTMAP neural network-based QSPR $\log K_{ow}$ model was superior to other neural network /QSPRs and multilinear regression/QSPRs reported in the literature. The present evaluation of the fuzzy ART classifier and the fuzzy ARTMAP cognitive system show that such a neural network system can be used to establish reasonably accurate quantitative structure−property relationships for heterogeneous compounds based on a set of descriptors calculated from quantum mechanics and graph theory. Further optimization and expansion of the set of chemical descriptors is currently underway to better classify isomers and other complex chemical structures.

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