A Fuzzy ARTMAP-Based Quantitative Structure−Property Relationship (QSPR) for the Henry's Law Constant of Organic Compounds

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Quantitative structure−property relationships (QSPRs) for estimating a dimensionless Henry's Law constant of organic compounds at 25 °C were developed based on a fuzzy ARTMAP and back-propagation neural networks using a heterogeneous set of 495 organic compounds. A set of molecular descriptors developed from PM3 semiempirical MO-theory and topological descriptors (second-order molecular connectivity index) were used as input parameters to the neural networks. Quantum chemical input descriptors included average molecular polarizability, dipole moments (total point charge, total hybridization, and total sum), ionization potential, and heat of formation. The fuzzy ARTMAP/QSPR correlated Henry's Law constant for $-6.72 \leq \log H \leq 2.87$ with average absolute errors of 0.03 and 0.13 logH units for the overall data and the test set, respectively. The optimal 7−17−1 back-propagation/QSPR model was less accurate and exhibited larger average absolute errors of 0.28 and 0.27 logH units for the validation (recall) and test sets, respectively. The fuzzy ARTMAP-based QSPR was superior to the back-propagation and multiple linear regression/QSPR models for Henry's Law constant of organic compounds.

I. INTRODUCTION

The Henry's Law constant for chemical air−water partitioning, typically defined as the ratio of a chemical partial pressure P_a in air to its mole fraction x_a in water, is a key parameter for assessing the distribution of trace organic compounds among the various environmental media (e.g., air, water, vegetation, soil, sediment, and groundwater). Henry's Law constant data are also essential for the design of air stripping technologies for the remediation of organic-contaminated aqueous streams and groundwater. The Henry's Law constant, H, which is usually concentration-independent for dilute systems, is typically reported in units of atm.m^3/gmol. However, in most correlations, as is the case in the present work, H is reported as a dimensionless partition coefficient (i.e., $H=C_a/C_w$, where C_a and C_w are the chemical equilibrium concentrations in the air and water phases, respectively). Although H can vary with temperature,[1−3] its value (usually taken at 25 °C) is often (explicitly or implicit) assumed to be temperature invariant over the range of interest for most environmental applications. Since the dimensionless Henry's law constant varies over many orders of magnitude (10^{-7} to 10^3), it is commonly reported as logH.

Experimental determination of the Henry's Law constant for organic compounds is not a trivial task, especially for organic compounds of very low vapor pressures or low aqueous solubilities.[4,5] Brennan et al.,[6] note that experimentally measured Henry's Law constants have been reported in the literature for fewer than 600 organic chemicals out of the over 70 000 chemicals that are in current use. Moreover, *H* values reported by different sources, for a given compound, can often differ by factors of up to 7.0, with an average variation of a factor of 2.4.[6]

Given the limited Henry's Law constant data, several approaches for estimating Henry's Law have been developed.[1−3,7] The simplest estimation is based on the theoretical expression $H = \gamma_\infty P^s$, where γ_∞ and P^s are the chemical infinite dilution activity coefficient and saturation vapor pressure, respectively. Molecular activity coefficients at infinite dilution can be estimated with UNIFAC,[1,7,8] modified-UNIFAC,[7−10] and UNIQUAC[1] group contribution methods. The above methods require interaction parameters that are obtained from model fits to experimental phase-equilibrium data. Unfortunately, group interaction parameters for UNIFAC and reliable vapor pressure data are often lacking for chemicals of environmental interest, as well as for many heterocyclic aromatic compounds and compounds with functional groups containing sulfur and phosphorus.[7−10]

Group contribution[11,12] and quantitative structure−property relations (QSPRs)[4−6,13−16] have been popular estimation methods of the Henry's Law constant for organic compounds. For example, Hine and Mookerjee[11] proposed bond contribution and group contribution schemes for logH, based on data sets of 263 and 212 compounds ($-5 < \log H < 2$), with a reported standard deviations of 0.42 and 0.12 logH units, respectively, for the above two sets.[11] The bond contribution approach of Hine and Mookerjee,[11] which was not validated with an external chemical data set, was later revised by Meylan and Howard,[12] who expanded the bond contribution factors and added correction factors, based on a data set of

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345 chemicals, demonstrating a lower standard deviation of 0.34 logH units. Validation of the above model with a heterogeneous set of 74 chemicals ($-5 \leq \log H \leq 3$) demonstrated a standard deviation of 0.46 logH units.

An early example of a logH-linear QSPR was reported by Nirmalakhandan and Speece[4] based on a set of 180 compounds ($-4.99 \leq \log H \leq 2.32$) using a set of structural chemical descriptors (a first-order valence molecular connectivity index, a hydrogen bonding index and a polarizability parameter). The above QSPR was validated with a data set of 20 organic compounds ($-2.98 \leq \log H \leq -1.27$) with a reported average absolute error of 0.34 (26%) logH units. The Nirmalakhandan and Speece[4] QSPR was tested in a subsequent study by Nirmalakhandan et al.,[5] with a set of 105 organics ($-5.23 \leq \log H \leq 2.32$) of 'similar' structures (aliphatic hydrocarbons, halogenated aliphatic and aromatic, aromatic, PAHs, esters, acids, alcohols and phenols) performing with an average absolute error and standard deviation of 0.41 (68.8%) and 0.40 (179.3%) logH units, respectively. An update of the above model, with optimized contributions to the polarizability parameter and an additional set of 87 chemicals (aldehydes, ketones, amines, nitro compounds, pyridines, and sulfonated compounds), resulted in a reduced average absolute error and standard deviation of 0.33 (13%) and 0.36 (14%) logH units, respectively, for the range of $-6.06 \leq \log H \leq -0.94$. A test of the above model with a heterogeneous set of 70 chemicals ($-8.07 \leq \log H \leq -0.15$) led to logH estimations with an average absolute error and standard deviation of 0.56 and 0.61 logH, respectively. In a later study, Russell et al.,[17] reported an optimal logH-linear correlation, derived using a data set of 63 organic compounds ($-4.91 \leq \log H \leq 2.12$), with five structural descriptors (selected from a set of 165 descriptors) revealing an absolute logH errors of 0.375 and 0.34 for the training set and a test set consisting of only seven compounds.

Correlations of dimensionless water/air partition coefficients using a solvatochromic approach have also been proposed in the literature. For example, Abraham et al.[13] proposed a correlation of the so-called Ostwald solubility coefficient, L_w ($= H^{-1}$) using the linear solvation energy relationship (LSER) method with five solvatochromic parameters that included excess molar refraction, dipolarity/polarizability, effective hydrogen-bond acidity, effective hydrogen bond basicity, and McGowan characteristic volume. The $\log L_w$ correlation, for a training set of 408 chemicals (equivalent range of $-8 \leq \log H \leq 2.32$), performed with a standard deviation of 0.151 $\log L_w$ units;[13] however, model performance for an external data set was not demonstrated. Another example is the linear $\log L_w$ QSPR reported by Katritzky et al.,[14] based on using seven molecular descriptors and a data set of 406 chemicals from Abraham et al.,[13] which performed with a standard deviation and average absolute error of 0.52 and 0.42 $\log L_w$ units, respectively. In a later study Katritzky et al.,[15] correlated $\log L_w$ (for an equivalent Henry's law constant range of $-6.99 \leq \log H \leq 2.32$), where L_w values were estimated from aqueous solubility and vapor pressure QSPRs, with a standard deviation of 0.63 $\log L_w$ units.

In recent years, a variety of QSPRs for physicochemical properties that are based on neural networks (NNs) have gained popularity as alternatives to regression-based QSPRs that make use of *a priori* analytical correlation equations. The advantage of NNs, over classical regression analysis methods, is their inherent ability to incorporate nonlinear relationships between chemical structural parameters and physicochemical properties.[16−21] Neural network/QSPR models for estimating the Henry's Law constant for a data set of 357 organic compounds ($-7.08 \leq \log H \leq 2.32$) have been recently reported by English and Carroll (2001).[16] The above authors reported QSPRs based on 12-4-1 and 10-3-1 back-propagation neural network architectures (trained using 303 compounds) that performed with absolute errors of 0.237 and 0.281 logH units for the test set (54 compounds), respectively.

Recently, neural network-based QSPR models that are based on the cognitive classifier fuzzy ARTMAP have been proposed for the estimation of boiling temperature,[18,19] critical properties,[19] aqueous solubility,[20] and octanol−water partition coefficients[21] of organics. The approach was shown to be superior to the popular back-propagation neural network approach as well as other statistical QSPR correlations reported in the literature. The application of fuzzy ARTMAP network for NN-based QSPR development has several advantages since it does not require problem-specific crafting or choice of initial weights, it does not get trapped in local minima (a problem that typically increases with data set size), and it is capable of classifying and analyzing noisy data.[22−27] The recent success of NN-based QSPRs suggests that there is merit in exploring the applicability of the approach for estimating the Henry' law constant for organic compounds, which is the focus of the present study.

In the present study we report on the development of a QSPR for the Henry's law constant based on both a fuzzy ARTMAP and back-propagation neural networks. The above approaches were evaluated based on a heterogeneous set of 495 organic compounds and chemical descriptors obtained from PM3 semiempirical MO-theory calculations. The performance of the proposed models and that of other published approaches were compared to demonstrate the potential application and reliability of the fuzzy ARTMAP approach.

II. METHODOLOGY

Data Set and Molecular Descriptors. The overall approach of developing the present neural network-based logH QSPRs is summarized in Figure 1. The first step involved the compilation of experimental Henry's Law constants at 25 °C for a diverse set of 495 organic compounds.[5−7,11−13] The compiled dimensionless H data, presented in Tables 1 and 2 as logH, covered a range of $-6.72 \leq \log H \leq 2.87$. The heterogeneous data set of compounds included 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 Henry's Law constant 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 logH values, respectively, and X_{min} and X_{max} are the minimum and maximum logH values in the data set, respectively.

Molecular descriptors for each compound were calculated based on the chemical molecular structure. Molecular

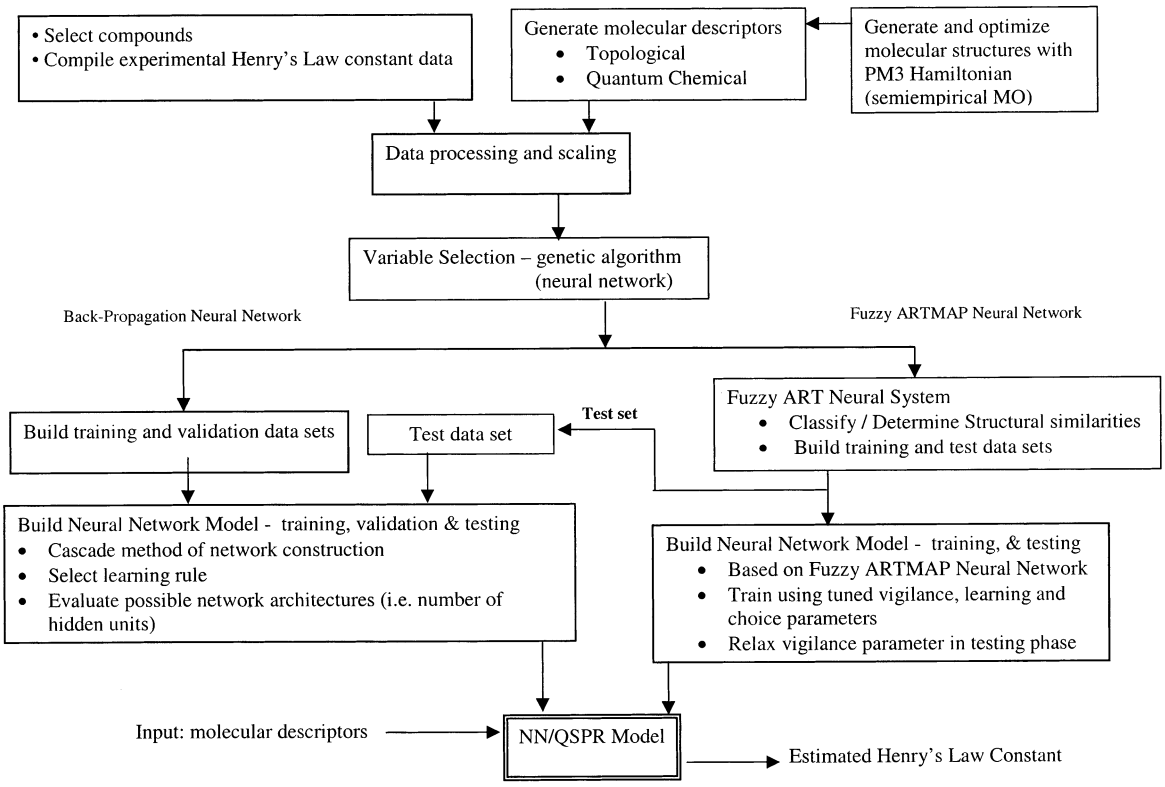

Figure 1. Process flow diagram for developing fuzzy ARTMAP and back-propagation QSPR/neural networks for predicting Henry's Law constant.

structures were drawn using Molecular Modeling Pro 3.01 (ChemSW Software Inc.)[28] and converted to 3-dimensional structures using the CAChe Software (Oxford Molecular Ltd.).[29] The geometries of the 3-dimensional structures were subsequently optimized using MOPAC,[30] a semiempirical molecular orbital modeling program, with the PM3 (parametric model 3) Hamiltonian[31] 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 (point-charge, hybridization, total) moments of inertia (x, y, and z directions), ionization potential, number of doubly occupied (filled) MO levels, molecular weight, heat of formation, total energy, and energy components that included the one-center (three descriptors) and two-center terms (seven descriptors). The total energy, in terms of the PM3 MO, is the sum of the total one-center and two-center terms both also used as independent descriptors. The one-center energy terms include electron−electron repulsion, and electron−nuclear attraction as well as the sum of these two energy terms. The two-center energy terms consisted of the following descriptors: resonance energy, exchange energy, electron−electron repulsion, electron−nuclear attraction, nuclear−nuclear repulsion, the sum of the exchange and resonance energies and the total two-center energy terms. Finally, the total electrostatic interaction was also used as a descriptor. This latter descriptor is the sum of the three two-center energy terms: electron−electron repulsion, electron−nuclear attraction, and nuclear−nuclear repulsion energy.

Molecular topological descriptors, which were also utilized in the present QSPRs, included the four valance molecular connectivity indices of orders 1, 2, 3, and 4 ($^1\chi^v$, $^2\chi^v$, $^3\chi^v$, $^4\chi^v$)[32,33] and the second Kappa shape index, $^2\kappa$.[34] The above molecular indices were generated from the 2-dimensional molecular structure using Molecular Modeling Pro 3.01 software. Molecular connectivity indices, which encode 2-dimensional structural information, are determined from a molecular structure 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 valance-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, $^2\kappa$, is included to characterize the level of branching among isomers.

The set of input descriptors for the final QSPR was selected, from the initial set of 28 descriptors, using a nonlinear variable selection method based on a dynamic neural network genetic algorithm.[35] Variable selection analysis was performed based on the generation of eleven different back-propagation neural networks to identify the optimal set of descriptors based on a frequency distribution (of the descriptors selected in each run). The final set of seven

Table 1. Molecular Descriptors and Experimental Henry's Law Constants at 25 °C

compound	H[a]	m_P[b]	μ_H[c]	m_S[d]	IP[e]	PO[f]	$^2\chi^v$[g]	logH
1,1,1,2-tetrachloro-2,2-difluoroethane	−122.92	1.52	0.39	1.13	11.09	49.22	3.74	−0.78
1,1,1,2-tetrachloroethane	−31.90	0.51	0.70	1.21	10.73	47.38	3.52	−0.95
1,1,1-trichloroethane	−31.91	0.78	0.60	1.38	10.75	40.13	3.62	−0.18
1,1,1-trichloropropane	−36.57	0.87	0.57	1.42	10.72	46.76	3.48	−0.88
1,1,2,2-tetrabromoethane	10.14	0.63	0.38	1.01	10.36	60.04	7.06	−3.24
1,1,2,2-tetrachloroethane	−29.54	0.57	0.95	1.52	10.74	46.34	2.99	−1.82
1,1,2-trichloroethane	−27.70	0.53	0.55	1.08	10.67	38.51	2.13	−1.32
1,1,2-trichloropropane	−34.93	0.83	0.58	1.39	10.57	45.77	2.86	−1.89
1,1,3-trimethylcyclopentane	−41.76	0.02	0.05	0.04	11.21	54.14	4.01	1.81
1,1-dichlorobutane	−37.03	1.06	0.62	1.66	10.55	44.78	2.45	−0.51
1,1-dichloroethane	−26.53	0.97	0.65	1.62	10.58	30.76	2.05	−0.63
1,1-dichloroethene	3.11	0.11	0.67	0.78	9.74	31.89	1.44	0.03
1,1-difluoroethene	−79.64	1.42	0.17	1.59	10.76	16.88	0.34	1.16
1,2,3-trichloropropane	−32.98	1.23	1.06	2.29	10.57	44.11	2.14	−1.85
1,2,3-trimethylbenzene	−2.82	0.55	0.03	0.52	9.25	70.68	2.52	−0.89
1,2,4,5-tetramethylbenzene	−12.39	0.03	0.05	0.02	8.95	79.74	3.02	0.01
1,2,4-trichlorobenzene	4.80	0.14	0.58	0.67	9.24	76.04	2.81	−0.76
1,2,4-trimethylbenzene	−3.87	0.28	0.05	0.23	9.08	71.24	2.59	−0.62
1,2-dibromo-3-chloropropane	−15.21	1.97	0.63	2.45	10.11	50.35	3.15	−2.22
1,2-dibromoethane	−3.41	0.01	0.00	0.01	11.22	40.17	1.96	−1.56
1,2-dibromopropane	−12.52	0.54	0.07	0.52	11.15	47.62	3.14	−1.22
1,2-dichlorobenzene (o)	11.14	0.37	0.98	1.35	9.29	64.47	2.23	−1.11
1,2-dichloroethane	−24.68	0.01	0.00	0.01	10.67	30.35	1.13	−1.31
1,2-dichloroethylene	3.56	0.00	0.00	0.00	9.52	32.74	0.75	−0.78
1,2-dichloropropane	−32.17	0.33	0.09	0.37	10.65	37.75	1.99	−0.94
1,2-diethylbenzene	−8.15	0.55	0.04	0.53	9.28	76.68	2.48	−0.97
1,3,5-trichlorobenzene	3.98	0.00	0.00	0.00	9.59	76.51	2.89	−1.02
1,3,5-trimethlybenzene	−4.47	0.01	0.00	0.00	9.28	71.01	2.67	−0.62
1,3-butadiene	31.03	0.00	0.00	0.00	9.47	35.26	0.47	0.48
1,3-dibromopropane	−8.68	1.59	0.23	1.82	11.08	44.30	2.31	−1.44
1,3-dichlorbenzene (m)	10.20	0.34	0.54	0.88	9.42	65.47	2.31	−0.97
1,3-dichloropropane	−30.44	0.84	0.66	1.50	10.55	36.98	1.49	−1.14
1,3-dimethylnaphthalene	23.18	0.35	0.01	0.36	8.64	101.82	3.30	−1.81
1,4-dichlorobenzene (p)	10.11	0.00	0.00	0.00	9.23	65.99	2.31	−1.01
1,4-dichlorobutane	−36.23	0.02	0.00	0.02	10.53	44.28	1.84	−1.70
1,4-diethylbenzene	−4.03	0.10	0.05	0.09	9.23	77.34	2.52	−0.51
1,4-dimethylbenzene (*p*-xylene)	4.78	0.02	0.03	0.05	9.18	62.95	2.15	−0.55
1,4-dimethylnaphthalene	24.67	0.02	0.01	0.01	8.59	101.17	3.24	−2.07
1,4-pentadiene	26.58	0.08	0.00	0.08	10.05	39.50	0.81	0.68
1,5-dichloropentane	−41.70	0.87	0.65	1.52	10.50	51.34	2.19	−1.64
1,5-dimethylnaphthalene	24.70	0.01	0.00	0.01	8.60	100.98	3.24	−1.83
1,5-hexadiene	21.06	0.14	0.01	0.15	10.10	46.40	1.15	0.84
1,6-heptadiene	15.65	0.08	0.00	0.08	10.14	53.70	1.51	0.44
1-bromo-2-chloroethane	−13.95	0.59	0.39	0.21	10.73	34.82	1.55	−1.43
1-bromo-2-methylpropane	−57.68	1.41	0.29	1.66	11.11	33.23	1.52	−0.02
1-bromobutane	−22.10	1.72	0.11	1.82	10.93	40.18	1.83	−0.45
1-bromoheptane	−38.33	1.74	0.14	1.85	10.93	61.58	2.89	0.27
1-bromohexane	−32.91	1.75	0.11	1.84	10.93	54.47	2.54	0.19
1-bromonaphthalene	49.28	1.02	0.14	1.13	8.99	95.91	3.31	−1.93
1-bromooctane	−43.75	1.76	0.11	1.84	10.93	68.70	3.25	0.38
1-bromopentane	−27.50	1.73	0.14	1.84	10.93	47.36	2.19	−0.09
1-bromopropane	−16.69	1.69	0.14	1.81	10.93	32.94	1.48	−0.52
1-butanol	−67.57	0.92	0.62	1.42	10.89	32.28	1.08	−3.43
1-butene	1.43	0.23	0.03	0.21	10.15	30.32	0.70	1.01
1-chloro-1,1-difluoroethane	−119.79	1.74	0.41	2.02	11.27	24.57	1.44	0.71
1-chloro-2-methylpropane	−32.94	0.97	0.55	1.51	10.37	35.82	1.86	−1.31
1-chlorobutane	−32.80	1.07	0.50	1.56	10.41	36.47	1.42	−0.17
1-chlorohexane	−43.63	1.09	0.49	1.58	10.41	50.68	2.13	0.06
1-chloronaphthalene	34.65	0.39	0.56	0.91	8.80	93.35	2.87	−1.84
1-chlorooctane	−54.47	1.11	0.49	1.58	10.42	64.88	2.83	0.19
1-chloropentane	−38.22	1.07	0.51	1.57	10.41	43.60	1.77	−0.01
1-chloropropane	−27.41	1.04	0.52	1.55	10.41	29.32	1.07	−0.27
1-cyanobutane	7.74	2.49	0.84	3.33	11.80	40.24	1.26	−2.67
1-cycanopropane	13.13	2.44	0.87	3.30	11.89	33.12	0.91	−2.58
1-decanol	−100.09	0.91	0.62	1.41	10.89	74.65	3.20	−2.71
1-dodecanol	−110.93	0.91	0.62	1.41	10.89	88.82	3.91	−2.67
1-ethyl-2-methylbenzene	0.63	0.48	0.03	0.45	9.32	69.38	2.28	−0.76
1-ethyl-4-methylbenzene	0.56	0.07	0.03	0.04	9.18	70.30	2.34	−0.69
1-ethylnaphthalene	27.90	0.34	0.04	0.31	8.70	99.72	2.99	−1.07
1-heptadecanol	−138.04	0.88	0.65	1.40	10.89	124.20	5.67	−2.05
1-heptanol	−83.82	0.89	0.65	1.41	10.89	53.45	2.14	−2.64
1-heptyne	19.41	0.55	0.18	0.37	10.76	49.93	1.66	0.44
1-hexadecanol	−132.62	0.91	0.62	1.41	10.90	117.18	5.32	−2.40
1-hexene	−9.42	0.23	0.03	0.21	10.15	44.67	1.43	1.23

Table 1. (Continued)

compound	H[a]	m_P[b]	μ_H[c]	m_S[d]	IP[e]	PO[f]	$^2\chi^v$[g]	logH
1-hexyne	24.83	0.55	0.19	0.37	10.76	42.78	1.31	0.23
1-iodobutane	−8.29	1.76	0.05	1.79	9.45	43.96	2.10	−0.19
1-iodopropane	−2.95	1.73	0.07	1.77	9.45	36.63	1.75	−0.43
1-methoxy-2-propanol	−97.69	0.49	0.38	0.61	10.63	36.28	1.30	−4.42
1-methylcyclohexene	−14.28	0.20	0.07	0.16	9.33	51.61	2.30	0.48
1-methylnaphthalene	32.60	0.28	0.01	0.27	8.71	92.33	2.80	−1.97
1-nitropropane	−26.30	3.73	0.53	4.21	12.07	34.44	1.03	−2.45
1-nonanol	−94.67	0.88	0.65	1.41	10.89	67.60	2.84	−2.90
1-nonene	−25.69	0.23	0.03	0.21	10.15	65.97	2.49	1.51
1-nonyne	8.57	0.55	0.18	0.38	10.76	64.15	2.37	0.77
1-octadecanol	−143.47	0.91	0.63	1.40	10.89	131.34	6.03	−0.89
1-octanol	−89.23	0.91	0.62	1.40	10.89	60.52	2.49	−3.00
1-octene	−20.27	0.23	0.03	0.21	10.15	58.88	2.14	1.59
1-octyne	14.00	0.56	0.19	0.37	10.77	57.03	2.01	0.52
1-pentadecanol	−127.20	0.88	0.65	1.40	10.89	110.04	4.97	−2.80
1-pentanol	−73.00	0.89	0.65	1.41	10.89	39.32	1.43	−3.27
1-pentene	−4.01	0.22	0.03	0.21	10.14	37.55	1.08	1.21
1-pentyne	30.23	0.53	0.17	0.36	10.76	35.61	0.95	−0.05
1-propanol	−62.20	0.89	0.64	1.43	10.88	25.23	0.72	−3.52
1-propene	6.40	0.23	0.00	0.23	10.11	23.25	0.41	0.90
1-tetradecanol	−121.77	0.91	0.62	1.41	10.90	102.98	4.61	−2.37
2,2,2-trifluoroethanol	−209.06	2.64	0.84	3.48	12.04	18.86	0.77	−3.15
2,2′,3,3′,4,6′-hexachloro-1,1′-biphenyl	17.48	0.11	1.58	1.61	9.26	158.75	5.79	−2.75
2,2′,3,4,4′,5′-hexachloro-1,1′-biphenyl	15.90	0.03	0.99	1.02	9.21	162.76	5.85	−3.08
2,2′,3,4′,5′,6-hexachloro-1,1′-biphenyl	16.53	0.08	1.00	1.05	9.22	160.29	5.87	−2.68
2,2,3-trimethyl-3-pentanol	−87.38	0.95	0.69	1.52	10.96	59.52	3.88	−3.43
2,2,3-trimethylbutane	−43.40	0.05	0.03	0.05	11.33	49.06	3.52	1.99
2,2′,4,5,5′-pentachloro-1,1′-biphenyl	19.98	0.16	0.57	0.70	9.25	150.83	5.43	−2.43
2,2,4-trimethylpentane	−50.35	0.16	0.08	0.08	11.24	56.36	4.16	2.12
2,2′,5-trichloro-1,1′-biphenyl	41.70	0.47	0.54	0.98	9.03	131.27	4.35	−2.00
2,2,5-trimethylhexane	−56.04	0.03	0.04	0.04	11.14	63.35	4.49	2.15
2,2′,6,6′-tetrachloro-1,1′-biphenyl	28.55	0.03	0.02	0.04	9.36	134.71	4.82	−2.09
2,2′3,3′-tetrachloro-1,1′-biphenyl	27.11	0.39	1.37	1.76	9.31	135.97	4.77	−2.21
2,2′4,4′,5,5′-hexachloro-1,1′-biphenyl	15.04	0.03	0.03	0.01	9.20	163.88	5.93	−2.85
2,2-dimethyl propanoic acid	−115.59	2.27	0.45	1.88	11.20	41.06	2.56	−3.94
2,2-dimethyl-1-butanol	−75.93	0.75	0.68	1.30	10.90	45.74	2.68	−2.85
2,2-dimethyl-3-pentanol	−83.02	1.00	0.66	1.56	10.83	52.62	3.29	−3.00
2,2-dimethylbutane	−39.59	0.09	0.03	0.07	11.48	42.24	2.91	1.84
2,2-dimethylpentane	−45.34	0.11	0.05	0.06	11.19	49.41	3.31	2.11
2,2-dimethylpropane	−35.83	0.00	0.00	0.00	12.06	35.06	3.00	1.95
2,3,4-trimethylpentane	−48.41	0.05	0.01	0.04	11.08	56.57	3.35	1.88
2,3′-dichloro-1,1′-biphenyl	40.80	0.71	0.43	1.07	9.06	121.30	3.83	−2.00
2,3-dichloro-1,1′-biphenyl	42.13	0.08	1.12	1.19	9.05	121.18	3.75	−2.04
2,3-dichlorobutane	−38.78	0.38	0.05	0.43	10.58	45.13	2.73	−0.53
2,3-dichloropropene	−2.87	0.35	0.03	0.38	9.95	38.18	1.45	−0.84
2,3-dimethy-2-butanol	−78.78	0.92	0.72	1.50	11.17	45.63	2.81	−3.39
2,3-dimethyl-1,3-butadiene	15.15	0.00	0.00	0.00	9.28	48.95	1.56	0.93
2,3-dimethyl-2-pentanol	−84.30	0.93	0.72	1.47	11.12	52.80	2.96	−3.33
2,3-dimethyl-3-pentanol	−83.54	1.03	0.69	1.58	11.03	52.74	2.87	−3.36
2,3-dimethylbutane	−39.22	0.00	0.00	0.00	11.30	42.63	2.49	1.72
2,3-dimethylnaphthalene	24.13	0.52	0.06	0.47	8.64	101.55	3.28	−2.04
2,3-dimethylpentane	−44.08	0.04	0.02	0.04	11.25	49.71	2.63	1.85
2,3-dimethylphenol	−39.27	1.05	0.67	1.66	8.99	67.15	2.22	−4.52
2,3-dimethylpyridine	12.27	0.76	1.33	1.91	9.60	60.56	1.91	−3.54
2,4,4′-trichloro-1,1′-biphenyl	34.39	0.37	0.60	0.75	8.88	138.12	4.41	−2.10
2,4,6-triclorophenol	−39.42	0.30	0.70	1.00	9.12	81.18	2.97	−3.97
2,4′-dichloro-1,1′-biphenyl	36.46	0.56	0.94	1.49	9.15	119.08	3.83	−2.03
2,4-dichloro-1,1′-biphenyl	41.11	0.21	0.69	0.83	8.92	124.28	3.83	−1.92
2,4-dimethyl-2-pentanol	−85.85	1.07	0.65	1.55	11.19	53.04	3.41	−3.16
2,4-dimethyl-3-pentanol	−82.15	0.95	0.70	1.51	10.75	52.98	2.98	−2.98
2,4-dimethyl-3-pentanone	−72.03	2.07	0.37	2.44	10.35	52.44	2.71	−1.84
2,4-dimethylpentane	−45.01	0.11	0.08	0.03	11.49	49.70	3.02	2.08
2,4-dimethylphenol	−38.83	0.39	0.71	0.93	8.85	68.05	2.29	−4.41
2,4-dimethylpyridine	11.61	0.77	1.34	2.08	9.75	60.70	1.97	−3.57
2,5-cyclohexzdiene-1,4-dione	−31.55	0.02	0.00	0.02	10.92	54.40	1.47	−1.71
2,5-dichloro-1,1′-biphenyl	40.81	0.27	0.11	0.28	9.01	122.12	3.83	−1.92
2,5-dimethylphenol	−40.23	0.63	0.66	1.19	8.96	67.78	2.29	−4.34
2,5-dimethylpyridine	11.64	0.53	1.35	1.87	9.53	61.30	1.98	−3.46
2,6-dichloro-1,1′-biphenyl	49.75	0.74	0.29	1.03	9.00	120.66	3.78	−2.03
2,6-dichlorophenol	−33.25	0.53	0.83	1.34	9.19	69.83	2.38	−3.96
2,6-diethylaniline	−1.83	0.82	1.18	1.28	8.46	86.37	2.70	−4.34
2,6-dimethyl-4-heptanone	−81.87	1.88	0.59	2.48	10.51	66.24	3.73	−2.32
2,6-dimethylnaphthalene	24.70	0.01	0.00	0.01	8.60	100.98	3.24	−1.93
2,6-dimethylphenol	−38.70	0.49	0.70	1.18	8.96	67.47	2.24	−3.86

Table 1. (Continued)

compound	H[a]	m_P[b]	μ_H[c]	m_S[d]	IP[e]	PO[f]	$^2\chi^v$[g]	logH
2-bromoethyl benzene	18.47	0.93	0.11	1.00	9.61	72.94	2.80	−1.21
2-bromopropane	−20.85	1.93	0.11	2.04	10.86	33.96	2.84	−0.35
2-butanol	−68.72	0.95	0.69	1.50	11.01	32.06	1.26	−3.43
2-butanone	−57.44	2.24	0.47	2.70	10.66	31.69	1.06	−2.63
2-chloro-1-nitrobenzene	11.82	4.64	0.93	5.38	9.94	70.28	2.04	−2.74
2-chloro2-methylpropane	−37.75	1.22	0.50	1.72	10.41	36.82	3.20	0.80
2-chlorobutane	−34.60	1.19	0.49	1.68	10.42	36.95	1.93	−0.01
2-chloroethanol	−59.98	0.72	0.72	1.41	10.51	25.27	0.79	−4.51
2-chloronaphthalene	33.91	0.54	0.53	1.07	8.90	95.54	2.93	−1.87
2-chloropentane	−40.09	1.24	0.46	1.70	10.41	44.14	2.31	−0.22
2-chlorophenol	−28.15	0.44	0.26	0.67	9.21	59.63	1.86	−3.34
2-chloropropane	−29.77	1.16	0.51	1.66	10.42	29.82	1.88	−0.15
2-chloropyridine	23.36	0.82	1.63	2.44	9.65	54.27	1.54	−3.22
2-ethylbutyric acid	−120.54	2.29	0.49	1.89	11.23	48.91	1.85	−4.18
2-ethylnaphthalene	27.59	0.40	0.04	0.39	8.75	100.87	3.04	−1.48
2-ethylpyridine	17.81	0.38	1.39	1.67	9.76	59.75	1.67	−3.17
2-fluorophenol	−64.56	1.28	0.58	0.94	9.40	52.17	1.45	−3.88
2-heptanone	−73.73	2.16	0.51	2.66	10.68	52.80	2.16	−2.23
2-hexanol	−79.75	0.98	0.68	1.52	11.00	46.34	1.99	−3.00
2-hexanone	−68.31	2.20	0.48	2.66	10.68	45.76	1.81	−2.42
2-iodophenol	4.49	0.47	0.69	0.68	9.04	67.68	2.59	−4.55
2-iodopropane	−5.25	2.06	0.03	2.08	9.43	38.15	3.46	−0.55
2-methyl-1,3-butadiene	22.15	0.20	0.02	0.19	9.36	39.36	1.05	0.50
2-methyl-1-butanol	−72.01	0.82	0.65	1.35	10.91	39.11	1.70	−3.24
2-methyl-1-pentene	−12.44	0.33	0.06	0.37	9.79	44.55	1.71	1.05
2-methyl-1-propanol	−67.25	0.82	0.65	1.39	10.91	31.98	1.58	−2.96
2-methyl-2-butanol	−75.18	1.03	0.71	1.56	11.18	38.80	2.17	−3.25
2-methyl-2-butene	−12.00	0.19	0.05	0.22	9.40	39.03	1.37	0.95
2-methyl-2-hexanol	−85.62	0.98	0.72	1.52	11.17	52.84	2.92	−3.20
2-methyl2-pentanol	−80.89	1.05	0.68	1.55	11.11	46.03	2.56	−2.84
2-methyl-2-propanol	−71.27	0.98	0.71	1.54	11.28	31.57	2.17	−3.28
2-methyl-3-pentanol	−78.09	1.01	0.67	1.57	10.83	46.07	2.22	−2.85
2-methyl-3-pentanone	−66.68	2.19	0.42	2.61	10.45	45.78	1.97	−2.20
2-methylaziridine	22.54	0.52	1.42	1.79	9.83	27.63	1.31	−3.46
2-methylbutane (isopentane)	−34.39	0.06	0.03	0.04	11.43	35.73	1.80	1.76
2-methylhexane	−45.40	0.05	0.03	0.04	11.18	49.86	2.54	2.15
2-methylnaphthalene	31.23	0.30	0.02	0.31	8.76	93.38	2.85	−1.78
2-methylpentane	−39.60	0.06	0.05	0.02	11.31	42.70	2.18	1.84
2-methylpropane	−29.53	0.05	0.04	0.01	11.59	28.62	1.73	1.68
2-methylpyridine	21.16	0.48	1.34	1.75	9.80	52.34	1.47	−3.40
2-nitropropane	−27.14	3.64	0.53	4.16	11.92	34.20	1.32	−2.31
2-nitrotoluene	9.54	4.37	0.63	5.00	10.24	68.72	2.01	−2.63
2-nonanone	−84.40	2.15	0.48	2.62	10.68	66.94	2.87	−1.82
2-octanone	−79.03	2.19	0.46	2.63	10.68	59.90	2.51	−2.11
2-pentanol	−74.37	1.02	0.66	1.53	11.00	39.28	1.64	−3.22
2-pentanone	−62.93	2.19	0.50	2.68	10.67	38.71	1.45	−2.47
2-pentene	−7.76	0.04	0.02	0.04	9.60	38.37	0.98	0.99
2-phenyl-1-ethanol	−27.70	0.72	0.59	1.26	9.46	65.10	1.96	−4.98
2-propanol	−63.95	0.98	0.66	1.52	11.04	25.03	1.09	−3.35
2-undecanone	−95.28	2.15	0.49	2.62	10.68	81.06	3.57	−1.58
3,3′,5-trichloro-1,1′-biphenyl	34.41	0.67	0.39	1.05	9.11	132.63	4.41	−2.16
3,3-dimethyl-2-butanol	−77.47	0.87	0.68	1.46	10.94	45.54	3.04	−3.00
3,3-dimethyl-2-butanone	−67.05	2.28	0.43	2.71	10.50	45.07	2.81	−2.28
3,3-dimethylpentane	−43.59	0.06	0.01	0.06	11.46	49.35	2.87	1.88
3,4-dichloro-1,1-biphenyl	35.33	0.62	0.96	1.57	8.92	124.94	3.81	−2.23
3,4-dichlorotoluene	1.72	0.69	0.96	1.65	9.17	73.65	2.73	−0.98
3,4-dimethylphenol	−39.55	0.99	0.68	1.47	8.87	67.93	2.27	−4.77
3,4-dimethylpyridine	11.84	1.17	1.27	2.41	9.72	60.45	1.96	−3.83
3,5-dimethylphenol	−40.31	0.73	0.70	1.24	9.04	67.63	2.35	−4.60
3,5-dimethylpyridine	11.35	0.89	1.30	2.19	9.62	60.76	2.04	−3.55
3-chlorophenol	−28.35	0.78	1.20	1.94	9.28	60.70	1.92	−4.85
3-chloropropane	3.60	0.87	0.55	1.43	10.23	30.47	0.75	−3.35
3-chloropyridine	24.25	0.55	1.15	1.70	9.67	53.34	1.61	−2.94
3-ethyl-3-pentanol	−83.17	0.98	0.67	1.55	10.81	53.36	2.29	−3.43
3-ethylphenol	−34.58	0.45	0.71	0.88	9.08	66.66	2.02	−4.59
3-formylpyridine	−3.60	1.63	0.91	1.08	10.41	56.21	1.40	−5.21
3-heptanol	−84.48	1.02	0.67	1.60	10.93	53.35	2.20	−2.94
3-heptanone	−72.38	2.10	0.48	2.58	10.57	52.98	2.00	−2.43
3-hexanol	−79.19	1.02	0.67	1.60	10.92	46.26	1.85	−3.00
3-hexanone	−67.00	2.09	0.50	2.59	10.57	45.90	1.64	−2.29
3-methyheptane	−49.90	0.08	0.01	0.08	11.19	56.94	2.66	2.18
3-methyhexane	−44.55	0.10	0.04	0.08	11.25	49.88	2.30	1.99
3-methyl-1-butanol	−72.99	0.95	0.60	1.44	10.78	39.14	1.91	−3.26
3-methyl-1-butene	−3.94	0.18	0.04	0.16	10.27	37.08	1.48	1.34

Table 1. (Continued)

compound	H[a]	m_P[b]	μ_H[c]	m_S[d]	IP[e]	PO[f]	$^2\chi^{v\,g}$	logH
3-methyl-2-butanol	−73.09	0.91	0.68	1.48	11.01	39.03	1.98	−3.15
3-methyl-2-butanone	−62.51	2.18	0.43	2.60	10.56	38.25	1.77	−2.38
3-methyl-2-pentanol	−77.29	0.89	0.68	1.45	10.97	45.94	2.13	−2.85
3-methyl-3-hexanol	−84.65	1.04	0.67	1.63	11.12	53.01	2.60	−3.28
3-methyl-3-pentanol	−79.37	0.99	0.71	1.56	11.07	45.90	2.20	−3.14
3-methylpentane	−38.99	0.07	0.01	0.07	11.44	42.74	1.92	1.84
3-methylpyridine	20.86	0.81	1.29	2.07	9.80	52.21	1.53	−3.50
3-methylthiophene	21.08	0.71	1.66	0.95	9.31	50.77	2.08	−0.53
3-nitrotoluene	5.10	4.97	0.49	5.46	10.28	68.60	2.07	−2.53
3-pentanol	−73.67	1.04	0.68	1.61	10.92	39.19	1.47	−3.19
3-pentanone	−61.52	2.15	0.47	2.61	10.55	38.86	1.25	−2.50
4-bromochlorobenzene	24.57	0.68	0.45	0.24	9.51	68.42	2.79	−1.23
4-bromophenol	−14.12	0.95	0.71	1.52	9.31	63.15	2.39	−5.21
4-bromotoluene	21.65	1.41	0.09	1.49	9.55	66.60	2.71	−1.02
4-chloro-2-nitrophenol	−38.86	4.06	0.51	3.64	9.63	76.39	2.25	−3.29
4-chloro-3-methylphenol	−36.96	0.72	0.98	1.56	8.94	68.77	2.34	−4.98
4-chloroaniline	14.42	1.16	1.22	1.97	8.58	66.59	1.99	−4.32
4-chlorophenol	−28.39	0.49	0.93	1.39	9.01	60.76	1.91	−5.16
4-ethylpyridine	17.13	1.09	1.29	2.37	10.04	59.34	1.71	−3.47
4-fluorophenol	−64.98	1.33	0.71	1.84	9.27	52.46	1.48	−4.54
4-formylpyridine	−2.71	1.67	1.02	1.68	10.38	55.92	1.40	−5.14
4-heptanone	−72.50	2.04	0.53	2.58	10.58	52.99	2.04	−2.14
4-methyl-1-pentene	−8.93	0.27	0.05	0.25	10.02	44.26	1.92	1.41
4-methyl-2-methoxyphenyol	−23.80	0.68	0.36	1.04	8.90	68.80	2.02	−4.26
4-methyl-2-pentanol	−79.61	0.99	0.66	1.52	10.97	46.22	2.48	−2.74
4-methyl-2-pentanone	−67.84	2.11	0.52	2.62	10.65	45.28	2.30	−2.25
4-methyl-2-pentyl acetate	−120.31	1.69	0.09	1.77	11.15	64.75	3.05	−1.62
4-methylphenol (*p*-cresol)	−30.91	0.68	0.68	1.18	8.95	59.63	1.84	−4.39
4-methylpyridine	20.78	0.97	1.31	2.27	10.06	51.97	1.52	−3.62
4-*n*-propylphenol	−39.70	0.78	0.64	1.23	8.93	74.57	2.42	−4.33
4-*tert*-butylphenol	−43.56	0.72	0.67	1.20	9.00	80.56	3.80	−4.34
4-vinylcyclohexene	16.12	0.19	0.06	0.14	9.59	59.27	2.28	0.26
5-methyl-2-hexanone	−73.51	2.21	0.47	2.67	10.66	52.52	2.63	−2.23
a,a,a-triflluorotoluene	3.87	1.27	0.57	1.84	10.07	81.14	4.14	−1.19
acenaphthene	38.84	0.59	0.03	0.56	8.59	98.45	3.43	−2.20
acenaphthylene	73.13	0.22	0.07	0.30	9.06	101.78	3.13	−2.33
acetaldehyde	−43.60	2.07	0.40	2.46	10.70	17.30	0.24	−2.57
acetamide	−50.96	2.86	1.01	3.31	10.09	24.71	0.61	−6.74
acetic acid	−102.00	2.16	0.41	1.83	11.44	20.52	0.52	−5.39
acetone (propanone)	−53.32	2.32	0.46	2.78	10.77	24.53	0.91	−2.79
acetonitrile	23.29	2.29	0.91	3.21	12.33	18.63	0.22	−2.85
acetophenone	−17.67	2.36	0.44	2.79	10.00	65.37	1.92	−3.37
a-chlorotoluene	12.14	0.75	0.59	1.33	9.66	61.49	1.89	−1.59
allylbenzene (2-propenyl)	35.30	0.09	0.06	0.15	9.39	71.47	1.98	−0.55
amyl formate (pentyl)	−106.12	3.34	0.61	3.91	11.16	51.27	1.67	−1.26
amyl propionate (pentyl)	−119.14	1.83	0.08	1.83	11.16	65.25	2.28	−1.46
aniline	21.30	0.62	1.17	1.30	8.61	55.86	1.41	−4.08
anthracene	61.67	0.00	0.00	0.00	8.25	131.41	3.55	−2.62
benz[*a*]pyrene (3,4-benzo)	81.68	0.05	0.03	0.02	8.04	198.33	5.45	−1.86
benzaldehyde	−10.65	2.27	0.42	2.69	10.05	58.35	1.53	−2.95
benzene	23.46	0.00	0.00	0.00	9.75	45.60	1.15	−0.64
benzo[*b*]fluoroanthene (2,3-benzo)	95.90	0.12	0.02	0.14	8.40	193.18	5.42	−1.69
benzo[g,h,I]perylene	83.43	0.04	0.02	0.03	8.14	207.39	6.20	−1.96
benzo[*k*]fluoroanthene (8,9-benzo)	93.62	0.24	0.03	0.27	8.66	188.39	5.45	−1.75
benzoic acid methyl ester	−57.88	2.12	0.06	2.08	10.08	70.27	1.86	−2.88
benzonitrile	58.48	2.75	0.86	3.61	10.09	61.85	1.48	−3.09
benzyl acetate	−63.52	1.88	0.08	1.85	9.58	77.08	2.27	−3.34
biphenyl	47.58	0.00	0.00	0.00	8.92	102.00	2.73	−1.95
bromobenzene	31.05	1.09	0.09	1.18	9.80	57.59	2.21	−1.00
bromodichloromethane	−4.95	1.21	0.62	1.51	10.56	26.20	1.57	−1.06
bromoethane	−11.37	1.71	0.14	1.85	10.91	25.99	1.39	−0.51
bromomethane	−1.98	1.36	0.19	1.55	11.01	17.07	0.00	−0.67
butane	−29.06	0.00	0.00	0.00	11.35	28.95	1.00	1.59
butanethiol	14.16	1.24	1.14	2.38	11.20	39.08	1.52	−0.73
butyl acetate	−109.50	1.90	0.03	1.91	11.25	50.81	1.69	−1.94
butyraldehyde	−54.56	2.21	0.35	2.54	10.62	31.72	0.96	−2.33
chlorobenzene	16.71	0.39	0.54	0.93	9.38	55.14	1.73	−0.85
chlorodifluoromethane	−109.70	1.26	0.43	1.52	11.36	17.11	0.58	0.09
chloroethane	−22.06	1.02	0.53	1.55	10.41	22.24	0.80	−0.46
chloroethene	9.72	0.32	0.59	0.91	9.84	22.96	0.46	−0.02
chloromethane	−14.68	0.81	0.57	1.38	10.48	14.02	0.00	−0.42
chlorotrifluoromethane	−169.25	1.32	0.27	1.04	11.88	17.01	0.86	1.75
cis-1,2-dibromoethene	32.50	0.00	0.00	0.00	10.42	40.26	1.31	−0.78
cis-1,2-dichloroethene	3.56	0.01	0.00	0.00	9.52	32.74	0.75	−0.51

Table 1. (Continued)

compound	H[a]	m_P[b]	μ_H[c]	m_S[d]	IP[e]	PO[f]	$^2\chi^v$[g]	logH
cis-1,2-dimethylcyclohexane	−40.33	0.00	0.01	0.01	10.96	55.26	3.24	1.17
cis-2-pentene	−7.76	0.04	0.02	0.04	9.60	38.37	0.98	0.96
cumene	5.49	0.26	0.03	0.25	9.51	68.10	2.57	−0.33
cycloheptane	−30.25	0.06	0.05	0.02	11.03	48.56	2.47	0.58
cyclohexane	−31.03	0.00	0.00	0.00	11.29	41.86	2.12	0.86
cyclohexanol	−71.06	1.02	0.67	1.50	10.89	45.08	2.29	−3.94
cyclohexanone	−60.14	2.46	0.37	2.81	10.48	44.80	2.10	−3.43
cyclohexene	1.26	0.16	0.01	0.17	9.52	43.64	1.76	0.27
cyclopentane	−23.87	0.03	0.02	0.01	11.09	33.86	1.77	−0.87
cyclopentanone	−55.16	2.39	0.32	2.71	10.60	37.02	1.75	−3.39
cyclopentene	3.02	0.16	0.01	0.15	9.52	35.87	1.40	0.42
cyclopropane	16.27	0.00	0.00	0.00	11.77	20.85	1.06	0.55
decalin (decahydronaphthalene)	−44.49	0.00	0.00	0.00	11.02	68.41	4.09	1.28
decan-2-one	−89.86	2.18	0.46	2.62	10.68	74.00	3.22	−1.72
di(*n*-butyl) ether	−78.73	0.74	0.38	1.12	10.49	62.05	2.32	−0.61
di(*n*-propyl) ether	−68.06	0.70	0.41	1.11	10.48	47.83	1.61	−1.05
dibromochloromethane	−94.09	0.64	0.10	0.54	11.17	33.63	3.48	−1.49
dibromomethane	7.87	1.13	0.32	1.45	10.59	27.97	2.72	−1.47
dichlorodifluoromethane	−116.05	1.18	0.39	0.80	11.33	26.94	1.57	1.21
dichlorofluoromethane	−61.98	0.98	0.56	1.25	10.99	25.13	1.23	−0.36
dichloromethane	−17.14	0.68	0.68	1.36	10.58	22.36	0.91	−0.97
diethyl ether	−57.44	0.78	0.37	1.15	10.48	33.58	0.78	−1.30
diethylamine	−19.51	0.18	1.31	1.18	9.15	35.68	0.96	−2.98
diethyl sulfide	−17.18	0.37	1.57	1.94	8.86	43.08	2.34	−1.07
difluoromethane	−103.76	1.46	0.36	1.81	12.86	8.19	0.10	−1.88
diisobutylamine	−39.93	0.28	1.36	1.08	9.08	63.39	3.45	−1.64
di-isopropyl ether	−69.37	0.92	0.39	1.31	10.55	47.40	2.23	−1.03
di-isopropylamine	−32.00	0.30	1.35	1.22	9.18	49.42	2.48	−2.36
di-isopropylsulfide	−25.57	0.51	1.49	2.00	8.92	57.82	4.38	−0.88
dimethyl ether	−48.31	0.85	0.40	1.26	10.69	18.64	0.41	−1.27
dimethylamine	−7.89	0.09	1.32	1.27	9.22	21.09	0.50	−3.15
dimethyl sulfide	−10.96	0.36	1.60	1.96	8.88	26.75	1.22	−1.18
di-*n*-butylamine	−40.95	0.22	1.34	1.15	9.19	64.01	2.46	−2.38
di-*n*-propylamine	−30.15	0.21	1.35	1.16	9.18	49.82	1.75	−2.68
dipropylsulfide	−27.83	0.26	1.63	1.89	8.86	57.40	2.83	−0.94
ethane	−18.14	0.00	0.00	0.00	11.98	14.95	0.00	1.31
ethanol	−56.85	0.93	0.62	1.45	10.90	18.20	0.32	−3.69
ethene	16.63	0.00	0.00	0.00	10.64	15.01	0.00	0.94
ethyl acetate	−98.89	1.90	0.05	1.92	11.25	36.43	0.92	−2.26
ethyl formate	−90.00	3.33	0.60	3.91	11.16	29.72	0.55	−1.80
ethyl mercaptan	25.06	1.17	1.16	2.33	11.21	24.64	0.95	−0.73
ethyl propionate	−103.13	1.81	0.11	1.83	11.15	43.77	1.16	−2.05
ethyl propyl ether	−62.75	0.74	0.39	1.13	10.48	40.70	1.20	−1.33
ethylbenzene	10.58	0.35	0.03	0.33	9.40	61.53	1.84	−0.46
ethylbenzoate	−62.67	2.09	0.04	2.09	10.06	78.21	2.09	−2.67
ethylbutyrate	−108.58	1.77	0.13	1.81	11.17	50.92	1.56	−1.79
ethylcyclohexane	−40.72	0.05	0.02	0.05	10.95	55.73	2.91	1.09
ethylene oxide (oxirane)	−8.13	1.88	0.10	1.78	11.34	17.18	0.61	−2.22
fluorene	49.02	0.36	0.01	0.37	8.84	108.81	3.49	−2.46
fluorobenzene	−20.23	1.49	0.11	1.60	9.80	46.96	1.30	−0.59
fluoromethane	−53.80	1.14	0.30	1.44	12.92	7.92	0.00	−0.10
formaldehyde	−34.08	1.83	0.34	2.16	10.63	9.92	0.00	−2.02
formic acid	−90.12	3.02	0.91	3.94	11.29	13.66	0.11	−5.15
furan	−4.03	0.07	0.15	0.22	9.38	32.09	0.79	−0.66
heptanal	−70.79	2.26	0.33	2.59	10.63	53.03	2.02	−1.96
heptanoic acid	−127.94	2.18	0.49	1.78	11.36	55.94	2.20	−4.86
hexachloro-1-propene	−18.82	1.06	0.06	1.07	9.65	78.94	4.67	−0.71
hexachlorobenzene	−9.10	0.00	0.00	0.00	9.31	108.70	4.15	−2.70
hexachlorocyclopentadiene	4.55	0.74	0.05	0.78	9.04	97.73	4.66	0.04
hexachloroethane	−36.48	0.01	0.00	0.01	10.84	64.76	5.54	−0.28
hexanal	−65.42	2.26	0.34	2.58	10.63	45.94	1.66	−2.06
hexanoic acid	−122.57	2.15	0.47	1.80	11.36	48.86	1.85	−4.51
indane	11.26	0.47	0.02	0.45	9.22	67.86	2.62	−1.07
iodobenzene	44.75	0.82	0.03	0.79	9.04	63.21	2.52	−1.28
iodoethane	2.09	1.77	0.06	1.83	9.44	29.61	1.77	−0.55
iodomethane	9.45	1.32	0.12	1.44	9.47	19.95	0.00	−0.67
isoamyl acetate	−114.83	1.83	0.05	1.87	11.15	57.73	2.52	−1.62
isoamyl formate	−105.98	3.39	0.58	3.94	11.14	51.17	2.15	−1.56
isobutane	−29.52	0.05	0.04	0.01	11.59	28.61	1.73	1.69
isobutene	−3.32	0.34	0.02	0.36	9.80	30.72	1.21	0.95
iso-butylamine	−23.16	0.24	1.53	1.36	9.43	34.54	1.39	−3.26
isobutyl formate	−100.34	3.22	0.65	3.84	11.14	43.76	1.82	−1.67
isobutyl propanoate	−113.19	1.88	0.12	1.87	11.15	57.81	1.93	−1.17
isobutylbenzene	0.30	0.34	0.09	0.34	9.39	76.02	3.08	0.12

Table 1. (Continued)

compound	H[a]	m_P[b]	μ_H[c]	m_S[d]	IP[e]	PO[f]	$^2\chi^v$[g]	logH
isobutylisobutanoate	−117.77	1.95	0.11	1.89	11.04	64.61	3.18	−1.24
isobutyraldehyde	−54.56	2.07	0.39	2.45	10.54	31.39	1.38	−2.10
isophorone	−48.87	3.32	0.42	3.74	10.07	69.91	3.97	−3.57
2-propanol	−63.94	0.98	0.66	1.52	11.05	25.03	1.09	−3.48
isoproplyamine	−17.32	0.20	1.43	1.32	9.38	27.54	1.24	−2.73
isopropylbenzene	4.80	0.23	0.04	0.21	9.53	67.96	2.57	−0.22
isopropyl acetate	−104.31	1.78	0.11	1.82	11.17	43.30	1.66	1.94
isopropyl formate	−96.29	3.43	0.61	4.02	11.09	36.70	1.28	−1.50
m-bromotoluene	21.63	1.28	0.07	1.36	9.65	66.45	2.71	−0.56
m-chlorotoluene	7.30	0.63	0.52	1.12	9.32	63.78	2.23	−0.18
m-cresol	−31.02	0.49	0.69	0.96	9.11	59.21	1.84	−4.45
methanethiol	28.74	1.00	1.24	2.23	11.26	18.55	0.00	−0.99
methanol	−51.88	0.93	0.62	1.49	11.14	10.94	0.00	−3.73
methyl acetate	−94.10	1.84	0.07	1.83	11.27	28.71	0.70	−2.33
methyl hexanoate	−114.61	1.74	0.15	1.74	11.18	57.35	2.03	−1.82
methyl isobutyl ether	−63.26	0.72	0.43	1.15	10.57	39.98	1.85	−1.04
methyl isopropyl ether	−58.57	0.85	0.41	1.25	10.64	33.00	1.28	−1.43
methyl *n*-butyl ether	−63.62	0.80	0.39	1.18	10.58	40.32	1.35	−1.14
methyl propionate	−98.35	1.78	0.12	1.76	11.17	36.00	0.93	−2.15
methyl propyl ether	−52.93	0.82	0.39	1.21	10.57	26.13	0.58	−1.22
methyl *tert*-butyl ether	−64.13	0.85	0.44	1.28	10.63	39.57	2.32	−1.62
methylamine	−5.19	0.08	1.45	1.40	9.40	13.55	0.00	−3.34
methylbutyrate	−103.80	1.75	0.13	1.74	11.18	43.14	1.33	−2.08
methylcyclohexane	−35.73	0.00	0.02	0.02	11.06	48.58	2.74	1.21
methylcyclopentane	−29.68	0.03	0.02	0.04	11.11	40.70	2.39	1.17
methylformate	−85.18	3.26	0.61	3.86	11.15	21.98	0.33	−2.04
methylthiobenzene	23.25	0.35	1.62	1.63	8.56	69.94	2.39	−2.00
methyltrimethyl acetate	−107.36	1.92	0.11	1.84	11.01	49.43	2.74	−1.76
m-xylene	4.81	0.25	0.02	0.26	9.31	62.57	2.16	−0.53
n,n-diethylformamide	−42.85	3.02	0.44	3.46	9.26	33.34	1.07	−5.52
n,n-dimethylaniline	20.05	0.76	0.94	1.21	8.44	72.30	2.23	−2.53
n-amyl acetate	−114.89	1.94	0.03	1.94	11.25	57.94	2.05	−1.80
naphthalene	40.68	0.00	0.00	0.00	8.84	83.80	2.35	−1.75
n-butyl acetate	−109.51	1.90	0.03	1.92	11.25	50.77	1.69	−1.94
n-butyl propionate	−113.73	1.81	0.09	1.83	11.16	58.11	1.93	−1.69
n-butylamine	−21.89	0.19	1.45	1.34	9.38	34.76	1.14	−3.11
n-butylbenzene	−0.14	0.36	0.04	0.34	9.41	76.07	2.59	−0.28
n-butylformate	−100.69	3.36	0.58	3.91	11.16	44.11	1.32	−1.68
n-decanal	−87.02	2.29	0.32	2.60	10.63	74.34	3.08	−1.13
n-decane	−61.59	0.00	0.00	0.00	11.27	71.26	3.12	2.33
n-ethylaniline	14.89	0.81	1.08	1.27	8.54	72.04	1.90	−3.18
n-heptane	−45.32	0.03	0.03	0.00	11.27	50.06	2.06	1.92
n-heptylamine	−38.13	0.21	1.47	1.33	9.40	55.97	2.20	−2.78
n-hexane	−39.90	0.00	0.00	0.00	11.28	43.01	1.71	1.84
n-hexyl acetate	−120.34	1.90	0.03	1.92	11.25	64.99	2.40	−1.70
n-hexylamine	−32.72	0.21	1.45	1.33	9.39	48.88	1.85	−2.90
n-hexylbenzene	−10.97	0.37	0.04	0.35	9.41	90.40	3.30	−0.03
nitrobenzene	14.54	4.76	0.48	5.24	10.60	59.94	1.56	−3.02
nitroethane	−21.39	3.53	0.55	4.06	12.08	27.19	0.61	−2.72
nitromethane	−15.94	3.40	0.59	3.99	12.17	19.98	0.42	−2.95
n-methylaniline	21.18	0.73	1.06	1.28	8.55	64.04	1.62	−3.44
n-nonane	−56.17	0.03	0.03	0.00	11.28	64.18	2.77	2.30
n-octadecane	−104.91	0.00	0.01	0.00	11.26	128.06	5.95	−0.18
n-octane	−50.74	0.00	0.00	0.00	11.27	57.13	2.41	2.08
n-octylamine	−43.56	0.21	1.45	1.33	9.40	63.02	2.56	−2.68
nonan-5-one	−83.25	2.05	0.49	2.54	10.58	67.15	2.75	−1.94
nonanal	−81.77	2.24	0.35	2.59	10.64	67.20	2.72	−1.52
nonanoic acid	−138.56	2.17	0.50	1.76	11.36	70.07	2.91	−4.33
n-pentyl acetate	−114.92	1.93	0.03	1.92	11.25	57.89	2.05	−1.84
n-pentylamine	−27.31	0.21	1.47	1.33	9.39	41.80	1.50	−3.00
n-pentylbenzene	−5.56	0.36	0.06	0.34	9.41	83.26	2.94	−0.17
n-pentylcyclopentane	−50.70	0.04	0.03	0.05	11.04	69.11	3.65	1.87
n-propyl acetate	−104.13	1.91	0.04	1.91	11.25	43.60	1.34	−2.05
n-propylbenzene	5.26	0.35	0.06	0.34	9.40	68.88	2.24	−0.55
n-propylcyclopentane	−40.25	0.09	0.04	0.06	11.05	54.97	2.94	1.56
n-propylpropionate	−108.36	1.83	0.10	1.83	11.16	50.96	1.57	−1.79
n-tetradecane	−83.23	0.00	0.00	0.00	11.27	99.70	4.54	1.14
n-undecane	−66.98	0.03	0.03	0.00	11.27	78.43	3.47	2.87
o-cresol	−30.88	0.77	0.67	1.40	9.06	58.99	1.79	−4.31
octanal	−76.36	2.25	0.35	2.59	10.64	60.13	2.37	−1.68
octanoic acid	−133.31	2.16	0.48	1.78	11.37	63.02	2.56	−4.47
o-ethylphenol	−31.05	0.99	0.65	1.64	8.99	66.91	1.98	−3.72
o-xylene	5.53	0.45	0.01	0.46	9.30	62.31	2.08	−0.66
p-chloronitrobenzene	8.44	4.66	0.07	4.59	10.22	71.82	2.09	−2.65

Table 1. (Continued)

compound	H[a]	m_P[b]	μ_H[c]	m_S[d]	IP[e]	PO[f]	$^2\chi^{v}$[g]	logH
pentachlorobenzene	−4.77	0.18	0.61	0.43	9.25	97.46	3.73	−0.40
pentanal	−60.12	2.21	0.36	2.56	10.63	38.88	1.31	−2.22
pentane	−34.48	0.03	0.03	0.00	11.30	35.97	1.35	1.70
pentanoic acid	−117.16	2.17	0.48	1.80	11.36	41.82	1.50	−4.52
phenanthrene	55.04	0.05	0.02	0.03	8.74	123.59	3.51	−2.79
phenol	−21.67	0.53	0.69	1.14	9.18	50.76	1.34	−4.87
phenylacetic acid	−69.98	1.69	0.32	1.54	9.60	67.36	2.06	−5.78
phenylacetylene	74.67	0.34	0.17	0.17	9.40	66.17	1.51	−0.55
phenylmethyl sulfide	23.25	0.35	1.62	1.63	8.56	69.92	2.39	−2.00
p-isopropyl toluene	−3.59	0.05	0.06	0.03	9.22	77.13	3.07	−0.30
p-methylacetophenone	−27.20	2.60	0.43	3.02	9.72	74.73	2.42	−3.45
prop-2-en-1-ol	−31.26	0.88	0.64	1.48	10.07	26.12	0.47	−3.69
propane	−23.62	0.03	0.03	0.00	11.51	21.93	0.71	1.46
propionaldehyde	−49.16	2.15	0.36	2.51	10.62	24.59	0.57	−2.52
propiophenone	−21.48	2.23	0.46	2.69	10.00	72.87	2.14	−2.27
propoinic acid	−106.32	2.16	0.46	1.80	11.35	27.69	0.75	−4.74
propyl benzene	5.26	0.35	0.06	0.34	9.40	68.88	2.24	−0.39
propyl formate	−95.34	3.33	0.61	3.90	11.16	36.95	0.97	−1.75
propylamine	−16.49	0.19	1.46	1.34	9.38	27.71	0.79	−3.22
propylene oxide	−16.53	1.94	0.11	1.83	11.29	24.63	1.14	−2.55
propyne	40.22	0.51	0.15	0.36	10.89	20.97	0.29	−0.35
pyridine	30.38	0.62	1.31	1.93	10.10	43.62	1.02	−3.44
pyrrole	27.11	1.89	0.29	2.18	8.93	35.76	0.88	−3.13
pyrrolidine	−11.97	0.22	1.37	1.46	9.27	32.80	1.46	−4.01
quinoline	47.54	0.56	1.33	1.85	9.24	81.74	2.20	−4.17
sec-butyl acetate	−108.97	1.80	0.08	1.84	11.15	50.55	1.83	−1.77
sec-butylbenzene	0.05	0.30	0.04	0.27	9.52	75.50	2.72	−0.25
styrene	39.19	0.02	0.01	0.02	9.13	66.26	1.61	−0.95
tert-butyl alcohol	−71.28	0.98	0.70	1.54	11.28	31.58	2.17	−3.23
tert-butyl amine	−25.20	0.28	1.52	1.36	9.47	34.08	2.37	−2.83
tert-butylbenzene	0.32	0.30	0.02	0.30	9.50	74.90	3.62	−0.32
tetrachloroethene	−8.08	0.00	0.00	0.00	9.22	52.79	2.41	−0.14
tetrachloromethane	−25.96	0.01	0.00	0.01	10.99	42.79	3.85	0.06
tetrafluoromethene	−225.09	0.00	0.00	0.00	16.79	8.02	0.43	2.32
tetrahydrofuran	−51.32	1.29	0.38	1.67	10.26	30.42	1.32	−2.54
tetrahydropyran	−57.41	0.98	0.40	1.38	10.57	38.59	1.67	−2.29
thiophene	30.72	1.01	1.68	0.67	9.54	42.24	1.61	−0.92
thiophenol	−7.94	0.60	2.28	1.69	9.27	47.46	1.87	−1.86
toluene	14.11	0.25	0.02	0.26	9.44	45.60	1.65	−0.57
trans 1,4-dimethylcyclohexane	−42.71	0.00	0.01	0.00	11.19	55.40	3.37	1.55
trans-2-butenal	−28.29	2.78	0.39	3.16	10.48	36.00	0.66	−3.10
trans-2-hexenal	−39.04	2.92	0.37	3.28	10.40	51.00	1.35	−2.70
trans-2-octenal	−49.87	2.96	0.35	3.31	10.40	65.48	2.06	−2.52
tribromomethane	17.56	0.60	0.35	0.95	10.84	39.97	6.66	−1.66
trichloroethene	−2.33	0.14	0.63	0.49	9.38	42.05	1.62	−0.44
trichlorofluoromethane	−67.33	0.98	0.42	0.56	11.16	35.44	2.57	0.60
trichloronitromethane	−20.10	2.88	0.08	2.80	11.30	46.67	2.87	−1.08
triethylamine	−25.74	0.14	1.16	1.06	9.04	50.43	1.62	−2.36
trifluorobenzene	−105.86	0.00	0.00	0.00	10.37	49.65	1.59	−0.18
trimethylamine	−10.84	0.05	1.20	1.15	9.07	28.46	1.34	−2.35
tripropylamine	−42.07	0.26	1.24	1.00	9.07	71.93	2.84	−1.81

[a] H = heat of formation, kcal/mol. [b] μ_P = total dipole moment (point−charge), Debye. [c] μ_H = dipole moment (hybridization), Debye. [d] μ_S = dipole moment (sum), Debye. [e] IP = ionization potential, eV. [f] PO = average polarizability, A.U. [g] $^2\chi^V$ = second-order valence molecular connectivity index.

descriptors selected to build the QSPRs were all at or above the level of selection of 70%. The final set of input parameters is listed in Table 1. We note that the dipole moment-total hybridization μ_H was the only parameter selected for all of the eleven NN runs. The dipole moment-total point-charge and heat of formation ranked at the 91st percentile range, while the second-order valence molecular connectivity index, ionization potential, and dipole moment-total sum ranked at the 82nd percentile range. Finally, the first-order average polarizability ranked at the 73rd percentile range.

Fuzzy ARTMAP Neural Network Systems. The present fuzzy ARTMAP neural network system was recently introduced for developing QSPRs for boiling temperatures,[18] critical properties,[19] aqueous solubilities,[20] and octanol−water partition coefficients.[21] This fuzzy ARTMAP network is the modification introduced by Giralt et al.,[27,36] to the original model of Carpenter et al.[22−26] Additional information about fuzzy ART and fuzzy ARTMAP systems can be found elsewhere.[37−41] 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 network consists of two fuzzy ART modules, *artA* and *artB*, that are linked together via an inter-ART module (Figure 2). Each

Table 2. Experimental and Predicted Henry's Law Constant [Dimensionless] Using Fuzzy ARTMAP and Back-Propagation QSPRs

	data sets[a]		logH			absolute logH error		absolute % logH error	
compounds	FAM[b]	Bk−Pr[c]	reported	FAM	Bk−Pr	FAM	Bk−Pr	FAM	Bk−Pr
1,1,1,2-tetrachloro-2,2-difluoroethane	Tr	Tr/V	−0.78	−0.78	−1.02	0.00	0.24	0.00	31.03
1,1,1,2-tetrachloroethane	Tr	V	−0.95	−0.97	−0.80	0.02	0.15	2.43	15.61
1,1,1-trichloroethane	Tr	Tr/V	−0.18	−0.18	−0.18	0.00	0.00	0.00	0.00
1,1,1-trichloropropane	Tr	Tr/V	−0.88	−0.89	−0.78	0.01	0.10	1.56	11.25
1,1,2,2-tetrabromoethane	Tr	Tr/V	−3.24	−3.24	−2.28	0.00	0.96	0.00	29.60
1,1,2,2-tetrachloroethane	Tr	V	−1.82	−1.82	−1.62	0.00	0.20	0.00	10.74
1,1,2-trichloroethane	Tr	Tr/V	−1.32	−1.33	−0.79	0.01	0.53	1.14	40.17
1,1,2-trichloropropane	Tr	Tr/V	−1.89	−1.89	−1.24	0.00	0.65	0.00	34.53
1,1,3-trimethylcyclopentane	Tr	Tr/V	1.81	1.81	1.30	0.00	0.51	0.00	28.14
1,1-dichlorobutane	Tr	Tr/V	−0.51	−0.53	−0.49	0.02	0.02	3.92	3.92
1,1-dichloroethane	Tr	V	−0.63	−0.64	−0.83	0.01	0.20	1.46	32.30
1,1-dichloroethene	Tr	Tr/V	0.03	0.03	0.03	0.00	0.00	0.00	0.00
1,1-difluoroethene	Tr	Tr/V	1.16	1.14	1.08	0.02	0.08	1.72	7.05
1,2,3-trichloropropane	Tr	Tr/V	−1.85	−1.86	−1.35	0.01	0.50	0.69	26.97
1,2,3-trimethylbenzene	Tr	V	−0.89	−0.89	−0.96	0.00	0.07	0.41	7.61
1,2,4,5-tetramethylbenzene	Tr	Tr/V	0.01	0.02	0.01	0.01	0.00	100.01	25.00
1,2,4-trichlorobenzene	Tr	Tr/V	−0.76	−0.78	−0.74	0.02	0.03	2.53	3.29
1,2,4-trimethylbenzene	Tr	Tr/V	−0.62	−0.64	−0.64	0.02	0.02	3.22	3.40
1,2-dibromo-3-chloropropane	Tr	Tr/V	−2.22	−2.20	−2.34	0.02	0.12	0.96	5.45
1,2-dibromoethane	Tr	Tr/V	−1.56	−1.59	−0.19	0.03	1.37	1.75	87.64
1,2-dibromopropane	Tr	Tr/V	−1.22	−1.23	−1.27	0.01	0.05	0.57	4.35
1,2-dichlorobenzene (o)	Tr	Tr/V	−1.11	−1.14	−1.24	0.03	0.13	2.70	11.98
1,2-dichloroethane	Tr	Tr/V	−1.31	−1.31	1.36	0.00	0.05	0.00	3.82
1,2-dichloroethylene	Ts	Ts	−0.78	−0.53	−0.71	0.25	0.07	32.05	8.54
1,2-dichloropropane	Tr	Tr/V	−0.94	−0.97	−0.63	0.03	0.31	3.19	32.98
1,2-diethylbenzene	Tr	Tr/V	−0.97	−0.97	−0.73	0.00	0.24	0.00	24.35
1,3,5-trichlorobenzene	Tr	V	−1.02	−1.05	−1.14	0.03	0.12	2.94	11.76
1,3,5-trimethlybenzene	Tr	Tr/V	−0.62	−0.64	−0.25	0.02	0.37	3.22	59.52
1,3-butadiene	Tr	V	0.48	0.48	0.11	0.00	0.37	0.00	77.22
1,3-dibromopropane	Tr	Tr/V	−1.44	−1.46	−0.99	0.02	0.45	1.39	31.24
1,3-dichlorbenzene (m)	Tr	Tr/V	−0.97	−0.97	−0.62	0.00	0.35	0.00	35.97
1,3-dichloropropane	Tr	Tr/V	−1.14	−1.14	−1.42	0.00	0.28	0.00	24.64
1,3-dimethylnaphthalene	Ts	Ts	−1.81	−2.06	−2.01	0.25	0.20	13.81	11.05
1,4-dichlorobenzene (p)	Tr	Tr/V	−1.01	−1.01	−0.42	0.00	0.59	0.00	58.59
1,4-dichlorobutane	Tr	Tr/V	−1.70	−1.70	−1.54	0.00	0.16	0.00	9.29
1,4-diethylbenzene	Tr	V	−0.51	−0.53	−0.44	0.02	0.07	3.92	12.76
1,4-dimethylbenzene (*p*-xylene)	Tr	Tr/V	−0.55	−0.56	−0.38	0.01	0.17	1.82	31.76
1,4-dimethylnaphthalene	Ts	Ts	−2.07	−1.96	−1.85	0.11	0.22	5.17	10.79
1,4-pentadiene	Tr	Tr/V	0.68	0.68	0.41	0.00	0.27	0.00	39.94
1,5-dichloropentane	Tr	Tr/V	−1.64	−1.64	−1.49	0.00	0.15	0.00	9.15
1,5-dimethylnaphthalene	Tr	Tr/V	−1.83	−1.86	−1.80	0.03	0.03	1.79	1.41
1,5-hexadiene	Tr	Tr/V	0.84	0.84	0.40	0.00	0.44	0.00	52.54
1,6-heptadiene	Tr	Tr/V	0.44	0.42	0.36	0.02	0.08	4.55	19.12
1-bromo-2-chloroethane	Tr	Tr/V	−1.43	−1.46	−1.48	0.03	0.05	2.10	3.68
1-bromo-2-methylpropane	Tr	V	−0.02	−0.02	−0.01	0.00	0.01	15.50	55.50
1-bromobutane	Tr	Tr/V	−0.45	−0.45	−0.63	0.00	0.18	0.00	40.68
1-bromoheptane	Tr	Tr/V	0.27	0.26	0.51	0.01	0.24	3.70	88.52
1-bromohexane	Ts	Ts	0.19	0.26	0.15	0.07	0.04	36.84	21.05
1-bromonaphthalene	Tr	Tr/V	−1.93	−1.96	−1.69	0.03	0.24	1.70	12.18
1-bromooctane	Tr	V	0.38	0.38	0.25	0.00	0.13	0.00	35.26
1-bromopentane	Tr	Tr/V	−0.09	−0.10	−0.07	0.01	0.02	15.78	25.56
1-bromopropane	Tr	Tr/V	−0.52	−0.53	−0.66	0.01	0.14	1.92	26.15
1-butanol	Ts	Ts	−3.43	−3.46	−3.40	0.03	0.03	0.87	0.83
1-butene	Tr	V	1.01	1.01	0.39	0.00	0.62	0.00	61.42
1-chloro-1,1-difluoroethane	Tr	Tr/V	0.71	0.68	0.75	0.03	0.04	4.23	5.77
1-chloro-2-methylpropane	Tr	Tr/V	−1.31	−1.33	−0.86	0.02	0.45	1.69	34.61
1-chlorobutane	Tr	V	−0.17	−0.18	−0.02	0.01	0.15	5.88	88.94
1-chlorohexane	Tr	V	0.06	0.06	0.09	0.00	0.03	0.00	51.67
1-chloronaphthalene	Ts	Ts	−1.84	−1.89	−2.30	0.05	0.46	2.72	24.75
1-chlorooctane	Tr	Tr/V	0.19	0.19	0.10	0.00	0.09	0.00	45.26
1-chloropentane	Tr	Tr/V	−0.01	−0.02	−0.02	0.01	0.01	131.00	60.00
1-chloropropane	Tr	Tr/V	−0.27	−0.30	−0.38	0.03	0.11	11.11	40.74
1-cyanobutane	Ts	Ts	−2.67	−2.58	−2.93	0.09	0.26	3.37	9.57
1-cycanopropane	Tr	Tr/V	−2.58	−2.58	−2.93	0.00	0.35	0.00	13.54
1-decanol	Tr	Tr/V	−2.71	−2.71	−2.13	0.00	0.58	0.00	21.49
1-dodecanol	Tr	V	−2.67	−2.71	−2.10	0.04	0.57	1.34	21.39
1-ethyl-2-methylbenzene	Tr	V	−0.76	−0.78	−0.25	0.02	0.51	2.63	67.16
1-ethyl-4-methylbenzene	Tr	Tr/V	−0.69	−0.71	−0.49	0.02	0.20	2.90	28.99
1-ethylnaphthalene	Tr	V	−1.07	−1.08	−1.09	0.01	0.02	0.93	1.50
1-heptadecanol	Tr	Tr/V	−2.05	−2.06	−2.57	0.01	0.52	0.54	25.40
1-heptanol	Tr	Tr/V	−2.64	−2.67	−3.29	0.03	0.65	1.14	24.64
1-heptyne	Tr	Tr/V	0.44	0.42	0.28	0.02	0.16	4.55	35.30

Table 2. (Continued)

compounds	data sets[a]		logH			absolute logH error		absolute % logH error	
	FAM[b]	Bk−Pr[c]	reported	FAM	Bk−Pr	FAM	Bk−Pr	FAM	Bk−Pr
1-hexadecanol	Ts	Ts	−2.39	−2.80	−2.29	0.40	0.10	16.53	4.18
1-hexene	Tr	V	1.23	1.21	1.36	0.02	0.13	1.63	10.88
1-hexyne	Tr	Tr/V	0.23	0.23	0.11	0.00	0.12	0.00	51.20
1-iodobutane	Tr	Tr/V	−0.19	−0.22	−0.18	0.03	0.01	15.79	5.79
1-iodopropane	Tr	Tr/V	−0.43	−0.45	−0.76	0.02	0.33	4.65	76.66
1-methoxy-2-propanol	Tr	Tr/V	−4.42	−4.42	−3.99	0.00	0.43	0.00	9.80
1-methylcyclohexene	Tr	Tr/V	0.48	0.48	0.41	0.00	0.07	0.00	14.00
1-methylnaphthalene	Tr	Tr/V	−1.97	−1.97	−1.85	0.00	0.12	0.00	6.09
1-nitropropane	Tr	Tr/V	−2.45	−2.46	−2.48	0.01	0.03	0.41	1.04
1-nonanol	Tr	V	−2.90	−2.90	−2.75	0.00	0.15	0.00	5.34
1-nonene	Ts	Ts	1.51	1.56	1.37	0.05	0.14	3.31	9.27
1-nonyne	Tr	Tr/V	0.77	0.77	0.81	0.00	0.04	0.00	5.03
1-octadecanol	Tr	Tr/V	−0.89	−0.89	−0.92	0.00	0.03	0.00	2.94
1-octanol	Ts	Ts	−3.00	−2.90	−2.57	0.10	0.43	3.33	14.37
1-octene	Tr	V	1.59	1.56	1.36	0.03	0.23	1.89	14.72
1-octyne	Tr	Tr/V	0.52	0.52	0.55	0.00	0.03	0.00	5.69
1-pentadecanol	Tr	V	−2.80	−2.80	−2.61	0.00	0.19	0.00	6.78
1-pentanol	Tr	Tr/V	−3.27	−3.29	−3.60	0.02	0.33	0.61	10.09
1-pentene	Tr	Tr/V	1.21	1.21	0.38	0.00	0.83	0.00	68.82
1-pentyne	Tr	Tr/V	−0.05	−0.06	−0.07	0.01	0.02	18.01	35.20
1-propanol	Ts	Ts	−3.52	−3.48	−3.69	0.04	0.17	1.14	4.87
1-propene	Tr	Tr/V	0.90	0.90	0.47	0.00	0.43	0.00	48.13
1-tetradecanol	Tr	Tr/V	−2.37	−2.38	−2.28	0.01	0.09	0.35	3.88
2,2,2-trifluoroethanol	Tr	Tr/V	−3.15	−3.18	−3.55	0.03	0.40	0.95	12.85
2,2′,3,3′,4,6′-hexachloro-1,1′-biphenyl	Tr	Tr/V	−2.75	−2.75	−2.85	0.00	0.10	0.00	3.65
2,2′,3,4,4′,5′-hexachloro-1,1′-biphenyl	Tr	Tr/V	−3.08	−3.11	−2.54	0.03	0.54	0.97	17.38
2,2′,3,4′,5′,6-hexachloro-1,1′-biphenyl	Tr	Tr/V	−2.68	−2.71	−2.55	0.03	0.13	1.12	4.99
2,2,3-trimethyl-3-pentanol	Tr	Tr/V	−3.43	−3.46	−3.49	0.03	0.06	0.87	1.75
2,2,3-trimethylbutane	Ts	Ts	1.99	2.11	1.68	0.12	0.31	6.03	15.33
2,2′,4,5,5′-pentachloro-1,1′-biphenyl	Tr	Tr/V	−2.43	−2.46	−1.73	0.03	0.70	1.23	28.88
2,2,4-trimethylpentane	Ts	Ts	2.12	1.81	1.51	0.31	0.61	14.62	28.75
2,2′,5-trichloro-1,1′-biphenyl	Ts	Ts	−2.00	−2.16	−2.19	0.16	0.19	8.00	9.64
2,2,5-trimethylhexane	Tr	Tr/V	2.15	2.15	1.80	0.00	0.35	0.00	16.36
2,2′,6,6′-tetrachloro-1,1′-biphenyl	Tr	Tr/V	−2.09	−2.11	−2.17	0.02	0.08	0.96	3.72
2,2′3,3′-tetrachloro-1,1′-biphenyl	Ts	Ts	−2.21	−2.75	−2.69	0.53	0.48	24.15	21.82
2,2′4,4′,5,5′-hexachloro-1,1′-biphenyl	Tr	Tr/V	−2.84	−2.85	−2.61	0.00	0.23	0.02	7.94
2,2-dimethyl propanoic acid	Tr	Tr/V	−3.94	−3.97	−3.29	0.03	0.65	0.76	16.43
2,2-dimethyl-1-butanol	Ts	Ts	−2.85	−3.00	−3.30	0.15	0.45	5.38	15.62
2,2-dimethyl-3-pentanol	Tr	Tr/V	−3.00	−3.00	−2.57	0.00	0.43	0.00	14.47
2,2-dimethylbutane	Ts	Ts	1.84	1.88	1.69	0.04	0.15	2.17	8.39
2,2-dimethylpentane	Tr	Tr/V	2.11	2.11	1.55	0.00	0.56	0.00	26.32
2,2-dimethylpropane	Tr	Tr/V	1.95	1.94	2.01	0.01	0.06	0.51	2.91
2,3,4-trimethylpentane	Tr	V	1.88	1.88	1.84	0.00	0.04	0.00	2.37
2,3′-dichloro-1,1′-biphenyl	Tr	V	−2.00	−2.03	−2.32	0.03	0.32	1.35	16.08
2,3-dichloro-1,1′-biphenyl	Ts	Ts	−2.04	−2.03	−2.48	0.01	0.44	0.63	21.80
2,3-dichlorobutane	Tr	Tr/V	−0.53	−0.53	−0.11	0.00	0.42	0.00	79.07
2,3-dichloropropene	Tr	V	−0.84	−0.85	−0.42	0.01	0.42	1.44	50.18
2,3-dimethy-2-butanol	Tr	Tr/V	−3.39	−3.40	−2.95	0.01	0.44	0.29	12.94
2,3-dimethyl-1,3-butadiene	Tr	Tr/V	0.93	0.93	0.95	0.00	0.02	0.00	2.26
2,3-dimethyl-2-pentanol	Tr	Tr/V	−3.33	−3.36	−3.09	0.03	0.23	1.00	7.04
2,3-dimethyl-3-pentanol	Tr	Tr/V	−3.36	−3.36	−3.13	0.00	0.23	0.00	6.84
2,3-dimethylbutane	Tr	Tr/V	1.72	1.72	1.78	0.00	0.06	0.00	3.36
2,3-dimethylnaphthalene	Tr	Tr/V	−2.04	−2.06	−2.22	0.02	0.18	0.98	8.85
2,3-dimethylpentane	Tr	Tr/V	1.85	1.84	1.88	0.01	0.03	0.54	1.86
2,3-dimethylphenol	Tr	Tr/V	−4.52	−4.54	−4.54	0.02	0.02	0.44	0.37
2,3-dimethylpyridine	Ts	Ts	−3.54	−3.46	−3.42	0.08	0.12	2.26	3.46
2,4,4′-trichloro-1,1′-biphenyl	Tr	V	−2.10	−2.11	−2.76	0.01	0.66	0.48	31.54
2,4,6-triclorophenol	Tr	V	−3.97	−3.97	−3.38	0.00	0.59	0.00	14.99
2,4′-dichloro-1,1′-biphenyl	Tr	Tr/V	−2.03	−2.03	−2.81	0.00	0.78	0.00	38.41
2,4-dichloro-1,1′-biphenyl	Tr	Tr/V	−1.92	−1.92	−2.47	0.00	0.55	0.04	28.57
2,4-dimethyl-2-pentanol	Ts	Ts	−3.15	−3.00	−2.03	0.15	1.12	4.81	35.47
2,4-dimethyl-3-pentanol	Tr	Tr/V	−2.98	−3.00	−3.45	0.02	0.47	0.78	15.89
2,4-dimethyl-3-pentanone	Tr	Tr/V	−1.84	−1.84	−1.92	0.00	0.08	0.00	4.57
2,4-dimethylpentane	Ts	Ts	2.08	1.88	1.79	0.20	0.29	9.62	14.10
2,4-dimethylphenol	Tr	Tr/V	−4.41	−4.42	−4.13	0.01	0.28	0.23	6.27
2,4-dimethylpyridine	Ts	Ts	−3.57	−3.57	−3.59	0.00	0.02	0.00	0.68
2,5-cyclohexadiene-1,4-dione	Tr	V	−1.71	−1.71	−1.30	0.00	0.41	0.00	23.98
2,5-dichloro-1,1′-biphenyl	Tr	Tr/V	−1.92	−1.92	−2.30	0.00	0.38	0.00	19.81
2,5-dimethylphenol	Ts	Ts	−4.34	−3.88	−4.57	0.46	0.23	10.60	5.21
2,5-dimethylpyridine	Tr	Tr/V	−3.46	−3.46	−2.93	0.00	0.53	0.00	15.32
2,6-dichloro-1,1′-biphenyl	Ts	Ts	−2.03	−2.03	−2.28	0.00	0.25	0.00	12.29
2,6-dichlorophenol	Tr	Tr/V	−3.96	−3.97	−4.30	0.01	0.34	0.25	8.62

Table 2. (Continued)

compounds	data sets[a]		logH			absolute logH error		absolute % logH error	
	FAM[b]	Bk−Pr[c]	reported	FAM	Bk−Pr	FAM	Bk−Pr	FAM	Bk−Pr
2,6-diethylaniline	Tr	Tr/V	−4.34	−4.34	−3.52	0.00	0.82	0.00	18.88
2,6-dimethyl-4-heptanone	Tr	Tr/V	−2.32	−2.33	−2.12	0.01	0.20	0.43	8.75
2,6-dimethylnaphthalene	Tr	V	−1.93	−1.96	−1.80	0.03	0.13	1.70	6.52
2,6-dimethylphenol	Tr	V	−3.86	−3.88	−4.42	0.02	0.56	0.52	14.45
2-bromoethyl benzene	Tr	Tr/V	−1.21	−1.23	−1.00	0.02	0.21	1.40	17.34
2-bromopropane	Tr	Tr/V	−0.35	−0.36	−0.29	0.01	0.06	2.86	17.95
2-butanol	Tr	Tr/V	−3.43	−3.46	−3.64	0.03	0.21	0.87	6.27
2-butanone	Tr	V	−2.63	−2.63	−2.51	0.00	0.12	0.00	4.62
2-chloro-1-nitrobenzene	Tr	Tr/V	−2.74	−2.75	−3.41	0.01	0.67	0.19	24.42
2-chloro2-methylpropane	Tr	V	0.80	0.77	0.45	0.03	0.35	3.75	44.29
2-chlorobutane	Tr	Tr/V	−0.01	−0.02	−0.02	0.01	0.01	131.00	127.00
2-chloroethanol	Tr	V	−4.51	−4.54	−4.44	0.03	0.07	0.67	1.47
2-chloronaphthalene	Tr	Tr/V	−1.87	−1.89	−2.16	0.02	0.29	1.07	15.57
2-chloropentane	Tr	Tr/V	−0.22	−0.22	−0.56	0.00	0.34	0.00	154.55
2-chlorophenol	Tr	V	−3.34	−3.36	−3.44	0.02	0.10	0.65	3.13
2-chloropropane	Tr	Tr/V	−0.15	−0.18	−0.16	0.03	0.01	20.00	6.67
2-chloropyridine	Tr	Tr/V	−3.22	−3.22	−2.35	0.00	0.87	0.00	27.15
2-ethylbutyric acid	Tr	Tr/V	−4.18	−4.18	−4.08	0.00	0.10	0.00	2.37
2-ethylnaphthalene	Tr	Tr/V	−1.48	−1.48	−2.00	0.00	0.52	0.00	35.13
2-ethylpyridine	Tr	V	−3.17	−3.18	−2.88	0.01	0.29	0.32	9.16
2-fluorophenol	Tr	Tr/V	−3.88	−3.88	−3.96	0.00	0.08	0.00	2.06
2-heptanone	Ts	Ts	−2.23	−2.46	−2.21	0.23	0.02	10.31	0.84
2-hexanol	Tr	Tr/V	−3.00	−3.00	−3.34	0.00	0.34	0.11	11.39
2-hexanone	Ts	Ts	−2.42	−2.29	−2.25	0.13	0.17	5.37	7.19
2-iodophenol	Tr	V	−4.55	−4.55	−4.59	0.00	0.04	0.00	0.81
2-iodopropane	Tr	Tr/V	−0.55	−0.56	−0.03	0.01	0.52	1.82	94.08
2-methyl-1,3-butadiene	Tr	Tr/V	0.50	0.48	0.31	0.02	0.19	4.00	38.60
2-methyl-1-butanol	Tr	Tr/V	−3.24	−3.24	−2.84	0.01	0.40	0.42	12.34
2-methyl-1-pentene	Tr	Tr/V	1.05	1.05	0.35	0.00	0.70	0.00	66.83
2-methyl-1-propanol	Tr	Tr/V	−2.96	−2.96	−3.44	0.00	0.48	0.00	16.08
2-methyl-2-butanol	Ts	Ts	−3.25	−3.29	−3.07	0.04	0.18	1.23	5.45
2-methyl-2-butene	Tr	Tr/V	0.95	0.93	0.97	0.02	0.02	2.11	1.58
2-methyl-2-hexanol	Tr	Tr/V	−3.20	−3.22	−2.87	0.02	0.33	0.62	10.18
2-methyl2-pentanol	Tr	Tr/V	−2.84	−2.85	−2.83	0.01	0.01	0.35	0.45
2-methyl-2-propanol	Tr	Tr/V	−3.28	−3.29	−2.90	0.01	0.38	0.30	11.45
2-methyl-3-pentanol	Tr	Tr/V	−2.85	−2.85	−3.19	0.00	0.34	0.00	11.79
2-methyl-3-pentanone	Ts	Ts	−2.20	−2.38	−2.29	0.18	0.09	8.18	4.09
2-methylaziridine	Tr	Tr/V	−3.46	−3.46	−2.93	0.00	0.53	0.00	15.42
2-methylbutane (isopentane)	Ts	Ts	1.76	1.84	1.51	0.08	0.25	4.55	13.94
2-methylhexane	Tr	Tr/V	2.15	2.15	1.86	0.00	0.29	0.00	13.31
2-methylnaphthalene	Tr	Tr/V	−1.78	−1.78	−1.78	0.00	0.00	0.00	0.28
2-methylpentane	Tr	Tr/V	1.84	1.84	1.63	0.00	0.21	0.00	11.30
2-methylpropane	Tr	Tr/V	1.68	1.68	1.23	0.00	0.45	0.00	26.78
2-methylpyridine	Tr	Tr/V	−3.40	−3.40	−3.49	0.00	0.09	0.00	2.65
2-nitropropane	Tr	V	−2.31	−2.33	−2.30	0.02	0.01	0.87	0.51
2-nitrotoluene	Ts	Ts	−2.63	−2.53	−3.03	0.10	0.40	3.80	15.09
2-nonanone	Tr	Tr/V	−1.82	−1.82	−1.80	0.00	0.02	0.00	0.95
2-octanone	Tr	Tr/V	−2.11	−2.11	−1.87	0.00	0.24	0.00	11.54
2-pentanol	Tr	Tr/V	−3.22	−3.22	−3.17	0.00	0.05	0.00	1.44
2-pentanone	Ts	Ts	−2.47	−2.53	−2.46	0.06	0.01	2.43	0.36
2-pentene	Ts	Ts	0.99	0.93	0.19	0.06	0.80	6.06	80.68
2-phenyl-1-ethanol	Tr	Tr/V	−4.98	−4.98	−4.75	0.00	0.24	0.00	4.72
2-propanol	Tr	Tr/V	−3.35	−3.36	−3.32	0.02	0.02	0.47	0.74
2-undecanone	Tr	V	−1.58	−1.59	−1.47	0.01	0.11	0.47	6.92
3,3′,5-trichloro-1,1′-biphenyl	Tr	V	−2.16	−2.16	−2.44	0.00	0.28	0.00	12.81
3,3-dimethyl-2-butanol	Tr	Tr/V	−3.00	−3.00	−2.83	0.00	0.17	0.11	5.77
3,3-dimethyl-2-butanone	Tr	Tr/V	−2.28	−2.29	−1.82	0.01	0.46	0.44	20.36
3,3-dimethylpentane	Tr	Tr/V	1.88	1.88	1.95	0.00	0.07	0.00	3.64
3,4-dichloro-1,1-biphenyl	Tr	Tr/V	−2.23	−2.26	−2.50	0.03	0.27	1.35	11.93
3,4-dichlorotoluene	Tr	V	−0.98	−1.01	−0.73	0.03	0.25	3.06	25.41
3,4-dimethylphenol	Tr	Tr/V	−4.77	−4.77	−4.74	0.00	0.03	0.00	0.65
3,4-dimethylpyridine	Tr	Tr/V	−3.83	−3.83	−4.39	0.00	0.56	0.00	14.55
3,5-dimethylphenol	Tr	Tr/V	−4.60	−4.60	−4.66	0.00	0.06	0.00	1.29
3,5-dimethylpyridine	Tr	V	−3.55	−3.57	−4.09	0.02	0.54	0.56	15.20
3-chlorophenol	Tr	Tr/V	−4.85	−4.87	−4.50	0.02	0.35	0.41	7.29
3-chloropropane	Tr	Tr/V	−3.35	−3.36	−3.21	0.01	0.14	0.35	4.21
3-chloropyridine	Tr	Tr/V	−2.94	−2.96	−2.80	0.02	0.14	0.68	4.67
3-ethyl-3-pentanol	Tr	V	−3.43	−3.46	−3.35	0.03	0.08	0.92	2.21
3-ethylphenol	Tr	Tr/V	−4.59	−4.56	−4.16	0.03	0.43	0.65	9.37
3-formylpyridine	Tr	Tr/V	−5.21	−5.21	−4.04	0.00	1.17	0.00	22.47
3-heptanol	Tr	Tr/V	−2.94	−2.96	−3.02	0.02	0.08	0.68	2.65
3-heptanone	Tr	V	−2.43	−2.46	−2.35	0.03	0.08	1.23	3.48

Table 2. (Continued)

compounds	data sets[a]		logH			absolute logH error		absolute % logH error	
	FAM[b]	Bk−Pr[c]	reported	FAM	Bk−Pr	FAM	Bk−Pr	FAM	Bk−Pr
3-hexanol	Tr	Tr/V	−3.00	−3.00	−3.22	0.00	0.22	0.11	7.18
3-hexanone	Tr	Tr/V	−2.29	−2.29	−2.54	0.00	0.25	0.00	11.13
3-methyheptane	Tr	Tr/V	2.18	2.15	1.99	0.03	0.19	1.38	8.70
3-methyhexane	Tr	V	1.99	1.99	1.86	0.00	0.13	0.00	6.67
3-methyl-1-butanol	Ts	Ts	−3.26	−3.18	−2.97	0.08	0.29	2.54	8.83
3-methyl-1-butene	Tr	Tr/V	1.34	1.34	0.19	0.00	1.15	0.00	85.59
3-methyl-2-butanol	Tr	Tr/V	−3.15	−3.18	−3.21	0.03	0.06	0.95	1.81
3-methyl-2-butanone	Tr	Tr/V	−2.38	−2.38	−2.16	0.00	0.22	0.00	9.37
3-methyl-2-pentanol	Ts	Ts	−2.85	−3.00	−3.34	0.15	0.49	5.38	17.17
3-methyl-3-hexanol	Ts	Ts	−3.28	−3.36	−2.36	0.08	0.92	2.49	27.97
3-methyl-3-pentanol	Ts	Ts	−3.14	−2.85	−3.21	0.29	0.07	9.24	2.39
3-methylpentane	Tr	V	1.84	1.84	1.89	0.00	0.05	0.00	2.57
3-methylpyridine	Ts	Ts	−3.50	−3.40	−3.88	0.10	0.38	2.86	10.81
3-methylthiophene	Tr	Tr/V	−0.53	−0.53	−0.49	0.00	0.04	0.00	6.68
3-nitrotoluene	Tr	Tr/V	−2.53	−2.53	−2.82	0.00	0.29	0.00	11.37
3-pentanol	Ts	Ts	−3.19	−3.22	−3.47	0.03	0.28	0.94	8.64
3-pentanone	Tr	Tr/V	−2.50	−2.53	−2.58	0.03	0.08	1.20	3.23
4-bromochlorobenzene	Tr	Tr/V	−1.23	−1.23	−1.39	0.00	0.16	0.00	13.07
4-bromophenol	Tr	Tr/V	−5.21	−5.21	−4.35	0.00	0.86	0.00	16.51
4-bromotoluene	Tr	Tr/V	−1.02	−1.05	−0.45	0.03	0.57	2.94	55.79
4-chloro-2-nitrophenol	Tr	V	−3.29	−3.29	−3.31	0.00	0.02	0.00	0.57
4-chloro-3-methylphenol	Tr	Tr/V	−4.98	−4.98	−4.59	0.00	0.39	0.00	7.87
4-chloroaniline	Tr	Tr/V	−4.32	−4.34	−4.29	0.02	0.03	0.46	0.65
4-chlorophenol	Tr	Tr/V	−5.16	−5.16	−4.22	0.00	0.94	0.00	18.26
4-ethylpyridine	Tr	V	−3.47	−3.48	−4.16	0.01	0.69	0.29	19.96
4-fluorophenol	Tr	Tr/V	−4.54	−4.54	−4.66	0.00	0.12	0.00	2.56
4-formylpyridine	Ts	Ts	−5.14	−5.21	−4.17	0.07	0.97	1.36	18.81
4-heptanone	Tr	Tr/V	−2.14	−2.16	−2.52	0.02	0.38	0.93	17.97
4-methyl-1-pentene	Tr	Tr/V	1.41	1.41	1.24	0.00	0.17	0.00	11.84
4-methyl-2-methoxyphenyl	Tr	V	−4.26	−4.26	−4.42	0.00	0.16	0.00	3.76
4-methyl-2-pentanol	Tr	V	−2.74	−2.75	−2.88	0.01	0.14	0.19	5.17
4-methyl-2-pentanone	Tr	Tr/V	−2.25	−2.26	−2.16	0.01	0.09	0.44	4.02
4-methyl-2-pentyl acetate	Tr	Tr/V	−1.62	−1.64	−1.55	0.02	0.07	1.23	4.47
4-methylphenol (*p*-cresol)	Ts	Ts	−4.39	−4.34	−4.56	0.05	0.17	1.14	3.76
4-methylpyridine	Ts	Ts	−3.62	−3.48	−4.08	0.14	0.46	3.87	12.67
4-*n*-propylphenol	Tr	Tr/V	−4.33	−4.34	−4.60	0.01	0.27	0.23	6.29
4-*tert*-butylphenol	Tr	Tr/V	−4.34	−4.34	−4.36	0.00	0.02	0.00	0.51
4-vinylcyclohexene	Tr	Tr/V	0.26	0.26	0.18	0.00	0.08	0.00	32.00
5-methyl-2-hexanone	Tr	Tr/V	−2.23	−2.26	−2.19	0.03	0.04	1.35	1.78
a,a,a-trifllluorotoluene	Tr	V	−1.19	−1.19	−0.70	0.00	0.49	0.00	40.95
acenaphthene	Tr	Tr/V	−2.20	−2.22	−2.13	0.02	0.07	1.00	3.27
acenaphthylene	Tr	Tr/V	−2.33	−2.33	−1.75	0.00	0.58	0.00	24.92
acetaldehyde	Tr	Tr/V	−2.57	−2.57	−2.62	0.00	0.05	0.00	1.98
acetamide	Tr	Tr/V	−6.74	−6.74	−6.07	0.00	0.67	0.00	9.88
acetic acid	Tr	Tr/V	−5.39	−5.39	−4.79	0.00	0.60	0.00	11.05
acetone (propanone)	Tr	Tr/V	−2.79	−2.80	−2.37	0.01	0.42	0.20	15.07
acetonitrile	Tr	Tr/V	−2.85	−2.85	−2.67	0.00	0.18	0.00	6.39
acetophenone	Tr	V	−3.37	−3.40	−3.08	0.03	0.29	0.89	8.66
a-chlorotoluene	Tr	Tr/V	−1.58	−1.59	−1.24	0.00	0.34	0.00	21.74
allylbenzene (2-propenyl)	Tr	V	−0.55	−0.56	−0.55	0.01	0.00	1.82	0.62
amyl formate (pentyl)	Tr	Tr/V	−1.26	−1.27	−1.49	0.01	0.23	0.79	17.98
amyl propionate (pentyl)	Tr	Tr/V	−1.46	−1.46	−1.85	0.00	0.39	0.00	26.71
aniline	Tr	Tr/V	−4.08	−4.08	−3.69	0.00	0.39	0.00	9.52
anthracene	Tr	Tr/V	−2.62	−2.63	−2.40	0.01	0.22	0.38	8.27
benz[*a*]pyrene (3,4-benzo)	Tr	Tr/V	−1.80	−1.86	−2.06	0.00	0.26	0.00	14.66
benzaldehyde	Tr	V	−2.95	−2.96	−2.86	0.01	0.09	0.34	3.19
benzene	Tr	Tr/V	−0.64	−0.64	−0.42	0.00	0.22	0.00	34.06
benzo[*b*]fluoroanthene (2,3-benzo)	Tr	Tr/V	−1.68	−1.70	−2.18	0.01	0.50	0.79	29.66
benzo[g,h,I]perylene	Tr	Tr/V	−1.96	−1.96	−1.74	0.00	0.22	0.00	11.18
benzo[*k*]fluoroanthene (8,9-benzo)	Ts	Ts	−1.75	−1.70	−2.21	0.05	0.46	2.90	26.18
benzoic acid methyl ester	Tr	Tr/V	−2.88	−2.90	−2.52	0.02	0.36	0.69	12.55
benzonitrile	Tr	Tr/V	−3.09	−3.11	−3.30	0.02	0.21	0.65	6.91
benzyl acetate	Tr	Tr/V	−3.34	−3.36	−3.46	0.02	0.12	0.65	3.67
biphenyl	Tr	Tr/V	−1.95	−1.96	−1.82	0.01	0.13	0.66	6.75
bromobenzene	Tr	Tr/V	−1.00	−1.01	−0.77	0.01	0.23	1.37	22.73
bromodichloromethane	Tr	Tr/V	−1.06	−1.08	−0.69	0.02	0.37	1.89	34.71
bromoethane	Tr	Tr/V	−0.51	−0.53	−0.54	0.02	0.03	3.92	6.09
bromomethane	Tr	V	−0.67	−0.67	−0.64	0.00	0.03	0.00	3.84
butane	Tr	Tr/V	1.59	1.56	1.18	0.03	0.41	1.89	25.48
butanethiol	Ts	Ts	−0.73	−0.73	−0.50	0.00	0.23	0.00	31.64
butyl acetate	Tr	Tr/V	−1.94	−1.96	−1.73	0.02	0.21	1.18	10.76
butyraldehyde	Ts	Ts	−2.33	−2.22	−2.22	0.11	0.11	4.72	4.86

Table 2. (Continued)

compounds	data sets[a]		logH			absolute logH error		absolute % logH error	
	FAM[b]	Bk−Pr[c]	reported	FAM	Bk−Pr	FAM	Bk−Pr	FAM	Bk−Pr
chlorobenzene	Tr	Tr/V	−0.85	−0.85	−0.74	0.00	0.11	0.00	12.56
chlorodifluoromethane	Tr	Tr/V	0.09	0.08	0.08	0.01	0.01	7.67	6.67
chloroethane	Tr	Tr/V	−0.46	−0.45	−0.43	0.01	0.03	2.10	6.65
chloroethene	Tr	Tr/V	−0.02	−0.02	−0.05	0.00	0.03	0.00	116.45
chloromethane	Tr	Tr/V	−0.42	−0.45	−0.54	0.03	0.12	7.14	28.57
chlorotrifluoromethane	Tr	V	1.75	1.72	1.41	0.03	0.34	1.71	19.43
cis-1,2-dibromoethene	Tr	Tr/V	−0.78	−0.78	−0.79	0.00	0.01	0.00	1.43
cis-1,2-dichloroethene	Tr	Tr/V	−0.51	−0.53	−0.71	0.02	0.20	3.92	39.22
cis-1,2-dimethylcyclohexane	Tr	V	1.17	1.14	1.45	0.03	0.28	2.56	24.06
cis-2-pentene	Tr	Tr/V	0.96	0.93	0.19	0.03	0.77	3.12	80.08
cumene	Tr	Tr/V	−0.33	−0.33	−0.17	0.00	0.16	0.00	48.26
cycloheptane	Tr	Tr/V	0.58	0.58	0.50	0.00	0.08	0.00	13.38
cyclohexane	Tr	Tr/V	0.86	0.84	1.40	0.02	0.54	2.33	63.12
cyclohexanol	Tr	Tr/V	−3.94	−3.97	−3.07	0.03	0.87	0.76	22.09
cyclohexanone	Tr	Tr/V	−3.43	−3.46	−2.15	0.03	1.28	0.87	37.26
cyclohexene	Tr	Tr/V	0.27	0.26	0.15	0.01	0.12	3.70	43.62
cyclopentane	Tr	Tr/V	−0.87	−0.89	−0.52	0.02	0.35	2.72	40.23
cyclopentanone	Tr	Tr/V	−3.39	−3.40	−2.21	0.01	1.18	0.29	34.68
cyclopentene	Tr	Tr/V	0.42	0.42	0.17	0.00	0.25	0.00	60.34
cyclopropane	Tr	Tr/V	0.55	0.52	0.06	0.03	0.49	5.45	89.09
decalin (decahydronaphthalene)	Tr	Tr/V	1.28	1.28	1.66	0.00	0.38	0.00	30.03
decan-2-one	Ts	Ts	−1.72	−1.82	−1.56	0.10	0.16	5.81	9.47
di(*n*-butyl) ether	Tr	Tr/V	−0.61	−0.64	−0.81	0.03	0.20	4.92	33.46
di(*n*-propyl) ether	Tr	Tr/V	−1.05	−1.05	−1.80	0.00	0.75	0.00	71.28
dibromochloromethane	Tr	V	−1.49	−1.52	−1.77	0.03	0.28	2.01	18.46
dibromomethane	Tr	Tr/V	−1.47	−1.48	−0.29	0.01	1.18	0.68	80.29
dichlorodifluoromethane	Tr	Tr/V	1.21	1.21	0.59	0.00	0.62	0.00	51.46
dichlorofluoromethane	Tr	V	−0.36	−0.36	−0.28	0.00	0.08	0.00	22.22
dichloromethane	Tr	Tr/V	−0.97	−0.97	−1.47	0.00	0.50	0.00	52.00
diethyl ether	Tr	V	−1.30	−1.33	−1.71	0.03	0.41	2.31	31.79
diethylamine	Ts	Ts	−2.98	−3.11	−3.34	0.13	0.36	4.36	12.24
diethyl sulfide	Tr	Tr/V	−1.07	−1.08	−1.20	0.01	0.13	0.93	12.47
difluoromethane	Tr	V	−1.88	−1.89	−1.48	0.01	0.40	0.53	21.28
diisobutylamine	Tr	V	−1.64	−1.64	−2.13	0.00	0.49	0.00	29.97
di-isopropyl ether	Tr	Tr/V	−1.03	−1.05	−1.04	0.02	0.01	1.94	0.81
di-isopropylamine	Tr	Tr/V	−2.36	−2.38	−2.36	0.02	0.00	0.85	0.10
di-isopropylsulfide	Tr	Tr/V	−0.88	−0.89	−1.39	0.01	0.51	1.56	57.76
dimethyl ether	Tr	Tr/V	−1.27	−1.27	−1.60	0.00	0.33	0.00	25.76
dimethylamine	Ts	Ts	−3.15	−3.22	−3.71	0.07	0.56	2.22	17.81
dimethyl sulfide	Tr	Tr/V	−1.18	−1.19	−1.46	0.01	0.28	0.63	23.90
di-*n*-butylamine	Tr	V	−2.38	−2.38	−2.58	0.00	0.20	0.00	8.49
di-*n*-propylamine	Tr	Tr/V	−2.68	−2.71	−2.76	0.03	0.08	1.12	2.99
dipropylsulfide	Ts	Ts	−0.94	−1.08	−1.20	0.14	0.26	14.89	27.91
ethane	Tr	Tr/V	1.31	1.28	1.45	0.03	0.14	2.29	10.66
ethanol	Tr	Tr/V	−3.69	−3.69	−3.48	0.00	0.21	0.00	5.56
ethene	Tr	V	0.94	0.93	0.87	0.01	0.07	1.06	7.06
ethyl acetate	Tr	V	−2.26	−2.26	−1.96	0.00	0.30	0.00	13.14
ethyl formate	Tr	Tr/V	−1.80	−1.82	−1.75	0.02	0.05	1.11	2.58
ethyl mercaptan	Tr	Tr/V	−0.73	−0.73	−1.10	0.00	0.37	0.00	50.81
ethyl propionate	Tr	V	−2.05	−2.06	−2.14	0.01	0.09	0.49	4.25
ethyl propyl ether	Tr	Tr/V	−1.33	−1.33	−1.76	0.00	0.43	0.00	32.10
ethylbenzene	Tr	Tr/V	−0.46	−0.46	−0.14	0.00	0.32	0.00	68.58
ethylbenzoate	Tr	Tr/V	−2.67	−2.67	−2.49	0.00	0.18	0.00	6.74
ethylbutyrate	Ts	Ts	−1.79	−1.82	−2.03	0.03	0.24	1.68	13.64
ethylcyclohexane	Tr	Tr/V	1.09	1.09	1.12	0.00	0.03	0.00	2.33
ethylene oxide (oxirane)	Tr	Tr/V	−2.22	−2.22	−1.18	0.00	1.04	0.00	46.77
fluorene	Tr	Tr/V	−2.46	−2.46	−2.10	0.00	0.36	0.00	14.45
fluorobenzene	Tr	V	−0.59	−0.59	−0.70	0.00	0.11	0.00	18.26
fluoromethane	Tr	Tr/V	−0.10	−0.10	−0.16	0.00	0.05	0.00	50.67
formaldehyde	Tr	Tr/V	−2.02	−2.03	−2.33	0.01	0.31	0.35	15.13
formic acid	Tr	V	−5.15	−5.16	−5.33	0.01	0.18	0.19	3.45
furan	Tr	Tr/V	−0.66	−0.67	−0.09	0.01	0.57	1.51	86.67
heptanal	Tr	V	−1.96	−1.96	−1.70	0.00	0.26	0.15	13.36
heptanoic acid	Tr	V	−4.86	−4.87	−3.93	0.01	0.93	0.21	19.13
hexachloro-1-propene	Tr	Tr/V	−0.71	−0.71	−0.75	0.00	0.04	0.00	5.47
hexachlorobenzene	Tr	Tr/V	−2.70	−2.71	−2.71	0.01	0.02	0.56	0.59
hexachlorocyclopentadiene	Tr	Tr/V	0.04	0.04	0.01	0.00	0.03	4.58	65.00
hexachloroethane	Tr	Tr/V	−0.28	−0.30	−0.18	0.02	0.10	7.14	36.07
hexanal (hexaldehyde)	Tr	Tr/V	−2.06	−2.06	−1.87	0.00	0.19	0.00	9.17
hexanoic acid	Tr	Tr/V	−4.51	−4.54	−3.91	0.03	0.60	0.67	13.32
indane	Tr	Tr/V	−1.07	−1.08	−1.82	0.01	0.75	0.93	69.83
iodobenzene	Tr	Tr/V	−1.28	−1.28	−1.19	0.00	0.09	0.00	7.10

Table 2. (Continued)

compounds	data sets[a]		logH			absolute logH error		absolute % logH error	
	FAM[b]	Bk−Pr[c]	reported	FAM	Bk−Pr	FAM	Bk−Pr	FAM	Bk−Pr
iodoethane	Ts	Ts	−0.55	−0.45	−0.59	0.10	0.04	18.18	7.85
iodomethane	Tr	Tr/V	−0.67	−0.67	−0.90	0.00	0.23	0.00	34.27
isoamyl acetate	Tr	Tr/V	−1.62	−1.64	−1.51	0.02	0.11	1.23	6.89
isoamyl formate	Tr	Tr/V	−1.56	−1.59	−1.17	0.03	0.39	1.75	25.28
isobutane	Tr	Tr/V	1.69	1.68	1.23	0.01	0.46	0.59	27.33
isobutene	Tr	Tr/V	0.95	0.93	0.41	0.02	0.54	2.11	57.28
iso-butylamine	Ts	Ts	−3.26	−3.11	−2.93	0.15	0.33	4.60	10.24
isobutyl formate	Tr	Tr/V	−1.67	−1.70	−1.45	0.03	0.22	1.80	13.22
isobutyl propanoate	Tr	Tr/V	−1.17	−1.19	−2.07	0.02	0.90	1.49	76.69
isobutylbenzene	Tr	Tr/V	0.12	0.12	0.14	0.00	0.02	0.00	20.00
isobutylisobutanoate	Tr	V	−1.24	−1.27	−1.44	0.03	0.20	2.42	16.33
isobutyraldehyde	Tr	Tr/V	−2.10	−2.11	−2.16	0.01	0.06	0.48	3.01
isophorone	Tr	Tr/V	−3.57	−3.57	−3.57	0.00	0.00	0.00	0.03
2-propanol	Tr	Tr/V	−3.48	−3.48	−3.32	0.00	0.16	0.00	4.49
iso-proplyamine	Tr	Tr/V	−2.73	−2.75	−3.17	0.02	0.44	0.55	15.97
isoproplybenzene (2-propyl)	Tr	Tr/V	−0.22	−0.22	−0.16	0.00	0.06	0.00	27.27
isopropyl acetate	Tr	Tr/V	1.94	1.94	1.53	0.00	0.41	0.00	21.01
isopropyl formate	Tr	Tr/V	−1.50	−1.52	−1.43	0.02	0.07	1.33	4.78
m-bromotoluene	Tr	Tr/V	−0.56	−0.56	−0.42	0.00	0.14	0.00	25.61
m-chlorotoluene	Tr	V	−0.18	−0.18	−0.19	0.00	0.01	0.00	55.54
m-cresol (3-methylphenol)	Tr	Tr/V	−4.45	−4.47	−4.21	0.02	0.24	0.45	5.40
methanethiol	Tr	Tr/V	−0.99	−1.01	−1.70	0.02	0.71	2.02	71.73
methanol	Tr	Tr/V	−3.73	−3.73	−3.08	0.00	0.65	0.00	17.39
methyl acetate	Tr	Tr/V	−2.33	−2.33	−1.91	0.00	0.42	0.00	18.09
methyl hexanoate	Tr	Tr/V	−1.82	−1.82	−1.95	0.00	0.13	0.00	7.10
methyl isobutyl ether	Ts	Ts	−1.04	−1.14	−1.59	0.10	0.55	9.62	52.54
methyl isopropyl ether	Tr	V	−1.43	−1.46	−1.44	0.03	0.01	2.10	0.97
methyl *n*-butyl ether	Tr	Tr/V	−1.14	−1.14	−1.41	0.00	0.27	0.00	23.58
methyl propionate	Tr	Tr/V	−2.15	−2.16	−2.09	0.01	0.06	0.47	2.61
methyl propyl ether	Tr	Tr/V	−1.22	−1.23	−1.68	0.01	0.46	0.57	37.62
methyl *tert*-butyl ether	Tr	Tr/V	−1.62	−1.64	−1.25	0.02	0.37	1.23	22.95
methylamine	Tr	Tr/V	−3.34	−3.36	−4.24	0.02	0.90	0.65	26.82
methylbutyrate	Ts	Ts	−2.08	−2.06	−2.01	0.02	0.07	0.96	3.34
methylcyclohexane	Tr	Tr/V	1.21	1.21	1.23	0.00	0.02	0.00	1.85
methylcyclopentane	Tr	Tr/V	1.17	1.14	1.30	0.03	0.13	2.56	10.78
methylformate	Tr	Tr/V	−2.04	−2.06	−1.86	0.02	0.18	0.98	8.95
methylthiobenzene	Tr	Tr/V	−2.00	−2.03	−1.96	0.03	0.04	1.35	1.96
methyltrimethyl acetate	Ts	Ts	−1.76	−1.64	−2.03	0.12	0.27	6.82	15.17
m-xylene	Tr	V	−0.53	−0.53	−0.20	0.00	0.33	0.00	63.01
n,n-diethylformamide	Tr	V	−5.52	−5.52	−5.69	0.00	0.17	0.00	3.09
n,n-dimethylaniline	Tr	Tr/V	−2.53	−2.53	−2.74	0.00	0.21	0.00	8.28
n-amyl acetate	Tr	Tr/V	−1.80	−1.82	−1.70	0.02	0.10	1.11	5.53
naphthalene	Tr	Tr/V	−1.75	−1.78	−1.54	0.03	0.21	1.71	12.24
n-butyl acetate	Tr	Tr/V	−1.94	−1.96	−1.73	0.02	0.21	1.18	11.01
n-butyl propionate	Ts	Ts	−1.69	−1.19	−1.87	0.50	0.18	29.74	10.56
n-butylamine	Tr	Tr/V	−3.11	−3.11	−3.22	0.00	0.11	0.00	3.61
n-butylbenzene	Ts	Ts	−0.28	−0.25	−0.28	0.03	0.00	10.71	0.42
n-butylformate	Tr	V	−1.68	−1.70	−1.51	0.02	0.17	1.19	9.88
n-decanal	Tr	V	−1.13	−1.14	−1.33	0.01	0.20	0.89	17.80
n-decane	Tr	Tr/V	2.33	2.30	2.02	0.03	0.31	1.29	13.52
n-ethylaniline	Tr	Tr/V	−3.18	−3.18	−3.78	0.00	0.60	0.00	18.79
n-heptane	Ts	Ts	1.92	1.99	1.94	0.07	0.02	3.65	0.79
n-heptylamine	Ts	Ts	−2.78	−2.71	−2.58	0.07	0.20	2.52	7.32
n-hexane	Ts	Ts	1.84	1.84	1.86	0.00	0.02	0.00	1.15
n-hexyl acetate	Tr	Tr/V	−1.70	−1.70	−1.55	0.00	0.15	0.00	8.88
n-hexylamine	Tr	Tr/V	−2.90	−2.90	−2.74	0.00	0.16	0.00	5.49
n-hexylbenzene	Tr	Tr/V	−0.03	−0.06	−0.04	0.03	0.01	96.68	42.33
nitrobenzene	Tr	V	−3.02	−3.02	−2.92	0.00	0.10	0.00	3.47
nitroethane	Tr	Tr/V	−2.72	−2.75	−2.72	0.03	0.00	0.92	0.04
nitromethane	Ts	Ts	−2.95	−2.75	−2.98	0.20	0.03	6.95	1.05
n-methylaniline	Ts	Ts	−3.44	−3.18	−3.65	0.26	0.21	7.56	6.03
n-nonane	Tr	Tr/V	2.30	2.30	2.02	0.00	0.28	0.00	12.20
n-octadecane	Tr	Tr/V	−0.18	−0.18	−0.12	0.00	0.06	0.00	34.00
n-octane	Ts	Ts	2.08	2.15	2.05	0.07	0.03	3.37	1.60
n-octylamine	Tr	Tr/V	−2.68	−2.71	−2.50	0.03	0.18	1.12	6.70
nonan-5-one	Ts	Ts	−1.94	−1.82	−2.06	0.12	0.12	6.19	5.94
nonanal	Tr	Tr/V	−1.52	−1.52	−1.49	0.00	0.03	0.00	2.23
nonanoic acid	Ts	Ts	−4.33	−4.47	−3.75	0.14	0.58	3.23	13.40
n-pentyl acetate	Ts	Ts	−1.84	−1.82	−1.71	0.02	0.13	1.09	7.25
n-pentylamine	Tr	V	−3.00	−3.00	−2.92	0.00	0.08	0.11	2.55
n-pentylbenzene	Tr	Tr/V	−0.17	−0.18	−0.24	0.01	0.07	5.88	41.17
n-pentylcyclopentane	Tr	Tr/V	1.87	1.84	1.88	0.03	0.01	1.60	0.74

Table 2. (Continued)

compounds	data sets[a]		logH			absolute logH error		absolute % logH error	
	FAM[b]	Bk−Pr[c]	reported	FAM	Bk−Pr	FAM	Bk−Pr	FAM	Bk−Pr
n-propyl acetate	Ts	Ts	−2.05	−2.06	−1.86	0.01	0.19	0.49	9.38
n-propylbenzene	Ts	Ts	−0.55	−0.40	−0.50	0.15	0.05	26.48	9.03
n-propylcyclopentane	Tr	Tr/V	1.56	1.56	1.36	0.00	0.20	0.00	12.53
n-propylpropionate	Tr	Tr/V	−1.79	−1.82	−2.04	0.03	0.25	1.68	14.15
n-tetradecane	Tr	Tr/V	1.14	1.14	1.35	0.00	0.21	0.00	18.81
n-undecane	Tr	Tr/V	2.87	2.87	1.92	0.00	0.95	0.00	33.00
o-cresol (2-methylphenol)	Tr	Tr/V	−4.31	−4.34	−4.39	0.03	0.08	0.70	1.83
octanal	Ts	Ts	−1.68	−2.11	−1.64	0.43	0.04	25.60	2.18
octanoic acid	Tr	Tr/V	−4.47	−4.47	−3.78	0.00	0.69	0.00	15.49
o-ethylphenol	Tr	Tr/V	−3.72	−3.73	−4.29	0.01	0.57	0.27	15.39
o-xylene	Tr	Tr/V	−0.66	−0.67	−0.55	0.01	0.11	1.51	16.53
p-chloronitrobenzene	Tr	Tr/V	−2.65	−2.67	−2.36	0.02	0.29	0.75	10.94
pentachlorobenzene	Tr	Tr/V	−0.40	−0.40	−0.39	0.00	0.01	0.00	2.56
pentanal	Tr	V	−2.22	−2.22	−2.09	0.00	0.13	0.00	5.66
pentane	Tr	Tr/V	1.70	1.68	1.37	0.02	0.33	1.18	19.44
pentanoic acid	Ts	Ts	−4.52	−4.54	−4.03	0.02	0.49	0.44	10.89
phenanthrene	Tr	Tr/V	−2.79	−2.80	−2.31	0.01	0.48	0.20	17.31
phenol	Tr	Tr/V	−4.87	−4.87	−4.10	0.00	0.77	0.00	15.75
phenylacetic acid	Tr	Tr/V	−5.78	−5.78	−4.91	0.00	0.87	0.00	15.05
phenylacetylene	Tr	Tr/V	−0.55	−0.56	−0.81	0.01	0.26	2.00	47.18
phenylmethyl sulfide	Ts	Ts	−2.00	−2.03	−1.96	0.03	0.04	1.35	2.07
p-isopropyl toluene	Tr	Tr/V	−0.30	−0.30	−0.51	0.00	0.21	0.00	70.86
p-methylacetophenone	Tr	Tr/V	−3.45	−3.46	−3.47	0.01	0.02	0.29	0.58
prop-2-en-1-ol (allyl alcohol)	Tr	V	−3.69	−3.69	−2.97	0.00	0.72	0.00	19.54
propane	Tr	V	1.46	1.46	0.70	0.00	0.76	0.00	51.72
propionaldehyde	Tr	V	−2.52	−2.53	−2.44	0.01	0.08	0.40	3.16
propiophenone	Tr	Tr/V	−2.27	−2.29	−2.87	0.02	0.60	0.88	26.54
propoinic acid	Tr	Tr/V	−4.74	−4.77	−4.00	0.03	0.74	0.63	15.70
propyl benzene	Tr	Tr/V	−0.39	−0.40	−0.24	0.01	0.15	3.68	38.28
propyl formate	Ts	Ts	−1.75	−1.52	−1.66	0.23	0.09	13.14	5.06
propylamine	Tr	V	−3.22	−3.22	−3.51	0.00	0.29	0.00	9.06
propylene oxide	Tr	V	−2.55	−2.57	−2.08	0.02	0.47	0.78	18.31
propyne	Tr	Tr/V	−0.35	−0.36	−0.30	0.01	0.05	2.86	15.20
pyridine	Tr	Tr/V	−3.44	−3.46	−3.11	0.02	0.33	0.58	9.60
pyrrole	Tr	Tr/V	−3.13	−3.13	−2.89	0.00	0.24	0.00	7.55
pyrrolidine	Tr	Tr/V	−4.01	−4.01	−2.57	0.00	1.44	0.00	35.82
quinoline	Tr	Tr/V	−4.17	−4.18	−4.35	0.01	0.18	0.24	4.27
sec-butyl acetate	Tr	Tr/V	−1.77	−1.78	−1.60	0.01	0.17	0.56	9.38
sec-butylbenzene	Tr	V	−0.25	−0.25	−0.22	0.00	0.03	0.00	11.98
styrene	Tr	Tr/V	−0.95	−0.97	−0.83	0.02	0.12	2.11	12.83
tert-butyl alcohol	Ts	Ts	−3.23	−3.29	−2.90	0.06	0.33	1.86	10.33
tert-butyl amine	Tr	Tr/V	−2.83	−2.85	−2.27	0.02	0.56	0.71	19.75
tert-butylbenzene	Tr	Tr/V	−0.32	−0.33	−0.40	0.01	0.08	3.12	25.86
tetrachloroethene	Tr	V	−0.14	−0.14	−0.14	0.00	0.00	0.00	0.00
tetrachloromethane	Tr	V	0.06	0.06	0.07	0.00	0.01	0.01	19.83
tetrafluoromethene	Tr	V	2.32	2.30	2.13	0.02	0.19	0.86	8.28
tetrahydrofuran	Tr	Tr/V	−2.54	−2.57	−1.67	0.03	0.87	1.18	34.13
tetrahydropyran	Tr	Tr/V	−2.29	−2.29	−1.84	0.00	0.45	0.00	19.49
thiophene	Tr	Tr/V	−0.92	−0.92	−0.67	0.00	0.25	0.00	27.54
thiophenol	Tr	Tr/V	−1.86	−1.86	−1.27	0.00	0.59	0.15	31.96
toluene	Tr	Tr/V	−0.57	−0.59	−0.43	0.02	0.14	3.51	24.56
trans 1,4-dimethylcyclohexane	Ts	Ts	1.55	1.14	1.79	0.41	0.24	26.45	15.34
trans-2-butenal	Tr	Tr/V	−3.10	−3.11	−2.82	0.01	0.28	0.32	9.10
trans-2-hexenal	Tr	V	−2.70	−2.71	−2.81	0.01	0.11	0.37	3.90
trans-2-octenal	Tr	Tr/V	−2.52	−2.53	−2.81	0.01	0.29	0.40	11.61
tribromomethane	Tr	Tr/V	−1.66	−1.66	−2.45	0.00	0.79	0.00	47.61
trichloroethene	Tr	V	−0.44	−0.45	−0.37	0.01	0.07	2.72	15.53
trichlorofluoromethane	Tr	V	0.60	0.58	0.72	0.02	0.12	3.33	20.00
trichloronitromethane	Tr	Tr/V	−1.08	−1.08	−0.26	0.00	0.82	0.00	75.93
triethylamine	Ts	Ts	−2.36	−2.71	−2.94	0.35	0.58	14.83	24.69
trifluorobenzene (benzotrifluoride)	Tr	Tr/V	−0.18	−0.18	−0.26	0.00	0.08	0.00	42.84
trimethylamine	Tr	V	−2.35	−2.38	−2.80	0.03	0.45	1.28	19.00
tripropylamine	Tr	Tr/V	−1.81	−1.82	−1.67	0.01	0.14	0.55	7.97

[a] Tr = training set, Ts = test set, V = validation set. [b] FAM = present fuzzy ARTMAP QSPR. [c] BK−Pr = present back-propagation QSPR.

ART system includes a field of nodes, F_o, that represents a current input vector; 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 input patterns (molecular descriptors), while *artB* module develops categories of target patterns (physical property) during supervised learning (training). During supervised learning, the *artA* module receives the molecular

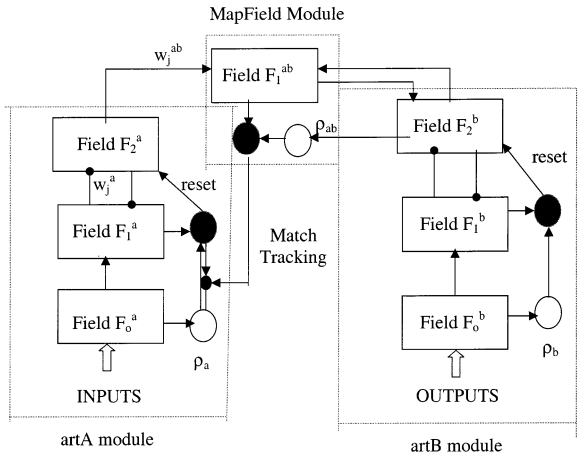

Figure 2. Block diagram of fuzzy ARTMAP neural network.

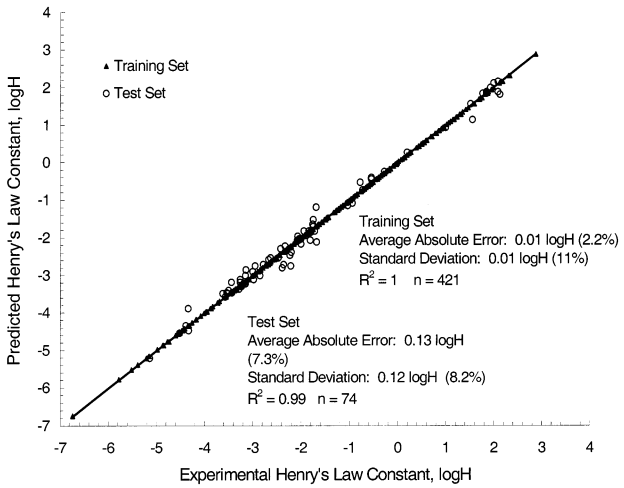

Figure 3. Henry's Law constant (dimensionless) estimates using the present fuzzy ARTMAP QSPR.

descriptors and the *artB* module receives the correct physical property prediction of the input presented to F_o^a. The *artA* module attempts a prediction through the *map field* of the category to which the current target belongs. The inter-ART module (*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 a *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 are relevant for such a category to be accepted. The vigilance parameter controls the degree of generalization. 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. In general, the degree of similarity among input features is determined by the vigilance and choice parameters.

The fuzzy ARTMAP-based QSPR for logH was developed following the methodology described in Figure 1. About 85% (421) of the 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 421 compounds, the hypothesis component of the *artB* module (F_o^b and F_1^b) was disconnected and the output in its category layer F_2^b was implemented.[27,36] Therefore, through the map field module F_1^{ab}, a prediction for the target physical property was obtained for any input of descriptors presented to module *artA*. The model was then evaluated with a test set containing 74 compounds.

Back-Propagation Neural Network System. The logH data and molecular descriptors, normalized from 0 to 1, were divided into training, validation (or recall) and test data sets. The test data set of 74 compounds (about 15% of the complete data set) was selected to be identical to the fuzzy ARTMAP test set to enable direct comparison of the QSPRs derived from two different networks. A random selection of 331 compounds of the remaining 421 compounds (about 67% of the total data set) made up the training set. To maintain an adequate size of the validation or recall set, the training set (331 compounds) and the remaining data not used for testing (90 compounds) were combined into a single validation set.

Model building with the back-propagation neural network proceeded with the same seven input descriptors and logH data set used for the fuzzy ARTMAP model. The neural network architecture was developed using a cascade method of network construction, together with a Kalman filtering learning rule.[35] In the above approach, hidden nodes were added one or two at a time with new hidden units having connections from both the input buffer and previously established hidden nodes. Construction was stopped when the validation (recall) set showed no further performance improvement. The optimal back-propagation neural network/QSPR for logH had a 7−17−1 architecture in which the hyperbolic tangent transfer function was chosen to correlate weighted inputs and outputs of the hidden layer. The resulting optimal neural network architecture was then validated and tested using the two data subsets described above.

III. RESULTS AND DISCUSSION

The optimal fuzzy ARTMAP/QSPR was obtained (i.e. training phase) for vigilance parameters $\rho_a = 0$, $\rho_b = 0.996$, $\rho_{ab} = 0.996$, learning rate parameters $\beta_a = 1$, $\beta_b = 1$, and choice parameter $\alpha = 0.0001$. The back-propagation QSPR was obtained for a 7−17−1 architecture using a set of seven molecular descriptors (Table 1). It is noted that, although errors of Henry's law estimation methods are often reported as absolute logH errors, these can be misleading since actual percent errors can be significant even for seemingly low absolute logH errors if, for example, the logH values for the corresponding range of compounds is small. Conversely, a reported high absolute logH error can also be misleading if it pertains to a range of high logH values. Therefore, in this study, to present a more balanced evaluation of model performance, both the absolute and absolute percent logH errors are reported. The performance of the present two models are presented in Table 2 and Figures 3 and 4, with an error analysis summary provided in Tables 3 and 4.

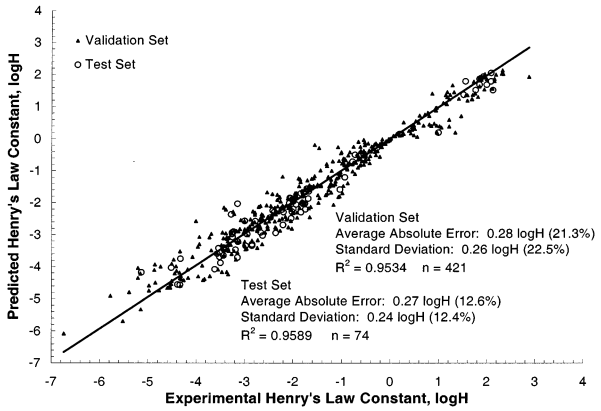

Figure 4. Henry's Law constant (dimensionless) estimates using the present back-propagation QSPR.

Table 3. Performance of the logH QSPRs Based on Fuzzy ARTMAP and Back-Propagation Neural Networks[a]

		average absolute error		maximum absolute error		standard deviation	
data set	records	logH	%	logH	%	logH	%
Fuzzy ARTMAP							
all data	495	0.03	2.9	0.53	131	0.06	11.1
training	421	0.01	2.2	0.04	131	0.01	11.4
test	74	0.13	7.3	0.53	37	0.12	8.2
Back-Propagation							
all data	495	0.28	20	1.4	154	0.26	21
training	331	0.29	21.8	1.4	154	0.27	22
validation	421	0.28	21.3	1.4	154	0.26	22
test	74	0.27	12.6	1.1	81	0.24	12.4

[a] Errors are expressed as |logH| estimation errors; H is dimensionless ($H = C_a/C_w$).

The performance of the fuzzy ARTMAP logH QSPR, for the complete set of 495 compounds, was with extremely low absolute average and maximum errors of 0.03 (2.9%) and 0.53 (131%) logH units, respectively, and a corresponding standard deviation of 0.06 (11.1%) logH units (Table 2). The performance of the fuzzy ARTMAP/QSPR for the test set of 74 compounds, with a relaxed vigilance parameter setting of $\rho_a = 0.9$, was with absolute average and maximum absolute errors and standard deviation of 0.13 (7.3%), 0.53 (37%), and 0.12 (8.2%) logH units, respectively. Although the performance of the logH fuzzy ARTMAP/QSPR was excellent for the heterogeneous set of compounds, there were several compounds, which were misclassified, thereby resulting in elevated logH errors. It appears that chemical input descriptors can be similar for some compounds (e.g., isomers), while there may be relatively large differences in their logH values. For example, 2,2′3,3′-PCB (logH = -2.21) was assigned to the category represented by 2,2′3,3′4,6-PCB (logH = -2.74) resulting in absolute error of 0.53 (24%) logH units. Another example of misclassification of structural isomers is the placing of *n*-butyl propionate (logH = -1.69) into a recognition category generated for isobutyl propionate (logH = -1.17). The condition of conflicting data, where two input patterns are very similar but have different outputs, was also observed for the pairs 2,5-dimethlyphenol (logH = −4.34) and 2,6-dimethlyphenol (logH = −3.86) as well as trans 1,4-dimethylcyclohexane (log H = 1.55) and 1,2-dimethylcyclohexane (logH = 1.17). Since the accuracy of the fuzzy ARTMAP based model depends on the quality of the training set, it is always desired to include a rich set comprised of many different chemical categories to arrive at a reasonable number of categories. If a given chemical in a test does not have a matching category, developed in the training phase, the fuzzy ARTMAP will match the compound with the closest available recognition category according to a tolerance set by the vigilance parameter. For example, during model evaluation with the test set, octanal (logH = −1.68), an aldehyde with a molecular formula of $C_8H_{16}O$, was classified with 2-octanone (logH = −2.11), a ketone also with a molecular formula of $C_8H_{16}O$. The above examples suggest that further improvements to the fuzzy ARTMAP logH QSPR would require a data set that contains a larger number of compounds per class and possibly a refined set of molecular descriptors to allow a greater ability to differentiate among complex or apparently very similar structures.

The logH QSPR, derived based on the optimal 7−17−1 back-propagation network, performed with absolute average and maximum errors, and standard deviation, for the training set, of 0.29 (21.8%), 1.4 (154%) and 0.27 (22%) logH units, respectively. LogH estimates for the validation set (recall phase) were obtained with absolute average and maximum errors, and standard deviation of 0.28 (21.3%), 1.4 (154%), and 0.26 (22%) logH units, respectively. Performance of the back-propagation/QSPR for the test set (same as that of the fuzzy ARTMAP based QSPR) was better, relative to the training and validation sets, with absolute average and maximum absolute errors, and standard deviation of 0.27 (12.6%), 1.1 (81%), and 0.24 (12.4%) logH units, respectively. However, the performance of the fuzzy ARTMAP based logH QSPR was superior as indicated in Table 3. Nonetheless, the overall performance of the back-propagation model is relatively good compared to other published methods of estimating logH. It is interesting to note that Brennan et al.[6] suggested that predictions of Henry's Law constant within a factor of 2.5 are a reasonable for many environmental applications given the variability among measured data, where standard deviations can range from less than 0.05 to about 0.5 logH units.[16]

The performance of the present logH QSPR models can also be assessed based on error analysis for specific chemical groups (Table 4). It is noted that the errors for the majority of the different chemical groups are within the same order of magnitude, for each respective model; however, errors for the fuzzy ARTMAP are generally about 2 orders of magnitude lower than for the back-propagation-based QSPR. Among the specific chemical groups, absolute average and percent logH errors for the fuzzy ARTMAP/QSPR reached up to 0.6 logH units and 10.17%, respectively. In contrast, the absolute average and percent logH errors for the back-propagation QSPR were higher ranging from 0.15 to 0.63 logH units or the equivalent of 6.48 to 46.76%, respectively. However, the performance (in terms of absolute percent logH error) of the back-propagation QSPR was better for aldehydes, nitriles, phenols (both halogenated and nonhalogenated), and amides, relative to the other groups (<10%). Eleven out of the twenty five chemical groups (i.e., representing 58% or 289 compounds of the total data set) exhibited average absolute errors of less than 0.27 logH units. The highest absolute average and percent errors of 0.63 logH and

Table 4. Error Analysis Based on Chemical Classes[a]

chemical classes and functional groups	no. of compds	average absolute logH error		average absolute percent logH error	
		Fuzzy ARTMAP	back-propagation	Fuzzy ARTMAP	back-propagation
alkanes	44	0.04	0.25	2.21	17.54
alkenes	23	0.01	0.37	1.46	42.17
alkynes	6	0.01	0.07	4.23	24.60
aromatics	27	0.02	0.15	10.17	30.10
carboxylic acids	11	0.02	0.58	0.56	12.39
aldehydes	14	0.04	0.15	2.43	6.94
ketones	27	0.04	0.26	1.79	10.15
alcohols	53	0.04	0.31	1.34	10.30
ethers	16	0.02	0.38	1.47	26.29
amines	19	0.05	0.32	1.87	12.15
PCBs	17	0.05	0.37	2.37	17.13
halogenated aliphatics	77	0.02	0.22	7.32	34.41
halogenated aromatics	24	0.01	0.23	1.04	20.85
nitriles	4	0.03	0.25	1.01	9.10
nitro compounds	9	0.04	0.26	1.46	14.77
esters	34	0.04	0.22	2.27	12.56
PAHs	23	0.03	0.27	1.43	17.33
aromatic amines	6	0.05	0.38	1.34	10.36
phenols	14	0.05	0.29	1.10	7.20
heterocyclic − nitrogen (e.g. pyridines)	19	0.02	0.50	0.68	13.17
sulfonated (mercaptans)	9	0.03	0.29	2.53	31.14
heterocyclic − oxygen (e.g. furans)	3	0.01	0.63	0.90	46.76
halogenated phenols	11	$<10^{-2}$	0.35	0.12	7.52
heterocyclic − sulfur (e.g. thiophene)	3	$<10^{-2}$	0.29	0.05	22.06
amides	2	$<10^{-2}$	0.42	$<10^{-2}$	6.48

[a] Errors are reported as |logH| estimation errors averaged for each listed chemical group.

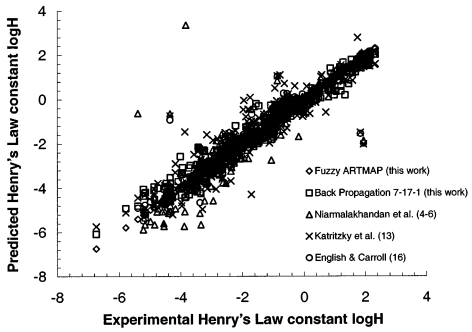

Figure 5. Comparison of selected methods of estimating the Henry's Law constant of organic compounds.

46.76%, respectively, obtained for the back-propagation based QSPR, were attributed to three heterocyclic oxygen compounds in the data set. In contrast, the highest absolute percent logH error of 10.17% for the fuzzy ARTMAP model occurred for aromatic hydrocarbons while less than 2% logH error were encountered for 17 of the 25 chemical groups. For both models, average absolute percent logH errors were relatively lower for amides, halogenated phenols, nitriles, alcohols, aromatic amines, and carboxylic acids. However, for both models, relatively high average absolute percent logH errors were encountered for aromatic and halogenated aliphatic compounds since many of those compounds possess relatively low logH values. Overall, the estimation errors for the specific chemical groups are largely attributed to logH data that 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 wells as for the overall data set.

The two QSPR models developed in this work were compared to previously reported multiple linear regression and neural network-based logH QSPRs. It is noted that the literature reports[4,5,13−16] a range of average absolute estimation error of about 0.24 to 0.56 logH units, for logH correlations spanning various ranges of the Henry's law constant. In contrast, the present back-propagation and fuzzy ARTMAP based models performed with average absolute errors of 0.13 and 0.27 logH units, respectively for a Henry's law constant range of $-6.72 \leq \log H \leq 2.87$. More specific comparisons of the performance of the present to previously published logH QSPRs,[4,5,15−16] for compounds common with the present data set, are provided in Table 5 and Figure 5. The predictions of the back-propagation and fuzzy ARTMAP models, for 277 compounds common with the data set of Nirmalakhandan and Speece,[4,5] were within an average absolute and maximum errors and standard deviation of 0.26 (19.5%), 1.3 (127%) and 0.25 (21.4%) and 0.03 (3.6%), 0.5 (131%), and 0.07 (13.2%) logH units, respectively. The above performance was somewhat better than for the Nirmalakhandan and Speece[4,5] model predictions that yielded higher average absolute error, maximum error and standard deviation of 0.38 (36.6%), 7.2 (1550%), and 0.67 (113.6%) logH units, respectively. Estimates for 308 compounds common with the data set of Katritzky et al.,[15] resulted in average absolute and maximum errors and standard deviation of 0.29 (20.5%), 1.4 (154%), and 0.26 (22.6%) and 0.025 (2.8%), 0.5 (131%) and 0.06 (11.4%) logH units, for the present back-propagation and fuzzy ARTMAP models, respectively. For the same 308 compounds, the multi-linear regression $\log L_w$ QSPR of Katritzky et al.,[15] resulted in higher average absolute and maximum errors and standard deviation of 0.50 (91.45), 3.96 (6700%), and 0.51 (521%) logH units (or $\log L_w^{-1}$ units), respectively. Finally, the present models were compared, for a common set of 275 compounds, to the 10-3-1 neural network/QSPR model of English and Carroll[16] which was reported to perform with

Table 5. Comparison of QSPR Models for Estimating the Henry's Law Constant at 25 °C

	LogH [dimensionless]					
compound	exptl	FAM[a]	Bk−Pr[b]	N&S[c]	Ketal[d]	E&C[e]
1,1,1,2-tetrachloro-2,2-difluoroethane	−0.78	−0.78	−1.02		1.1	
1,1,1,2-tetrachloroethane	−0.95	−0.97	−0.80	−1.13	−0.47	−1.05
1,1,1-trichloroethane	−0.18	−0.18	−0.18		−0.13	−0.29
1,1,1-trichloropropane	−0.88	−0.89	−0.78		−0.21	
1,1,2,2-tetrabromoethane	−3.24	−3.24	−2.28		−2.76	
1,1,2,2-tetrachloroethane	−1.82	−1.82	−1.62	−1.18	−0.44	
1,1,2-trichloroethane	−1.32	−1.33	−0.79	−0.91	−0.67	
1,1,2-trichloropropane	−1.89	−1.89	−1.24		−0.78	
1,1-dichlorobutane	−0.51	−0.53	−0.49		−0.52	−0.6
1,1-dichloroethane	−0.63	−0.64	−0.83	−0.54	−0.42	−0.09
1,1-dichloroethene	0.03	0.03	0.03		0.17	
1,1-difluoroethene	1.16	1.14	1.08		1.41	
1,2,3-trichloropropane	−1.85	−1.86	−1.35		−0.99	
1,2,3-trimethylbenzene	−0.89	−0.89	−0.96	−0.31	−0.06	−0.7
1,2,4-trichlorobenzene	−0.76	−0.78	−0.74	−1.61	−1.2	−0.92
1,2,4-trimethylbenzene	−0.62	−0.64	−0.64	−0.3	−0.07	−0.7
1,2-dibromo-3-chloropropane	−2.22	−2.20	−2.34		−2.71	
1,2-dibromoethane	−1.56	−1.59	−0.19	−1.27	−1.01	
1,2-dibromopropane	−1.22	−1.23	−1.27		−1.11	
1,2-dichlorobenzene (o)	−1.11	−1.14	−1.24	−1.32	−0.91	−1.07
1,2-dichloroethane	−1.31	−1.31	−1.36	−0.64	−0.73	−0.92
1,2-dichloroethylene	−0.78	−0.53	−0.71		−0.19	−0.83
1,2-dichloropropane	−0.94	−0.97	−0.63	−0.47	−0.84	−0.71
1,3,5-trichlorobenzene	−1.02	−1.05	−1.14	−1.61		
1,3,5-trimethlybenzene	−0.62	−0.64	−0.25	−0.3	−0.06	
1,3-butadiene	0.48	0.48	0.11	0.64		0.49
1,3-dibromopropane	−1.44	−1.46	−0.99		−1.14	
1,3-dichlorbenzene (m)	−0.97	−0.97	−0.62	−1.32		
1,3-dichloropropane	−1.14	−1.14	−1.42	−0.54	−0.87	
1,3-dimethylnaphthalene	−1.81	−2.06	−2.01	−2.67		−1.45
1,4-dichlorobenzene (p)	−1.01	−1.01	−0.42	−1.32	−1.03	
1,4-dichlorobutane	−1.70	−1.70	−1.54	−0.44	−0.98	−0.68
1,4-diethylbenzene	−0.51	−0.53	−0.44	−0.29		
1,4-dimethylnaphthalene	−2.07	−1.96	−1.85	−2.68		
1,4-pentadiene	0.68	0.67	0.41			0.61
1,5-dichloropentane	−1.64	−1.64	−1.49		−1.02	
1,5-hexadiene	0.84	0.84	0.40	0.84		0.73
1-bromo-2-chloroethane	−1.43	−1.46	−1.48		−1.63	
1-bromo-2-methylpropane	−0.02	−0.02	−0.01	−0.33		0
1-bromobutane	−0.45	−0.45	−0.63	−0.41	−0.01	−0.19
1-bromoheptane	0.27	0.26	0.51	−0.09	−0.14	0.19
1-bromohexane	0.19	0.26	0.15	−0.19	−0.12	0.07
1-bromonaphthalene	−1.93	−1.96	−1.69		−1.65	
1-bromooctane	0.38	0.38	0.25	0.01	−0.14	0.32
1-bromopentane	−0.09	−0.10	−0.07	−0.3	−0.1	−0.06
1-bromopropane	−0.52	−0.53	−0.66	−0.51	0.07	−0.32
1-butanol	−3.43	−3.46	−3.40	−3.39	−3.66	−3.37
1-butene	1.01	1.01	0.39	1.08	0.86	0.93
1-chloro-1,1-difluoroethane	0.71	0.68	0.75		−0.58	
1-chlorobutane	−0.17	−0.18	−0.02	−0.09	−0.53	−0.13
1-chlorohexane	0.06	0.06	0.09	0.12	−0.62	0.12
1-chloronaphthalene	−1.84	−1.89	−2.30		−1.43	
1-chlorooctane	0.19	0.19	0.10		−0.64	
1-chloropentane	−0.01	−0.02	−0.02	0.01	−0.6	−0.01
1-chloropropane	−0.27	−0.30	−0.38	−0.19	−0.46	−0.26
1-cyanobutane	−2.67	−2.58	−2.93	−1.57		−2.01
1-cycanopropane	−2.58	−2.58	−2.93	−1.68		−2.15
1-decanol	−2.71	−2.71	−2.13	−2.77	−3.39	
1-ethyl-2-methylbenzene	−0.76	−0.78	−0.25	−0.37	−0.1	
1-ethyl-4-methylbenzene	−0.69	−0.71	−0.49	−0.37		−0.63
1-ethylnaphthalene	−1.07	−1.08	−1.09	−2.74		−1.37
1-heptanol	−2.64	−2.67	−3.29	−3.09	−3.5	−3.09
1-heptyne	0.44	0.42	0.28	0.34		0.48
1-hexene	1.23	1.21	1.36	1.28	0.82	1.17
1-hexyne	0.23	0.23	0.11	0.24		0.36
1-iodobutane	−0.19	−0.22	−0.18	−0.27		−0.29
1-iodopropane	−0.43	−0.45	−0.76	−0.37	−0.45	−0.42
1-methoxy-2-propanol	−4.42	−4.42	−3.99		−3.94	
1-methylcyclohexene	0.48	0.48	0.41		0.41	0.22
1-methylnaphthalene	−1.97	−1.97	−1.85		−0.46	−1.58
1-nitropropane	−2.45	−2.46	−2.48	−2.07	−1.88	−2.46
1-nonanol	−2.90	−2.90	−2.75	−2.88	−3.4	

Table 5. (Continued)

compound	LogH [dimensionless]					
	exptl	FAM[a]	Bk−Pr[b]	N&S[c]	Ketal[d]	E&C[e]
1-nonene	1.51	1.56	1.37	1.59		1.53
1-nonyne	0.77	0.77	0.81			0.71
1-octanol	−3.00	−2.90	−2.57	−2.99	−3.49	−3
1-octene	1.59	1.56	1.36	1.48	0.85	1.41
1-octyne	0.52	0.52	0.55	0.44		0.59
1-pentanol	−3.27	−3.29	−3.60	−3.29	−3.52	−3.28
1-pentene	1.21	1.21	0.38	1.18	0.83	1.05
1-pentyne	−0.05	−0.06	−0.07	0.14		0.24
1-propanol	−3.52	−3.48	−3.69	−3.49	−3.62	−3.46
1-propene	0.90	0.90	0.47	0.99		0.81
2,2,2-trifluoroethanol	−3.15	−3.18	−3.55		−1.59	−3.23
2,2′,4,5,5′-pentachloro-1,1′-biphenyl	−2.43	−2.46	−1.73			−2.18
2,2,4-trimethylpentane	2.12	1.81	1.51	2.15		2.04
2,2′,5-trichloro-1,1′-biphenyl	−2.00	−2.16	−2.19			−2.17
2,2,5-trimethylhexane	2.15	2.15	1.79			2.16
2,2′3,3′-tetrachloro-1,1′-biphenyl	−2.21	−2.74	−2.69			−2.21
2,2-dimethyl propanoic acid	−3.94	−3.97	−3.29		−3.35	
2,2-dimethylbutane	1.84	1.88	1.69	1.88	1.48	1.81
2,2-dimethylpentane	2.11	2.11	1.55	1.99	1.51	2.05
2,2-dimethylpropane	1.95	1.94	2.01	1.81	1.46	1.7
2,3,4-trimethylpentane	1.88	1.88	1.84	2.1	1.56	2.04
2,3-dichlorobutane	−0.53	−0.53	−0.11		−0.89	
2,3-dichloropropene	−0.84	−0.85	−0.42		−0.69	
2,3-dimethy-2-butanol	−3.39	−3.40	−2.95		−3.17	
2,3-dimethyl-1,3-butadiene	0.93	0.93	0.95	0.93		
2,3-dimethylbutane	1.72	1.72	1.78	1.84	1.49	1.82
2,3-dimethylnaphthalene	−2.04	−2.06	−2.22	−2.52		
2,3-dimethylpentane	1.85	1.84	1.88	1.93	1.51	1.83
2,3-dimethylphenol	−4.52	−4.54	−4.54	−5.06		−4.46
2,3-dimethylpyridine	−3.54	−3.46	−3.42	−3.37	−3.87	−3.59
2,4,6-triclorophenol	−3.97	−3.97	−3.38		−4.65	
2,4-dimethyl-3-pentanone	−1.84	−1.84	−1.92		−1.5	−1.55
2,4-dimethylpentane	2.08	1.88	1.79	1.95	1.52	1.93
2,4-dimethylphenol	−4.41	−4.42	−4.13	−5.06	−4.22	−4.59
2,4-dimethylpyridine	−3.57	−3.57	−3.59	−3.36	−3.88	−3.64
2,5-cyclohexadiene-1,4-dione	−1.71	−1.71	−1.30		−4.28	
2,5-dimethylphenol	−4.34	−3.88	−4.57	−5.06		−4.55
2,5-dimethylpyridine	−3.46	−3.46	−2.93	−3.36	−3.85	−3.59
2,6-dichlorophenol	−3.96	−3.97	−4.30		−4.79	
2,6-diethylaniline	−4.34	−4.34	−3.52		−4.09	
2,6-dimethyl-4-heptanone	−2.32	−2.33	−2.12		−1.48	
2,6-dimethylnaphthalene	−1.93	−1.96	−1.80	−2.67		
2,6-dimethylphenol	−3.86	−3.88	−4.42	−5.06	−1.46	
2-bromoethyl benzene	−1.21	−1.23	−1.00		−1.51	−0.84
2-bromopropane	−0.35	−0.36	−0.29		0.09	−0.22
2-butanol	−3.43	−3.46	−3.64	−3.35	−3.15	−3.32
2-butanone	−2.63	−2.63	−2.51	−2.61	−1.87	−2.54
2-chloro-1-nitrobenzene	−2.74	−2.75	−3.41		−3.27	
2-chloro2-methylpropane	0.80	0.77	0.45	0.11		
2-chlorobutane	−0.01	−0.02	−0.02	−0.02	−0.68	−0.07
2-chloroethanol	−4.51	−4.54	−4.44		−4.62	
2-chloropentane	−0.22	−0.22	−0.56		−0.73	0.05
2-chlorophenol	−3.34	−3.36	−3.44	−5.65		
2-chloropropane	−0.15	−0.18	−0.16	−0.1	−0.56	−0.19
2-chloropyridine	−3.22	−3.22	−2.35	−4.57	−2.3	−2.86
2-ethylbutyric acid	−4.18	−4.18	−4.08		−3.29	
2-ethylpyridine	−3.17	−3.18	−2.88	−3.43	−3.78	
2-fluorophenol	−3.88	−3.88	−3.96	−5.72		
2-heptanone	−2.23	−2.46	−2.21	−2.25	−1.75	−2.21
2-hexanol	−3.00	−3.00	−3.34		−3.45	
2-hexanone	−2.42	−2.29	−2.25	−2.36	−1.77	−2.32
2-iodophenol	−4.55	−4.55	−4.59	−5.59		−4.56
2-iodopropane	−0.55	−0.56	−0.03		−0.38	−0.29
2-methyl-1,3-butadiene	0.50	0.48	0.31	0.78		0.6
2-methyl-1-butanol	−3.24	−3.25	−2.84	−3.23	−3.67	−3.07
2-methyl-1-pentene	1.05	1.05	0.35	1.33		1.29
2-methyl-2-butanol	−3.25	−3.29	−3.07	−3.17	−3.23	−3.27
2-methyl-2-butene	0.95	0.93	0.97	1.25	0.84	0.92
2-methyl-2-pentanol	−2.84	−2.85	−2.83		−3.22	−3.19
2-methyl-2-propanol	−3.28	−3.29	−2.90	−3.26		−3.35
2-methyl-3-pentanol	−2.85	−2.85	−3.19	−3.11		−2.96
2-methyl-3-pentanone	−2.20	−2.38	−2.29		−1.75	

Table 5. (Continued)

	LogH [dimensionless]					
compound	exptl	FAM[a]	Bk−Pr[b]	N&S[c]	Ketal[d]	E&C[e]
2-methylaziridine	−3.46	−3.46	−2.93		−3.58	
2-methylbutane	1.76	1.84	1.51	1.68	1.44	1.71
2-methylhexane	2.15	2.15	1.86	1.89	1.5	
2-methylnaphthalene	−1.78	−1.78	−1.78		−0.47	
2-methylpentane	1.84	1.84	1.63	1.78	1.46	1.82
2-methylpropane	1.68	1.68	1.23	1.6	1.43	1.59
2-methylpyridine	−3.40	−3.40	−3.49	−3.51	−3.72	−3.53
2-nitropropane	−2.31	−2.33	−2.30	−2.01	−1.72	−2.25
2-nitrotoluene	−2.63	−2.53	−3.03	−3.76		
2-nonanone	−1.82	−1.82	−1.80	−2.04	−1.51	−1.99
2-octanone	−2.11	−2.11	−1.87	−2.15	−1.69	−2.1
2-pentanol	−3.22	−3.22	−3.17	−3.25	−3.35	−3.24
2-pentanone	−2.47	−2.53	−2.46	−2.46	−1.68	
2-pentene	0.99	0.93	0.19	1.18	0.82	1.05
2-propanol	−3.35	−3.36	−3.32	−3.43		−3.41
2-undecanone	−1.58	−1.59	−1.47	−1.84		−1.76
3,3-dimethyl-2-butanone	−2.28	−2.29	−1.82	−2.29	−1.82	−2.05
3,3-dimethylpentane	1.88	1.88	1.95	1.96	1.51	2.05
3,4-dichlorotoluene	−0.98	−1.01	−0.73		−1.35	
3,4-dimethylphenol	−4.77	−4.77	−4.74	−5.06		−4.71
3,4-dimethylpyridine	−3.83	−3.83	−4.39	−3.36	−3.84	−3.54
3,5-dimethylphenol	−4.60	−4.60	−4.66	−5.06		−4.62
3,5-dimethylpyridine	−3.55	−3.57	−4.09	−3.36	−3.91	−3.48
3-chlorophenol	−4.85	−4.87	−4.50	−5.65	−4.77	−4.52
3-chloropyridine	−2.94	−2.96	−2.80	−4.56		−2.86
3-ethylphenol	−3.37	−3.40	−4.16	−5.13		−4.65
3-formylpyridine	−5.21	−5.21	−4.04	−4.97		−5.47
3-heptanol	−2.94	−2.96	−3.02		−3.12	
3-heptanone	−2.43	−2.46	−2.35		−1.54	
3-hexanol	−3.00	−3.00	−3.22	−3.17		−3.16
3-hexanone	−2.29	−2.29	−2.54		−1.72	
3-methyheptane	2.18	2.15	1.99	1.98		2.05
3-methyhexane	1.99	1.99	1.86	1.88		1.94
3-methyl-1-butanol	−3.26	−3.18	−2.97	−4.05		−3.07
3-methyl-1-butene	1.34	1.34	0.19	1.24	0.85	1.05
3-methyl-2-butanone	−2.38	−2.38	−2.16		−1.8	−2.2
3-methyl-2-pentanol	−2.85	−3.00	−3.34		−3.14	
3-methylpentane	1.84	1.84	1.89	1.76	1.47	1.82
3-methylpyridine	−3.50	−3.40	−3.88	−3.51	−3.76	−3.37
3-methylthiophene	−0.53	−0.53	−0.49		−0.65	
3-nitrotoluene	−2.53	−2.53	−2.82	−3.76		
3-pentanol	−3.19	−3.22	−3.47	−3.28	−3.09	−3.24
3-pentanone	−2.50	−2.53	−2.58		−1.83	−2.43
4-bromophenol	−5.21	−5.21	−4.35	−5.87		−4.94
4-bromotoluene	−1.02	−1.05	−0.45			−0.93
4-chloro-2-nitrophenol	−3.29	−3.29	−3.31		−4.95	
4-chloro-3-methylphenol	−4.98	−4.98	−4.59	−5.5		−4.62
4-chloroaniline	−4.32	−4.34	−4.29		−4.56	−4.13
4-chlorophenol	−5.16	−5.16	−4.22	−5.65	−4.87	−4.76
4-ethylpyridine	−3.47	−3.48	−4.16	−3.43	−3.86	−3.4
4-fluorophenol	−4.54	−4.54	−4.66	−5.72		−4.72
4-formylpyridine	−5.14	−5.21	−4.17	−4.97		−5.2
4-heptanone	−2.14	−2.16	−2.52	−2.28		−2.21
4-methyl-1-pentene	1.41	1.41	1.24		0.84	1.17
4-methyl-2-methoxyphenyl	−4.26	−4.26	−4.42		−5.19	
4-methyl-2-pentanol	−2.74	−2.75	−2.88	−3.08	−3.12	
4-methyl-2-pentanone	−2.25	−2.26	−2.16	−2.29	−1.62	−2.1
4-methyl-2-pentyl acetate	−1.62	−1.64	−1.55		−1.92	
4-methylphenol (*p*-cresol)	−4.39	−4.34	−4.56	−4.24		−4.62
4-methylpyridine	−3.62	−3.48	−4.08	−3.51	−3.77	−3.42
4-*n*-propylphenol	−4.33	−4.34	−4.60	−5.03		−4.46
4-*tert*-butylphenol	−4.34	−4.34	−4.36	−4.78		−4.22
4-vinylcyclohexene	0.26	0.26	0.18		0.18	
acenaphthene	−2.20	−2.22	−2.13	−2.42		
acetaldehyde	−2.57	−2.57	−2.62	−2.56	−2.28	−2.55
acetamide	−6.74	−6.74	−6.07		−5.73	
acetic acid	−5.39	−5.39	−4.79	−0.62	−4.43	−4.89
acetone (propanone)	−2.79	−2.80	−2.37	−2.71	−1.77	−2.8
acetonitrile	−2.85	−2.85	−2.67	−1.85	−4.04	−2.86
acetophenone	−3.37	−3.40	−3.08	−3.12	−2.68	
allylbenzene	−0.55	−0.56	−0.55	−0.85		
amyl formate (pentyl)	−1.26	−1.27	−1.49	−1.84		

Table 5. (Continued)

compound	LogH [dimensionless]					
	exptl	FAM[a]	Bk−Pr[b]	N&S[c]	Ketal[d]	E&C[e]
amyl propionate (pentyl)	−1.46	−1.46	−1.85	−1.74	−1.92	−1.63
aniline	−4.08	−4.08	−3.69		−3.87	
benzaldehyde	−2.95	−2.96	−2.86	−3.25	−2.77	−3.13
benzene	−0.64	−0.64	−0.42	−0.73	0.72	−0.73
benzoic acid methyl ester	−2.88	−2.90	−2.52		−2.87	
benzonitrile	−3.09	−3.11	−3.30	−2.57	−3.76	
benzyl acetate	−3.34	−3.36	−3.46		−3.13	
biphenyl	−1.95	−1.96	−1.82		−0.04	−1.8
bromobenzene	−1.00	−1.01	−0.77	−1.26	−0.85	−1.13
bromodichloromethane	−1.06	−1.08	−0.69		−0.9	
bromoethane	−0.51	−0.53	−0.54	−0.61	0.24	−0.44
bromomethane	−0.67	−0.67	−0.64			−0.47
butane	1.59	1.56	1.18	1.51		1.59
butanethiol	−0.73	−0.73	−0.50	−0.47	−0.79	−0.76
butyl acetate	−1.94	−1.96	−1.73	−1.81		−1.88
butyraldehyde	−2.33	−2.22	−2.22	−2.37	−2.13	−2.33
chlorobenzene	−0.85	−0.85	−0.74		−0.63	−1
chlorodifluoromethane	0.09	0.08	0.08		0.59	−0.32
chloroethane	−0.46	−0.45	−0.43	−0.29	−0.35	−0.38
chloromethane	−0.42	−0.45	−0.54			−0.41
chlorotrifluoromethane	1.75	1.72	1.41		2.78	
cis-1,2-dimethylcyclohexane	1.17	1.14	1.45	1.25		1.45
cumene	−0.33	−0.33	−0.17		−0.07	−0.47
cycloheptane	0.58	0.58	0.50		1.1	
cyclohexane	0.86	0.84	1.40	0.95	1.07	1.18
cyclohexanol	−3.94	−3.97	−3.07		−3.75	−4.01
cyclohexanone	−3.43	−3.46	−2.15	−3.14	−2.19	−3.35
cyclohexene	0.27	0.26	0.15	0.50	0.42	0.09
cyclopentane	−0.87	−0.89	−0.52	0.85	1.06	1.03
cyclopentanone	−3.39	−3.40	−2.21	−3.25	−2.23	−3.27
cyclopentene	0.42	0.42	0.17	0.40	0.46	−0.05
cyclopropane	0.55	0.52	0.06	0.65	1.02	0.74
decalin	1.28	1.28	1.66		0.79	
decan-2-one	−1.72	−1.82	−1.56			−1.88
di(*n*-butyl) ether	−0.61	−0.64	−0.81	−0.2		
di(*n*-propyl) ether	−1.05	−1.05	−1.80	−0.4	−1.44	
dibromochloromethane	−1.49	−1.52	−1.77		−1.6	
dibromomethane	−1.47	−1.48	−0.29		−0.83	
dichlorodifluoromethane	1.21	1.21	0.59		1.55	
dichlorofluoromethane	−0.36	−0.36	−0.28		−0.25	
dichloromethane	−0.97	−0.97	−1.47		−0.2	−0.65
diethyl ether	−1.30	−1.33	−1.71	−0.62	−1.48	−1.77
diethylamine	−2.98	−3.11	−3.34		−2.57	−2.89
diethyl sulfide	−1.07	−1.08	−1.20	−0.86	−0.81	−1.06
diisobutylamine	−1.64	−1.64	−2.13		−1.57	
di-isopropyl ether	−1.03	−1.05	−1.04	−0.3	−1.48	
di-isopropylamine	−2.36	−2.38	−2.36	−2.65	−2.22	−2.37
di-isopropylsulfide	−0.88	−0.89	−1.39	−0.46		
dimethyl ether	−1.27	−1.27	−1.60	−0.74	−1.32	
dimethylamine	−3.15	−3.22	−3.71	−3.13	−3.07	
dimethyl sulfide	−1.18	−1.19	−1.46	−1.21	−0.89	−1.08
di-*n*-butylamine	−2.38	−2.38	−2.58	−2.55		−2.46
di-*n*-propylamine	−2.68	−2.71	−2.76	−2.76		−2.68
dipropylsulfide	−0.94	−1.08	−1.20	−0.65		−0.88
ethane	1.31	1.28	1.45	1.27	1.43	1.36
ethanol	−3.69	−3.69	−3.48	−3.59	−3.48	−3.55
ethene	0.94	0.93	0.87	0.89		0.69
ethyl acetate	−2.26	−2.26	−1.96	−2.01	−2.05	−2.12
ethyl formate	−1.80	−1.82	−1.75	−2.15	−1.94	−1.81
ethyl mercaptan	−0.73	−0.73	−1.10	−0.68	−0.85	−0.95
ethyl propionate	−2.05	−2.06	−2.14	−1.94	−1.99	−2
ethyl propyl ether	−1.33	−1.33	−1.76		−1.48	
ethylbenzene	−0.46	−0.46	−0.14	−0.52	−0.01	−0.55
ethylbenzoate	−2.67	−2.67	−2.49	−2.73	−3.1	−3.22
ethylbutyrate	−1.79	−1.82	−2.03		−1.99	−1.88
ethylcyclohexane	1.09	1.09	1.12		1.08	
ethylene oxide (oxirane)	−2.22	−2.22	−1.18		−1.41	
fluorene	−2.46	−2.46	−2.10			−2.13
fluorobenzene	−0.59	−0.59	−0.70	−1.09	−0.5	
fluoromethane	−0.10	−0.10	−0.16			−0.28
formaldehyde	−2.02	−2.03	−2.33	−2.66	−2.19	−2.35
formic acid	−5.15	−5.16	−5.33		−4.28	

Table 5. (Continued)

compound	LogH [dimensionless] exptl	FAM[a]	Bk−Pr[b]	N&S[c]	Ketal[d]	E&C[e]
furan	−0.66	−0.67	−0.09		−1.46	
heptanal	−1.96	−1.96	−1.70	−2.05	−2.07	−1.99
heptanoic acid	−4.86	−4.87	−3.93		−4.03	
hexachlorocyclopentadiene	0.04	0.04	0.01		−0.77	
hexanal (hexaldehyde)	−2.06	−2.06	−1.87		−2.08	−2.11
hexanoic acid	−4.51	−4.54	−3.91	−4.62	−4.29	−4.44
indane	−1.07	−1.08	−1.82	−1.16		−1.25
iodobenzene	−1.28	−1.28	−1.19		−1.2	−0.76
iodoethane	−0.55	−0.45	−0.59	−0.47	−0.46	0.26
iodomethane	−0.67	−0.67	−0.89			0.28
isoamyl acetate	−1.62	−1.64	−1.51	−1.64	−1.97	−1.77
isoamyl formate	−1.56	−1.59	−1.17	−1.78	−1.92	−1.45
isobutene	0.95	0.93	0.41		0.88	0.92
isobutyl formate	−1.67	−1.70	−1.45	−1.88	−1.98	−1.58
isobutylbenzene	0.12	0.12	0.14	−0.24	−0.13	−0.28
isobutylisobutanoate	−1.24	−1.27	−1.44	−1.51		
isobutyraldehyde	−2.10	−2.11	−2.16	−2.31	−2.13	−2.11
isophorone	−3.57	−3.57	−3.57		−2.48	
2-propanol	−3.48	−3.48	−3.32		−3.43	
iso-proplyamine	−2.73	−2.75	−3.17		−2.89	
isopropybenzene (2-propyl)	−0.22	−0.22	−0.16	−0.36		−0.47
isopropyl acetate	1.94	1.94	1.53	−1.86	−2.02	−1.99
isopropyl formate	−1.50	−1.52	−1.43	−1.99	−1.97	−1.7
m-bromotoluene	−0.56	−0.56	−0.42		−1.29	
m-chlorotoluene	−0.18	−0.18	−0.19		−1.08	
m-cresol (3-methylphenol)	−4.45	−4.47	−4.21	−4.24	−4.62	
methanethiol	−0.99	−1.01	−1.70	−0.86	−0.72	
methanol	−3.73	−3.73	−3.08	−3.65	−3.6	−3.81
methyl acetate	−2.33	−2.33	−1.91	−1.98	−1.97	−2.24
methyl hexanoate	−1.82	−1.82	−1.95		−1.95	−1.76
methyl isobutyl ether	−1.04	−1.14	−1.59		−1.48	
methyl isopropyl ether	−1.43	−1.46	−1.44		−1.45	
methyl *n*-butyl ether	−1.14	−1.14	−1.41		−1.42	
methyl propionate	−2.15	−2.16	−2.09	−2	−1.99	−2.12
methyl propyl ether	−1.22	−1.23	−1.68		−1.42	
methyl *tert*-butyl ether	−1.62	−1.64	−1.25	−0.33	−1.42	−1.53
methylamine	−3.34	−3.36	−4.24	−3.14	−3.18	−3.44
methylbutyrate	−2.08	−2.06	−2.01		−1.98	−2
methylcyclohexane	1.21	1.21	1.23	1.11		1.32
methylcyclopentane	1.17	1.14	1.30	1.01	1.05	1.17
methylformate	−2.04	−2.06	−1.86	−2.2	−1.85	−1.93
methylthiobenzene	−2.00	−2.03	−1.96	−1.75		
methyltrimethyl acetate	−1.76	−1.64	−2.03	−1.66		−1.75
m-xylene	−0.53	−0.53	−0.20	−0.45	0.03	−0.62
n,n-dimethylaniline	−2.53	−2.53	−2.74	−3.78	−3.78	
n-amyl acetate	−1.80	−1.82	−1.70		−1.97	−1.76
naphthalene	−1.75	−1.78	−1.54	−1.9	0.09	−1.72
n-butyl acetate	−1.94	−1.96	−1.73		−2.01	−1.88
n-butyl propionate	−1.69	−1.19	−1.87	−1.67	−1.96	
n-butylamine	−3.11	−3.11	−3.22	−2.84	−3	−3.26
n-butylbenzene	−0.28	−0.25	−0.28		−0.15	−0.29
n-butylformate	−1.68	−1.70	−1.51		−1.94	
n-decanal	−1.13	−1.14	−1.33		−1.97	
n-decane	2.33	2.30	2.02	2.14	1.59	2.26
n-ethylaniline	−3.18	−3.18	−3.78		−3.88	
n-heptane	1.92	1.99	1.94	1.81	1.49	
n-heptylamine	−2.78	−2.71	−2.58	−2.53		−2.91
n-hexane	1.84	1.84	1.86	1.71	1.45	1.81
n-hexyl acetate	−1.70	−1.70	−1.55		−1.95	−1.63
n-hexylamine	−2.90	−2.90	−2.74	−2.64	−2.91	−3.03
n-hexylbenzene	−0.03	−0.06	−0.04	−0.09		−0.02
nitrobenzene	−3.02	−3.02	−2.92	−3.91	−2.85	
nitroethane	−2.72	−2.75	−2.72	−2.18		−2.89
nitromethane	−2.95	−2.75	−2.98	−2.26	−1.84	−3.19
n-methylaniline	−3.44	−3.18	−3.65	−3.83	−4.05	−3.26
n-nonane	2.30	2.30	2.02	2.03	1.56	
n-octane	2.08	2.15	2.05	1.91		2.04
n-octylamine	−2.68	−2.71	−2.50	−2.42		−2.79
nonan-5-one	−1.94	−1.82	−2.06	−2.07		−1.99
nonanal	−1.52	−1.52	−1.49	−1.84		−1.76
nonanoic acid	−4.33	−4.47	−3.75		−4.14	
n-pentyl acetate	−1.84	−1.82	−1.71	−1.71		−1.76

Table 5. (Continued)

	LogH [dimensionless]					
compound	exptl	FAM[a]	Bk−Pr[b]	N&S[c]	Ketal[d]	E&C[e]
n-pentylamine	−3.00	−3.00	−2.92	−2.74	−3	−3.14
n-pentylbenzene	−0.17	−0.18	−0.24	−0.2		−0.16
n-pentylcyclopentane	1.87	1.84	1.88	1.41		
n-propyl acetate	−2.05	−2.06	−1.86	−1.91	−2.01	−2
n-propylbenzene	−0.55	−0.40	−0.50		−0.1	−0.42
n-propylcyclopentane	1.56	1.56	1.36	1.2		
n-propylpropionate	−1.79	−1.82	−2.04	−1.84	−1.99	−1.88
o-cresol (2-methylphenol)	−4.31	−4.34	−4.39	−4.25	−4.06	−4.37
octanal	−1.68	−2.11	−1.64	−1.95	−2.05	−1.88
octanoic acid	−4.47	−4.47	−3.78		−4.16	
o-ethylphenol	−3.72	−3.73	−4.29		−3.89	
o-xylene	−0.66	−0.67	−0.55	−0.45	0.03	−0.62
p-chloronitrobenzene	−2.65	−2.67	−2.36		−3.59	
pentachlorobenzene	−0.40	−0.40	−0.39			
pentanal	−2.22	−2.22	−2.09	−2.26		−2.22
pentane	1.70	1.68	1.37	1.61		1.71
pentanoic acid	−4.52	−4.54	−4.03	−4.73	−3.86	−4.54
phenanthrene	−2.79	−2.80	−2.31	−3.08		
phenol	−4.87	−4.87	−4.10	−4.39	−4.23	−4.86
phenylacetic acid	−5.78	−5.78	−4.91		−5.1	
phenylacetylene	−0.55	−0.56	−0.81			
phenylmethyl sulfide	−2.00	−2.03	−1.96	−1.75		
p-isopropyl toluene	−0.30	−0.30	−0.51	−0.21	−0.13	−0.54
p-methylacetophenone	−3.45	−3.46	−3.47	−2.97		
prop-2-en-1-ol (allyl alcohol)	−3.69	−3.69	−2.97	−3.94	−4.04	−4.1
propane	1.46	1.46	0.70	1.41	1.42	1.47
propionaldehyde	−2.52	−2.53	−2.44	−2.47	−2.16	−2.44
propiophenone	−2.27	−2.29	−2.87		−2.85	
propoinic acid	−4.74	−4.77	−4.00	−4.92	−3.78	−4.75
propyl benzene	−0.39	−0.40	−0.24	−0.42		−0.42
propyl formate	−1.75	−1.52	−1.66	−2.04	−1.94	−1.68
propylamine	−3.22	−3.22	−3.51	−2.95	−3.11	
propylene oxide	−2.55	−2.57	−2.08		−1.5	
p-xylene	−0.55	−0.56	−0.38	−0.45		−0.62
pyridine	−3.44	−3.46	−3.11	−3.65	−2.35	−3.47
pyrrole	−3.13	−3.13	−2.89		−4.02	
pyrrolidine	−4.01	−4.01	−2.57		−3.32	
quinoline	−4.17	−4.18	−4.35	−4.92	−2.9	
sec-butyl acetate	−1.77	−1.78	−1.60		−2.04	
sec-butylbenzene	−0.25	−0.25	−0.22			−0.35
styrene	−0.95	−0.97	−0.83	−0.96	0.51	−0.91
tert-butyl amine	−2.83	−2.85	−2.27		−2.71	
tert-butylbenzene	−0.32	−0.33	−0.40	−0.17	−0.08	−0.35
tetrachloroethene	−0.14	−0.14	−0.14		0.61	0.11
tetrahydrofuran	−2.54	−2.57	−1.67		−1.77	−2.51
tetrahydropyran	−2.29	−2.29	−1.84		−1.81	−2.7
thiophene	−0.92	−0.92	−0.67		−0.23	−1.34
thiophenol	−1.86	−1.86	−1.27	−1.4	−1.66	−1.61
toluene	−0.57	−0.59	−0.43	−0.59	0.18	−0.61
trans 1,4-dimethylcyclohexane	1.55	1.14	1.79	1.26		1.45
trans-2-butenal	−3.10	−3.11	−2.82	−2.82		
trans-2-hexenal	−2.70	−2.71	−2.81	−2.62		−2.33
trans-2-octenal	−2.52	−2.53	−2.81	−2.41		−2.11
trichloroethene	−0.44	−0.45	−0.37		0	−0.43
trichlorofluoromethane	0.60	0.58	0.72		0.67	
trichloronitromethane	−1.08	−1.08	−0.26		−1.51	
triethylamine	−2.36	−2.71	−2.94	−2.91	−2.34	−2.52
trifluorobenzene	−0.18	−0.18	−0.26	−1.68		
trimethylamine	−2.35	−2.38	−2.80	−3.07	−2.6	−2.32
tripropylamine	−1.81	−1.82	−1.67		−2.02	
average absolute logH error		0.029	0.27	0.380	0.50	0.197
standard deviation logH		0.066	0.259	0.676	0.51	0.41
number of data points		422	422	277	308	275

[a] FAM = present fuzzy ARTMAP/QSPR. [b] Bk−Pr = back propagation (this work). [c] N&S = QSPR models of Nirmalakhandan and co−workers.[4−6] [d] Ketal = QSPR model of Katritzky et al.[14] [e] E&C = NN/QSPR model of English and Carroll.[16]

average absolute and maximum errors and standard deviations were 0.20 (28%), 3.93 (600%), and 0.41(75.4%) logH units, respectively. The present back-propagation model performed with nearly comparable or lower average absolute and maximum errors and standard deviations of 0.25 (19.7%), 1.27 (154%), and 0.25 (22.2%), respectively. In contrast, the present fuzzy ARTMAP QSPR performed with lower average absolute and maximum errors and standard

deviation of 0.03 (3.9%), 0.54 (131%), and 0.07 (13.3%) logH units, respectively.

In closure, the performances of the fuzzy ARTMAP/QSPR and back-propagation QSPRs suggest that quantum chemical descriptors are reasonable for characterizing the structural information of the present data set of 495 organic compounds (containing 25 different chemical groups) with respect to logH predictions. The fuzzy ARTMAP QSPR was superior to the back-propagation-based logH QSPR. Both QSPRs demonstrated equivalent or greater estimation accuracy, for the range of compounds studied, relative to other regression-based QSPRs and group contribution methods.

CONCLUSIONS

The success of using fuzzy ARTMAP and back-propagation networks for developing QSPRs for estimating Henry's Law constants was demonstrated using a set of molecular descriptors calculated from PM3 semiempirical MO-theory and a heterogeneous set of 495 organic compounds with a range of $-6.72 \leq \log H \leq 2.87$. The descriptors obtained from PM3 semiempirical MO-theory calculations represented different forms of 3-dimensional information for characterizing the various atoms and functional groups for a set of heterogeneous organic compounds. For the fuzzy ARTMAP-based QSPR, average absolute errors for logH predictions for the overall data set and test set were 0.03 and 0.13 logH units, respectively. In contrast, the 7−17−1 back-propagation logH QSPR performed with an average absolute errors for the validation (recall) and test sets of 0.28 and 0.27 logH units, respectively which was comparable to published NN/QSPR models. The fuzzy ARTMAP neural network-based QSPR model was also of higher accuracy relative to previously published multi-linear regression and neural network QSPR models for Henry's Law constant and Ostwald solubility coefficient. The study demonstrated that it is possible to develop reasonably accurate QSPRs for heterogeneous organic compounds based on the fuzzy ART classifier and the fuzzy ARTMAP cognitive system using a set of descriptors calculated from quantum mechanics and graph theory.

REFERENCES AND NOTES

(1) Reid, R. C.; Prausnitz, J. M.; Sherwood, T. K. *The Properties of Gases and Liquids*, 3rd ed.; McGraw-Hill: New York, 1977.

(2) Prausnitz, J. M.; Shair, F. H. A Thermodynamic correlation of gas solubilities. *AICHE J.* **1961**, *7*, 682−687.

(3) Yen, L.; McKetta, J. J. A Thermodynamic Correlation of Nonpolar Gas Solubilities in Polar, Nonassociated Liquids. *AICHE J.* **1962**, *8*, 501−507.

(4) Nirmalakhandan, N. N.; Speece, R. E. QSAR model for predicting Henry's Constant. *Environ. Sci. Technol.* **1988**, *22*(11), 1349−1361.

(5) Nirmalakhandan, N.; Brennan, R. A.; Speece, R. E. Predictive Henry's Law Constant and the effects of Temperature on Henry's Law Constant. *Water Res.* **1997**, *31*(6), 1471−1481.

(6) Brennan, R. A.; Nirmalakhandan, N.; Speece, R. E. Comparison of Predictive Methods for Henry's Law Constants of Organic Chemicals. *Water Res. 1998*, *32*(6), 1901−1911.

(7) Lohmann, J.; Joh, R.; Gmehling, J. From UNIFAC to modified UNIFAC (Dortmund). *Ind. Eng. Chem. Res.* **2001**, *40*, 957−964.

(8) Ornektekin, S.; Paksoy, H.; Demirel, Y. The performance of UNIFAC and related group. contribution models Part II. Prediction of Henry's Law Constant. *Thermochim. Acta* **1996**, *287*, 251−259.

(9) Hwang, S.-M.; Lee, J.-M.; Lin, H. New group-interaction parameters of the UNIFAC model: Aromatic methoxyl binaries. *Ind. Eng. Chem. Res.* **2001**, *40*, 1740−1747.

(10) Gmehling, J.; Lohmann, J.; Jakob, A.;, Li, J.; Joh, R. A modified UNIFAC (Dortmund) Model. 3. Revision and Extension. *Ind. Eng. Chem. Res.* **1998**, *37*, 4876−4882.

(11) Hine, J.; Mookerjee, P. K. The intrinsic hydrophilic character of organic compounds, correlations in terms of structural contribution. *J. Org. Chem.* **1975**, *40*, 292−298.

(12) Meylan, W. M.; Howard, P. H. Bond contribution method for estimating Henry's Law Constants. *Environ. Toxicol. Chem.* **1991**, *10*, 1283−1293.

(13) Abraham, M. H.; Andonian-Haftvan, J.; Whiting, g. S.; Leo, A.; Taft, S. Hydrogen bonding. Part 34. The factors that influence the solubility of gases and vapors in water at 398 K, and a new method for its determination. *J. Chem. Soc., Perkin. Trans.* **1994**, *2*, 1777−1791.

(14) Katritzky, A.; Mu, L.: A QSPR study of the solubility of gases and vapors in water. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 1162−1168.

(15) Katritzky, A. R.; Wang, Y.; Sild, S.; Tamm, T.; Karelson, M. QSPR Studies on Vapor Pressure, Aqueous Solubility, and the Prediction of Water−Air Partition Coefficients. *J. Chem. Inf. Comput. Sci*. **1998**, *38*, 720−725.

(16) English, N. J.; Carroll, D. G.; Prediction of Henry's Laws Constant by a Quantitative Structure−Property Relationship and Neural Networks. *J. Chem. Inf. Comput. Sci*. **2001**, *41*, 1150−1161.

(17) Russell, C. J.; Dixon, S. L.; Jurs, P. C.; Computer-Assisted Study of the Relationship between Molecular-Structure and Henry's Law. *Constant. Anal. Chem.* **1992**, *64*, 1350−1355.

(18) Espinosa, G.; Yaffe, D.; Cohen, Y.; Arenas, A.; Giralt, F. Neural Network Based Quantitative Structural Property Relations (QSPRs) for Predicting Boiling Points of Aliphatic Hydrocarbons. *J. Chem. Inf. Comput. Sci*. **2000**, *40*, 859−877.

(19) Espinosa, G.; Yaffe, D.; Cohen, Y.; Arenas, A.; Giralt, F. A fuzzy ARTMAP−Based Quantitative Structure−Property Relations (QSPRs) for Predicting Physical Properties of Organic Compounds. *Ind. Eng. Chem. Res.* **2001**, *40*, 2757−2766.

(20) Yaffe, D Espinosa, G.; Cohen, Y.; Arenas, A.; Giralt, F. A fuzzy ARTMAP based Quantitative Structure−Property Relationships (QSPRs) for predicting Aqueous Solubility of Organic Compounds *J. Chem. Inf. Comput. Sci*. **2001**, *41*, 1177−1207.

(21) Yaffe, D.; Cohen, Y.; Espinosa, G.; Giralt, F.; Arenas, A. Fuzzy ARTMAP and Back-Propagation Neural Networks based Quantitative Structure−Property Relationships (QSPRs) for Octanol−Water Partition Coefficient of Organic Compounds *J. Chem Inf. Comput Sci*. **2002**, *42*(2), 162−183.

(22) Carpenter, A.; Grossberg, S. A Massively Parallel Architecture for a Self-Organizing Neural Pattern Recognition Machine. *Computer Vision, Graphics, Image Processing* **1987**, *37*, 54.

(23) Carpenter, A.; Grossberg, S. The ART of Adaptative Pattern Recognition by a Self-organizing Neural Network. *Computer* **1988**, 77.

(24) Carpenter, G. A.; Grossberg, S.; Marcuzon, N.; Reynolds, J. H.; Rosen, D. B. fuzzy ARTMAP: A Neural Network Architecture for Incremental Supervised Learning of Analogue Multidimensional Maps. *IEEE Trans. Neural Networks* **1992**, *3*, 698.

(25) Carpenter, G. A.; Grossberg, S.; Marcuzon, N.; Rosen, D. B. Fuzzy ART: Fast Stable Learning and Categorization of Analogue Patterns by an Adaptive Resonance System. *Neural Networks* **1991**, *4*, 759.

(26) Carpenter, G.; Grossberg, S. A Self-Organizing Neural Network for Supervised Learning, Recognition, and Prediction. *IEEE Communications Magazine* **1992**, 38.

(27) Giralt, F.; Arenas, A.; Ferre-Giné, J.; Rallo R. The Simulation and Interpretation of Turbulence with a Cognitive Neural System. *Phys. Fluids* **2000**, *12*, 1826.

(28) Molecular Modeling Pro. Revision 3.14; ChemSM Inc. 1998.

(29) CAChe Version 3.2, CAChe Chemistry Products, Oxford Molecular Ltd.

(30) Stewart, J. J. P.; MOPAC 6.0, Quantum Chemistry Program Exchange No. 455, Bloomington, IN, 1989.

(31) Stewart, J. J. P. Optimization of Parameter for Semiemperical Methods I Method *J. Comput. Chem*. **1989**, *10*, 209−220.

(32) Kier, L. B.; Hall, L. H. *Molecular Connectivity in Chemistry and Drug Research;* Academic Press: New York, 1976.

(33) Kier, L. B.; Hall, L. H. *Molecular Connectivity in Structure−Activity Analysis;* John Wiley & Sons Inc.: New York, 1985.

(34) Kier, L. B. A Shape Index from Molecular Graphs. *Quantum Struct-Act. Relat*, **1985**, *4*, 109−116.

(35) NeuralSim Software; Aspen Technology, Inc., 1999.

(36) Ferre-Gine, J.; Rallo, R.; Arenas, A.; Giralt, F. Extraction of structures embedded in the velocity field of a turbulent wake, in Solving Engineering Problems with Neural Networks, Proceedings of the International Conference on Engineering Applications of Neural Networks (EANN'96), Ed. Bulsari, A. B.; Kallio, S.; Tsaptsinos; D. Turku; 1996; Vol. 1, 17−20.

(37) Bartfai, B. Hierarchical Clustering with ART Neural Netwoks. *Technical Report CS-TR-94/1*. 1994.

(38) Bartfai, B. On the Match Tracking Anomaly of ARTMAP Neural Network. *Technical Report CS-TR-95/1*. 1995.

(39) Bartfai, B. An Improved Learning Algorithm for the fuzzy ARTMAP Neural Network. *Technical Report CS-TR-95/10*, 1995.

(40) Bartfai, B.; White, R. A fuzzy ART-based Modular Neuro-fuzzy Architecture for Learning Hierarchical Clusterings. *Technical Report CS-TR-97/6,* 1997.
(41) Breindl, A.; Beck, B.; Clark, T. Prediction of the *n*-Octanol/Water Partition Coefficient, logP, using a combination of Semiempirical MO−Calculations and Neural Network. *J. Molecular Modeling* **1997**, *3,* 142−155.

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