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QSPR Modeling of Gibbs Free Energy of Organic Compounds by Weighting of Nearest Neighboring Codes

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We examine the encoding of chemical structure of organic compounds by Labeled Hydrogen-Filled Graphs (LHFGs). Quantitative Structure-Property Relationships (QSPR) for a representative set of 150 organic molecules have been derived by means of the optimization of correlation weights of local invariants of the LHFGs. We have tested as local invariants Morgan extended connectivity of zero- and first order, numbers of path of length 2 (P2) and valence shells of distance of 2 (S2) associated with each atom in the molecular structure, and the Nearest Neighboring Codes (NNC). The best statistical characteristics for the Gibbs free energy has been obtained for the NNC weighting. Statistical parameters corresponding to this model are the following $n = 100, r^2 = 0.9974$, $s = 5.136$ kJ/mol, $F = 38319$ (training set); $n = 50$, $r^2 = 0.9990$, $s = 3.405$ kJ/mol, $F = 48717$ (test set). Some possible further developments are pointed out.

KEY WORDS: QSPR; Gibbs free energy; local invariant; nearest neighboring code; correlation weights.

INTRODUCTION

Thermodynamics, the study of the laws governing interconvertibility of different forms of energy into heat, enables us to discuss physical chemistry properties quantitatively and to make useful predictions. In particular, chemical phenomena can be developed quite independently of the atomic and molecular theory by this powerful method. The energy changes associated with chemical reactions are themselves of considerable importance, and even greater chemical interest, however, stems from the fact that the equilibrium position of a reacting system can be related to these energy changes.

The supposition of the early thermochemists that equilibrium was always approached with a decrease in the internal energy of the system, a principle which applies to macroscale mechanical systems, has been shown to be inadequate for chemical systems. A more careful statement of the role of the internal energy or enthalpy is that in systems of constant entropy the equilibrium position is that of lowest energy. In systems of constant energy, the equilibrium position is that of highest entropy. However, in most chemical processes neither the energy nor entropy is held constant. Gibbs free energy is the suitable thermodynamic function when both energy and entropy change.

The free energy is often considered to be the most important quantity in thermodynamics. The free energy is usually expressed as the Helmholtz function, A, or the Gibbs function, G. The Helmholtz free energy is appropriate to a system with constant number of particles, temperature and volume (constant NVT), whereas the Gibbs free energy is appropriate to constant number of particles, temperature and pressure (constant NPT). Most experiments are conducted under conditions of constant temperature and pressure, where the Gibbs function is the suitable free energy quantity.

Unfortunately, the free energy is a difficult quantity to obtain experimentally for systems such as liquids or flexible macromolecules that have many minimum energy configurations separated by low-energy barriers. Associated quantities such as the entropy and the chemical potential are also difficult to calculate. The free energy

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Table I. Statistical Characteristics of Optimal Descriptors of Eq. (1) with r the Correlation Coefficient, s the Standard Error Estimation, and F is Fischer F-ratio

	Training set ($n = 100$)			Test set ($n = 50$)			Complete set ($n = 150$)		
Probes	r^2	s	F	r^2	s	F	r^2	s	F
D(a, ^{0}EC) 1	0.9770	15.417	4166	0.9910	10.214	5279	0.9822	13.865	8157
D(a, ^{0}EC) 2	0.9771	15.404	4173	0.9910	10.223	5272	0.9822	13.857	8167
D(a, ^{0}EC) 3	0.9771	15.386	4183	0.9911	10.162	5340	0.9823	13.829	8201
D(a, ^{1}EC) 1	0.9846	12.623	6262	0.9914	10.006	5505	0.9871	11.781	11356
D(a, ^{1}EC) 2	0.9843	12.743	6143	0.9909	10.249	5240	0.9868	11.935	11061
D(a, ^{1}EC) 3	0.9845	12.676	6209	0.9912	10.064	5435	0.9870	11.835	11250
D(a, P2) 1	0.9847	12.583	6303	0.9928	9.207	6637	0.9877	11.536	11866
D(a, P2) 2	0.9844	12.713	6172	0.9924	9.457	6291	0.9873	11.696	11540
D(a, P2) 3	0.9847	12.590	6296	0.9928	9.205	6624	0.9877	11.540	11855
D(a, S2) 1	0.9894	10.446	9189	0.9948	7.806	9134	0.9914	9.620	17112
D(a, S2) 2	0.9898	10.294	9466	0.9949	7.762	9279	0.9916	9.498	17562
D(a, S2) 3	0.9898	10.268	9514	0.9948	7.746	9254	0.9917	9.476	17639
D(a, NNC) 1	0.9974	5.136	38319	0.9990	3.405	48717	0.9980	4.620	74761
D(a, NNC) 2	0.9975	5.119	38572	0.9991	3.313	51051	0.9981	4.585	75846
D(a, NNC) 3	0.9975	5.115	38638	0.9991	3.319	50948	0.9981	4.583	75915

cannot be accurately determined from a standard molecular dynamics or Monte Carlo simulation because such simulations do not adequately sample from those regions of phase space that make important contributions to the free energy.

However, there is a suitable option to model thermodynamic properties within the realm of Quantitative Structure-Property Relationships (QSPR) theory. In fact, several previous theoretical studies for predicting these properties have shown to be rather valuable tools [1–10]. In particular, we have resorted to the modeling of free energy of 60 hydrocarbons employing the maximum topological distances based indices as molecular descriptors for QSPR [2]. But it is a well-known fact that there is a large set of options to choose molecular descriptors, so that we have deemed interesting and potentially valuable to complement this analysis for a larger set of organic compounds using different molecular descriptors.

The present study aims to model the Gibbs free energy (ΔG°) by means of QSPR for a set of 150 organic molecules whose experimental data were taken from Ref. [11].

METHOD

The QSPR analysis is performed by means of the Optimization of Correlation Weights of Local Graph Invariants (OCWLGI) in Labeled Hydrogen-Filled Graphs (LHFG) described elsewhere [12–16] have been used. As local invariants we have examined the following indices:

- standard vertex degree in the LHFG, ^{0}EC;
- Morgan extended connectivity index of first order in LHFG, ^{1}EC;
- numbers of path of length two associated with each vertex in LHFG as described in a recent article [17] and denoted as P2;
- valence shells values of distance two, as described before [17] and denoted as S2.

We do not describe the method for brevity sake since it has been presented before, so that the pertinent details can be consulted in the precedent article [17]. Standard ORIGIN software was employed for numerical calculations.

The molecular descriptors employed in this study are calculated with formula

$$\mathrm{D}(a_k, \mathrm{LI}_k) = \sum_k \mathrm{CW}(a_k) + \sum_k \mathrm{CW}(\mathrm{LI}_k) \qquad (1)$$

where the a_k is the chemical element that is image of k-th vertex in the LHFG, the LI_k is the numerical value of the local invariant in the LHFG. The $\mathrm{CW}(a_k)$ and the $\mathrm{CW}(\mathrm{LI}_k)$ are correlation weights associated with the chemical element and the local invariant values in the LHFG, respectively. The sum in Eq. (1) is extended over all vertices in the LHFG. The simple additive formula (1) is arbitrary and there is complete freedom to apply any other alternative algebraic relationship.

RESULTS AND DISCUSSION

Statistical characteristics of Gibbs free energies values (in kJ/mol) from a previous article [11] are presented in Table I. These results allow us to verify that the best linear approximation takes place when using the optimal descriptor D(a_k, NNC$_k$).

The NNC is calculated as

$$\mathrm{NNC}_k = 100\ N_\mathrm{t} + 10\ N_\mathrm{c} + N_\mathrm{h},$$

where N_t is total number of the k-the vertex neighbors in the LHFG, N_c is number of carbon atoms connected with the k-th vertex and the N_h is number of hydrogen atoms bonded with the k-th vertex in the LHFG.

We have tried several partitions of the entire molecular set in a training set and a test set, but final results do not depend significantly of the particular way to assign molecules to each set, so that we present results for a representative case. It must be pointed out that results derived for test set are true predictions since these molecules are not included in the training set. QSPRs under consideration have been obtained with software described in detail in a recent article [18]. This algorithm is based on the Monte Carlo technique. Starting values of all these correlation weights are defined as 1.0. The optimum values corresponding to the correlation weights are those yielding the largest possible correlation coefficient between property under consideration and the chosen descriptor/s calculated by means of Eq. (1) (Tables II–VI).

The analysis of the final results allows as to note that all the remaining local invariants provides reasonable satisfactory models to predict the Gibbs free energies. First probes from the Table I of the Gibbs free energies modeling are the following

$$\Delta G^\circ\,(\mathrm{kJ/mol}) = [12.975\,\mathrm{D}(a, {}^0\mathrm{EC}) - 52.838]\,\mathrm{kJ/mol} \quad (2)$$

$$\Delta G^\circ\,(\mathrm{kJ/mol}) = [9.877\,\mathrm{D}(a, {}^1\mathrm{EC}) - 29.514]\,\mathrm{kJ/mol} \quad (3)$$

Table II. Correlation Weights for the Molecular Descriptor of D(a, ^{0}EC)

Atom	Probe 1	Probe 2	Probe 3
H	0.025	0.037	0.050
C	0.667	0.467	0.267
N	5.649	5.501	5.854
O	−3.896	−3.950	−4.388
Cl	−0.675	−0.688	−0.750
Br	0.695	0.703	0.812
I	5.053	5.143	5.793
0001	−0.125	−0.075	0.037
0002	−3.755	−3.831	−4.291
0003	1.413	1.607	1.968
0004	0.100	0.175	0.200

Table III. Correlation Weights Corresponding to the Molecular Descriptor of D(a, ^{1}EC)

Atom	Probe 1	Probe 2	Probe 3
H	−0.338	−0.325	−0.263
C	0.293	0.479	0.304
N	0.506	1.038	0.536
O	−1.673	−0.991	−1.442
Cl	−1.139	−1.168	−1.069
Br	0.822	0.868	0.875
I	6.380	6.671	6.424
0003	2.263	2.027	2.116
0004	−0.075	−0.288	−0.188
0005	−1.764	−2.162	−1.860
0006	1.756	1.687	1.747
0007	−0.066	−0.071	−0.046
0008	−1.738	−1.963	−1.785
0009	3.247	3.413	3.285
0010	1.618	1.892	1.678
0011	−1.058	−1.050	−1.065
0012	8.262	8.972	8.352
0013	2.694	3.146	2.762
0014	0.400	0.675	0.437
0015	2.534	3.052	2.644
0016	4.897	5.614	4.960

$$\Delta G^\circ\,(\mathrm{kJ/mol}) = [9.535\,\mathrm{D(a, P2)} - 39.439]\,\mathrm{kJ/mol} \quad (4)$$

$$\Delta G^\circ\,(\mathrm{kJ/mol}) = [9.211\,\mathrm{D(a, S2)} - 7.306]\,\mathrm{kJ/mol} \quad (5)$$

$$\Delta G^\circ\,(\mathrm{kJ/mol}) = [9.963\,\mathrm{D(a, NNC)} - 53.177]\,\mathrm{kJ/mol} \quad (6)$$

Table IV. Correlation Weights of the Molecular Descriptor of D(a, P2)

Atom	Probe 1	Probe 2	Probe 3
H	−0.525	−0.250	−0.438
C	0.731	0.543	0.681
N	2.352	1.438	1.277
O	−8.090	−7.443	−6.900
Cl	−1.349	−1.050	−1.208
Br	0.937	1.195	0.927
I	6.580	6.691	6.186
0000	1.339	0.866	1.115
0001	0.143	−0.301	−0.254
0002	2.697	2.694	2.767
0003	−0.013	−0.225	−0.075
0004	−0.252	−0.452	−0.563
0005	3.936	4.141	3.976
0006	1.502	1.570	1.433
0007	0.417	0.492	0.154
0008	5.713	6.067	5.663
0009	3.055	3.336	2.970
0010	1.565	1.915	1.310
0011	2.435	3.265	2.760
0012	4.935	5.448	4.778

Table V. Correlation Weights for the Molecular Descriptor of D(a, S2)

Atom	Probe 1	Probe 2	Probe 3
H	−1.325	−1.277	−1.302
C	2.632	2.068	2.060
N	5.692	4.593	4.631
O	−12.863	−12.080	−11.778
Cl	−2.424	−2.212	−2.226
Br	−0.054	−0.103	−0.155
I	5.854	5.040	4.856
0000	−2.608	−2.313	−2.141
0002	−0.400	−0.227	−0.250
0003	0.562	0.498	0.486
0004	0.510	0.575	0.562
0005	0.494	0.519	0.518
0006	−0.275	−0.150	−0.138
0007	0.427	0.625	0.650
0008	1.168	1.173	1.164
0009	0.288	0.375	0.400
0010	0.975	1.090	1.000
0011	0.826	0.942	0.921
0012	0.782	0.892	0.889
0013	0.879	0.969	0.970
0014	0.411	0.633	0.654
0015	1.446	1.564	1.583
0016	0.879	1.027	1.051
0017	0.045	0.382	0.406
0018	1.921	1.986	2.027
0020	−0.122	0.320	0.398
0021	−0.144	0.523	0.808
0024	1.898	3.281	4.327

Table VI. Correlation Weights for the Molecular Descriptor of D(a, NNC)

Atom	Probe 1	Probe 2	Probe 3
H	−0.500	−0.263	−0.313
C	0.282	0.279	0.229
N	11.570	10.922	10.194
O	−3.918	−3.898	−4.336
Cl	−1.400	−1.544	−1.502
Br	1.924	1.890	1.693
I	6.640	6.731	6.166
0100	−2.205	−1.927	−1.931
0110	0.112	0.050	0.025
0220	−3.949	−4.865	−3.690
0312	1.470	1.332	1.512
0320	2.512	2.822	2.692
0321	2.928	2.896	2.755
0330	1.848	1.851	1.781
0400	4.375	5.468	5.275
0401	2.756	3.538	3.353
0402	1.982	2.367	2.330
0403	1.417	1.420	1.446
0410	3.505	4.266	4.173
0411	0.994	1.336	1.460
0412	0.300	0.287	0.439
0413	1.740	1.376	1.473
0420	−2.565	−2.256	−1.871
0421	−1.118	−1.114	−0.849
0422	1.340	1.035	1.164
0430	−1.959	−1.909	−1.591
0431	0.753	0.506	0.662
0440	0.159	−0.033	0.161

Results obtained from application of Eqs. (2)–(6) are shown in Tables VII–XI. In order to judge the relative merits of the present approach one must take into account that the experimental values vary within an ample range of values (i.e. 370 kJ/mol) and the average absolute deviation, for example, in the test molecular set calculated on the basis of Eq. (2) is only 8 kJ/mol. Since there are no available theoretical data of Gibbs free energies corresponding to the same molecular set, there is no possibility of a direct comparison of the relative merits with other possible theoretical approaches. There are other theoretical approaches to the calculation of this property within the realm of the QSPR theory and semiempirical molecular orbital methods [19, 20], but the molecular sets are rather restricted with respect to that one chosen in this study.

A relatively serious disadvantage of the present approach is the capability to discern among isomers, since in the majority of the cases the descriptors are the same. Evidently, in order to complement this sort of flexible topological descriptors it should be necessary to incorporate another complementary ones taking into account this feature.

CONCLUSIONS

The optimization of correlation weights of local graph invariants gives reasonable good models to mimic Gibbs free energies. The best linear approximation for this molecular set is that one based on the correlation weights of the nearest neighboring codes. However, the remaining molecular descriptors show a sensible behavior as predictor of this thermodynamic quantity.

A possible option to improve present results should be to employ fitting linear polynomials depending upon several variables or/and to try higher-order relationships instead of the linear ones or/and to apply other functional more complex relationship than the simplest polynomial mathematical structure. Besides, it is necessary to study the way to discern among isomers. Research along these lines is under development and results will be published elsewhere in the forthcoming future.

Table VII. Experimental and Theoretical Data for ΔG° (kJ/mol) Calculated with Eq. (2)

N	Molecule	D(a, ^{0}EC)	$\Delta G^{\circ}_{exp.}$	$\Delta G^{\circ}_{theor.}$	Residue
Training set					
1	Bromomethane	1.037	−28.158	−39.383	11.225
2	Chloromethane	−0.333	−62.886	−57.159	−5.727
3	Propane	1.501	−23.472	−33.363	9.891
4	Pentane	2.635	−8.368	−18.649	10.281
5	2-Methylbutane	2.635	−14.811	−18.649	3.838
6	2-Methylpentane	3.202	−5.021	−11.292	6.271
7	3-Methylpentane	3.202	−2.134	−11.292	9.158
8	3-Methylhexane	3.769	4.602	−3.935	8.537
9	2,2,3-Trimethylbutane	3.769	4.268	−3.935	8.203
10	Octane	4.336	16.401	3.422	12.979
11	4-Methylheptane	4.336	16.736	3.422	13.314
12	3-Ethylhexane	4.336	16.527	3.422	13.105
13	2,4-Dimethylhexane	4.336	11.715	3.422	8.293
14	2,5-Dimethylhexane	4.336	10.460	3.422	7.038
15	Ethylbenzene	13.014	130.583	116.019	14.564
16	*m*-Xylol	13.014	118.867	116.019	2.848
17	Propylbenzene	13.581	137.235	123.375	13.860
18	Cumol	13.581	136.984	123.375	13.609
19	*p*-Ethyltoluol	13.581	126.692	123.375	3.317
20	1,2,3-Trimethylbenzene	13.581	124.558	123.375	1.183
21	Butylbenzene	14.148	144.683	130.732	13.951
22	*m*-Diethylbenzene	14.148	136.691	130.732	5.959
23	1,2,3,4-Tetramethylbenzene	14.148	123.428	130.732	−7.304
24	1,2,3,5-Tetramethylbenzene	14.148	118.742	130.732	−11.990
25	Pentamethylbenzene	14.715	123.344	138.089	−14.745
26	Hexylbenzene	15.282	161.335	145.446	15.889
27	1,3,5-Triethylbenzene	15.282	144.683	145.446	−0.763
28	Hexamethylbenzene	15.282	130.206	145.446	−15.240
29	1-Phenylheptane	15.849	169.745	152.803	16.942
30	1,2,4,5-Tetraethylbenzene	16.416	155.352	160.160	−4.808
31	1-Methylnaphthalene	20.567	217.694	214.019	3.675
32	2-Ethylnaphthalene	21.134	224.430	221.376	3.054
33	1,2-Dimethylnaphthalene	21.134	216.229	221.376	−5.147
34	1,5-Dimethylnaphthalene	21.134	216.187	221.376	−5.189
35	1,6-Dimethylnaphthalene	21.134	214.430	221.376	−6.946
36	2,6-Dimethylnaphthalene	21.134	214.639	221.376	−6.737
37	2,7-Dimethylnaphthalene	21.134	214.639	221.376	−6.737
38	2-Ethyl-3-methylnaphthalene	21.701	224.011	228.732	−4.721
39	2-Ethyl-6-methylnaphthalene	21.701	220.204	228.732	−8.528
40	2-Butylnaphthalene	22.268	238.530	236.089	2.441
41	Dimethyl ether	−6.717	−112.926	−139.991	27.065
42	Ethyl methyl ether	−6.150	−117.654	−132.634	14.980
43	Methyl-tert-butyl ether	−5.016	−125.436	−117.921	−7.515
44	Ditertbutyl ether	−3.315	−97.696	−95.850	−1.846
45	Dipropyl ether	−4.449	−105.562	−110.564	5.002
46	Dibutyl ether	−3.315	−88.533	−95.850	7.317
47	Diiodomethane	10.423	101.085	82.400	18.685
48	Triiodomethane	15.451	177.946	147.639	30.307
49	1-Iodopropane	6.529	27.949	31.876	−3.927
50	2-Iodopropane	6.529	20.083	31.876	−11.793

Table VII. Continued

N	Molecule	D(a, ^{0}EC)	$\Delta G^\circ_{exp.}$	$\Delta G^\circ_{theor.}$	Residue
51	Methylamine	7.329	32.259	42.256	−9.997
52	Ethylamine	7.896	37.279	49.613	−12.334
53	Sec-Butylamine	9.030	40.627	64.326	−23.699
54	Tert-Butyl amine	9.030	28.870	64.326	−35.456
55	Trimethylamine	8.463	98.910	56.969	41.941
56	Triethylamine	10.164	110.290	79.040	31.250
57	Chloroform	−1.733	−68.534	−75.324	6.790
58	Carbon tetrachloride	−2.433	−58.241	−84.406	26.165
59	1,2-Dichloroethane	−0.466	−73.848	−58.884	−14.964
60	1,1,2-Trichloroethane	−1.166	−77.488	−67.967	−9.521
61	Hexachloroethane	−3.266	−56.819	−95.214	38.395
62	1-Chloropropane	0.801	−50.668	−42.445	−8.223
63	1,3-Dichloropropane	0.101	−82.592	−51.528	−31.064
64	2,2-Dichloropropane	0.101	−84.559	−51.528	−33.031
65	2-Chlorobutane	1.368	−53.472	−35.088	−18.384
66	1-Chloro-2-methylpropane	1.368	−49.664	−35.088	−14.576
67	1-Chloro-3-methylpropane	1.935	−43.681	−27.731	−15.950
68	2-Chloro-2-methylpropane	1.935	−56.484	−27.731	−28.753
69	*m*-Dichlorobenzene	10.480	78.576	83.140	−4.564
70	*p*-Dichlorobenzene	10.480	77.153	83.140	−5.987
71	Bromoethane	1.604	−26.317	−32.026	5.709
72	1,2-Dibromoethane	2.274	−10.586	−23.333	12.747
73	1,2-Dibromopropane	2.841	−17.656	−15.976	−1.680
74	1-Bromobutane	2.738	−12.887	−17.312	4.425
75	1,2-Dibromobutane	3.408	−13.138	−8.619	−4.519
76	2,3-Dibromo-2-methylbutane	3.975	−13.347	−1.262	−12.085
77	2-Bromo-2-methylpropane	2.738	−28.158	−17.312	−10.846
78	Hexachlorobenzene	7.680	44.183	46.810	−2.627
79	1,2,3-Trichloropropane	−0.599	−97.780	−60.610	−37.170
80	Pentachloroethane	−2.566	−66.651	−86.132	19.481
81	1,1-Dichloroethane	−0.466	−73.094	−58.884	−14.210
82	Dichloromethane	−1.033	−68.869	−66.241	−2.628
83	Dimethylamine	7.896	67.990	49.613	18.377
84	Diethylamine	9.030	72.090	64.326	7.764
85	Propylamine	8.463	39.790	56.969	−17.179
86	1,2-Diiodopropane	11.557	74.517	97.114	−22.597
87	1,4-Diiodobutane	12.124	82.090	104.471	−22.381
88	1,1-Diiodoethane	10.990	78.492	89.757	−11.265
89	Di-sec-butyl ether	−3.315	−104.056	−95.850	−8.206
90	Isopropyl-tertbutyl ether	−3.882	−128.825	−103.207	−25.618
91	Diisopropyl ether	−4.449	−121.880	−110.564	−11.316
92	1,2,3,4-Tetraethylbenzene	16.416	155.938	160.160	−4.222
93	1,2,3,5-Tetraethylbenzene	16.416	154.557	160.160	−5.603
94	1,2,3-Triethylbenzene	15.282	151.544	145.446	6.098
95	3,3-Dimethylhexane	4.336	13.263	3.422	9.841
96	Benzene	11.880	129.662	101.305	28.357
97	2,2-Dimethylhexane	4.336	10.711	3.422	7.289
98	2,2-Dimethylpentane	3.769	0.084	−3.935	4.019
99	2,2-Dimethylbutane	3.202	−9.623	−11.292	1.669
100	2,2-Dimethylpropane	2.635	−15.230	−18.649	3.419

Table VII. Continued

N	Molecule	D(a, ^{0}EC)	$\Delta G^\circ_{exp.}$	$\Delta G^\circ_{theor.}$	Residue
Test set					
1	2,3-Dibromobutane	3.408	−11.924	−8.619	−3.305
2	1-Bromopentane	3.305	−5.732	−9.956	4.224
3	2-Bromobutane	2.738	−25.773	−17.312	−8.461
4	1-Bromopropane	2.171	−22.468	−24.669	2.201
5	2-Bromopropane	2.171	−27.238	−24.669	−2.569
6	Chlorobenzene	11.180	99.161	92.222	6.939
7	*o*-Dichlorobenzene	10.480	82.676	83.140	−0.464
8	2-Chloro-2-methylpropane	1.368	−64.099	−35.088	−29.011
9	1-Chloropentane	1.935	−37.405	−27.731	−9.674
10	1-Chlorobutane	1.368	−38.786	−35.088	−3.698
11	2-Chloropropane	0.801	−62.509	−42.445	−20.064
12	1,2-Dichloropropane	0.101	−83.094	−51.528	−31.566
13	1,1,2,2-Tetrachloroethane	−1.866	−85.563	−77.049	−8.514
14	Chloroethane	0.234	−59.999	−49.802	−10.197
15	Butylamine	9.030	49.204	64.326	−15.122
16	Iodoethane	5.962	21.338	24.519	−3.181
17	Iodomethane	5.395	15.648	17.162	−1.514
18	Diethyl ether	−5.583	−122.340	−125.277	2.937
19	Methyl propyl ether	−5.583	−109.914	−125.277	15.363
20	2-Ethyl-7-methylnaphthalene	21.701	220.204	228.732	−8.528
21	1-Butylnaphthalene	22.268	240.078	236.089	3.989
22	1-Propylnaphthalene	21.701	232.630	228.732	3.898
23	2-Propylnaphthalene	21.701	230.999	228.732	2.267
24	1,7-Dimethylnaphthalene	21.134	213.719	221.376	−7.657
25	2,3-Dimethylnaphthalene	21.134	215.016	221.376	−6.360
26	1,3-Dimethylnaphthalene	21.134	213.719	221.376	−7.657
27	1,4-Dimethylnaphthalene	21.134	216.899	221.376	−4.477
28	2-Methylnaphthalene	20.567	216.145	214.019	2.126
29	1-Ethylnaphthalene	21.134	225.978	221.376	4.602
30	1,2,4-Triethylbenzene	15.282	145.227	145.446	−0.219
31	1,2,4,5-Tetramethylbenzene	14.148	119.453	130.732	−11.279
32	Pentylbenzene	14.715	152.925	138.089	14.836
33	*o*-Diethylbenzene	14.148	141.084	130.732	10.352
34	*p*-Diethylbenzene	14.148	137.863	130.732	7.131
35	1,2,4-Trimethylbenzene	13.581	116.943	123.375	−6.432
36	1,3,5-Triethylbenzene	13.581	117.947	123.375	−5.428
37	*m*-Ethyltoluene	13.581	126.440	123.375	3.065
38	*o*-Ethyltoluene	13.581	131.085	123.375	7.710
39	*o*-Xylol	13.014	122.089	116.019	6.070
40	*p*-Xylol	13.014	121.127	116.019	5.108
41	2,3-Dimethylhexane	4.336	17.698	3.422	14.276
42	2-Methylheptane	4.336	12.761	3.422	9.339
43	3-Methylheptane	4.336	13.724	3.422	10.302
44	3,3-Dimethylpentane	3.769	2.636	−3.935	6.571
45	2,3-Dimethylbutane	3.202	−4.100	−11.292	7.192
46	Hexane	3.202	−0.251	−11.292	11.041
47	Butane	2.068	−17.154	−26.006	8.852
48	2-Methylpropane	2.068	−20.878	−26.006	5.128
49	Ethane	0.934	−32.928	−40.719	7.791
50	Heptane	3.769	7.991	−3.935	11.926

Table VIII. Experimental and Theoretical Data for ΔG° (kJ/mol) Calculated with Eq. (3)

n	Molecule	D(a, ^{1}EC)	$\Delta G^{\circ}_{\text{exp.}}$	$\Delta G^{\circ}_{\text{theor.}}$	Residue
Training set					
1	Bromomethane	−0.274	−28.158	−32.220	4.062
2	Chloromethane	−2.235	−62.886	−51.589	−11.297
3	Propane	−0.939	−23.472	−38.789	15.317
4	Pentane	1.231	−8.368	−17.355	8.987
5	2-Methylbutane	0.623	−14.811	−23.361	8.550
6	2-Methylpentane	1.708	−5.021	−12.644	7.623
7	3-Methylpentane	1.708	−2.134	−12.644	10.510
8	3-Methylhexane	2.793	4.602	−1.928	6.530
9	2,2,3-Trimethylbutane	2.704	4.268	−2.807	7.075
10	Octane	4.486	16.401	14.794	1.607
11	4-Methylheptane	3.878	16.736	8.789	7.947
12	3-Ethylhexane	3.878	16.527	8.789	7.738
13	2,4-Dimethylhexane	3.270	11.715	2.784	8.931
14	2,5-Dimethylhexane	3.270	10.460	2.784	7.676
15	Ethylbenzene	14.373	130.583	112.448	18.135
16	*m*-Xylol	14.050	118.867	109.258	9.609
17	Propylbenzene	15.458	137.235	123.165	14.070
18	Cumol	18.789	136.984	156.065	−19.081
19	*p*-Ethyltoluol	14.942	126.692	118.068	8.624
20	1,2,3-Trimethylbenzene	14.619	124.558	114.878	9.680
21	Butylbenzene	16.543	144.683	133.881	10.802
22	*m*-Diethylbenzene	15.834	136.691	126.878	9.813
23	1,2,3,4-Tetramethylbenzene	15.188	123.428	120.498	2.930
24	1,2,3,5-Tetramethylbenzene	15.188	118.742	120.498	−1.756
25	Pentamethylbenzene	15.757	123.344	126.118	−2.774
26	Hexylbenzene	18.713	161.335	155.314	6.021
27	1,3,5-Triethylbenzene	17.295	144.683	141.309	3.374
28	Hexamethylbenzene	16.326	130.206	131.738	−1.532
29	1-Phenylheptane	19.798	169.745	166.031	3.714
30	1,2,4,5-Tetraethylbenzene	18.756	155.352	155.739	−0.387
31	1-Methylnaphthalene	24.865	217.694	216.078	1.616
32	2-Ethylnaphthalene	25.757	224.430	224.888	−0.458
33	1,2-Dimethylnaphthalene	25.434	216.229	221.698	−5.469
34	1,5-Dimethylnaphthalene	25.434	216.187	221.698	−5.511
35	1,6-Dimethylnaphthalene	25.434	214.430	221.698	−7.268
36	2,6-Dimethylnaphthalene	25.434	214.639	221.698	−7.059
37	2,7-Dimethylnaphthalene	25.434	214.639	221.698	−7.059
38	2-Ethyl-3-methylnaphthalene	26.326	224.011	230.508	−6.497
39	2-Ethyl-6-methylnaphthalene	26.326	220.204	230.508	−10.304
40	2-Butylnaphthalene	27.927	238.530	246.321	−7.791
41	Dimethyl ether	−8.831	−112.926	−116.738	3.812
42	Ethyl methyl ether	−9.404	−117.654	−122.397	4.743
43	Methyl-tert-butyl ether	−8.464	−125.436	−113.113	−12.323
44	Ditertbutyl ether	−8.097	−97.696	−109.488	11.792
45	Dipropyl ether	−7.807	−105.562	−106.624	1.062
46	Dibutyl ether	−5.637	−88.533	−85.191	−3.342
47	Diiodomethane	12.002	101.085	89.030	12.055
48	Triiodomethane	18.720	177.946	155.383	22.563
49	1-Iodopropane	5.779	27.949	27.565	0.384
50	2-Iodopropane	5.779	20.083	27.565	−7.482

Table VIII. Continued

n	Molecule	D(a, ^{1}EC)	$\Delta G^\circ_{\text{exp.}}$	$\Delta G^\circ_{\text{theor.}}$	Residue
51	Methylamine	6.922	32.259	38.855	−6.596
52	Ethylamine	7.814	37.279	47.665	−10.386
53	Sec-Butylamine	9.376	40.627	63.093	−22.466
54	Tert-Butyl amine	5.903	28.870	28.790	0.080
55	Trimethylamine	11.198	98.910	81.089	17.821
56	Triethylamine	13.874	110.290	107.519	2.771
57	Chloroform	−3.837	−68.534	−67.412	−1.122
58	Carbon tetrachloride	−4.638	−58.241	−75.324	17.083
59	1,2-Dichloroethane	−3.626	−73.848	−65.328	−8.520
60	1,1,2-Trichloroethane	−4.427	−77.488	−73.239	−4.249
61	Hexachloroethane	−6.830	−56.819	−96.974	40.155
62	1-Chloropropane	−1.740	−50.668	−46.700	−3.968
63	1,3-Dichloropropane	−2.541	−82.592	−54.611	−27.981
64	2,2-Dichloropropane	−2.541	−84.559	−54.611	−29.948
65	2-Chlorobutane	−0.655	−53.472	−35.983	−17.489
66	1-Chloro-2-methylpropane	−1.263	−49.664	−41.989	−7.675
67	1-Chloro-3-methylpropane	−0.178	−43.681	−31.272	−12.409
68	2-Chloro-2-methylpropane	−0.178	−56.484	−31.272	−25.212
69	*m*-Dichlorobenzene	11.310	78.576	82.195	−3.619
70	*p*-Dichlorobenzene	11.310	77.153	82.195	−5.042
71	Bromoethane	−0.864	−26.317	−38.048	11.731
72	1,2-Dibromoethane	0.296	−10.586	−26.590	16.004
73	1,2-Dibromopropane	1.381	−17.656	−15.874	−1.782
74	1-Bromobutane	1.306	−12.887	−16.615	3.728
75	1,2-Dibromobutane	2.466	−13.138	−5.157	−7.981
76	2,3-Dibromo-2-methylbutane	2.943	−13.347	−0.446	−12.901
77	2-Bromo-2-methylpropane	0.698	−28.158	−22.620	−5.538
78	Hexachlorobenzene	8.106	44.183	50.549	−6.366
79	1,2,3-Trichloropropane	−3.342	−97.780	−62.523	−35.257
80	Pentachloroethane	−6.029	−66.651	−89.062	22.411
81	1,1-Dichloroethane	−3.626	−73.094	−65.328	−7.766
82	Dichloromethane	−3.036	−68.869	−59.501	−9.368
83	Dimethylamine	7.298	67.990	42.568	25.422
84	Diethylamine	9.082	72.090	60.189	11.901
85	Propylamine	8.899	39.790	58.381	−18.591
86	1,2-Diiodopropane	12.497	74.517	93.919	−19.402
87	1,4-Diiodobutane	13.582	82.090	104.635	−22.545
88	1,1-Diiodoethane	11.412	78.492	83.202	−4.710
89	Di-sec-butyl ether	−7.645	−104.056	−105.024	0.968
90	Isopropyl-tertbutyl ether	−8.956	−128.825	−117.972	−10.853
91	Diisopropyl ether	−9.815	−121.880	−126.457	4.577
92	1,2,3,4-Tetraethylbenzene	18.756	155.938	155.739	0.199
93	1,2,3,5-Tetraethylbenzene	18.756	154.557	155.739	−1.182
94	1,2,3-Triethylbenzene	17.295	151.544	141.309	10.235
95	3,3-Dimethylhexane	4.397	13.263	13.915	−0.652
96	Benzene	12.912	129.662	98.018	31.644
97	2,2-Dimethylhexane	4.397	10.711	13.915	−3.204
98	2,2-Dimethylpentane	3.312	0.084	3.199	−3.115
99	2,2-Dimethylbutane	2.227	−9.623	−7.518	−2.105
100	2,2-Dimethylpropane	1.142	−15.230	−18.234	3.004

Table VIII. Continued

n	Molecule	D(a, ^{1}EC)	$\Delta G^\circ_{exp.}$	$\Delta G^\circ_{theor.}$	Residue
Test set					
1	2,3-Dibromobutane	2.466	−11.924	−5.157	−6.767
2	1-Bromopentane	2.391	−5.732	−5.898	0.166
3	2-Bromobutane	1.306	−25.773	−16.615	−9.158
4	1-Bromopropane	0.221	−22.468	−27.331	4.863
5	2-Bromopropane	0.221	−27.238	−27.331	0.093
6	Chlorobenzene	12.111	99.161	90.106	9.055
7	*o*-Dichlorobenzene	11.310	82.676	82.195	0.481
8	2-Chloro-2-methylpropane	−1.263	−64.099	−41.989	−22.110
9	1-Chloropentane	0.430	−37.405	−25.267	−12.138
10	1-Chlorobutane	−0.655	−38.786	−35.983	−2.803
11	2-Chloropropane	−1.740	−62.509	−46.700	−15.809
12	1,2-Dichloropropane	−2.541	−83.094	−54.611	−28.483
13	1,1,2,2-Tetrachloroethane	−5.228	−85.563	−81.151	−4.412
14	Chloroethane	−2.825	−59.999	−57.417	−2.582
15	Butylamine	9.984	49.204	69.098	−19.894
16	Iodoethane	4.694	21.338	16.849	4.489
17	Iodomethane	5.284	15.648	22.676	−7.028
18	Diethyl ether	−9.977	−122.340	−128.057	5.717
19	Methyl propyl ether	−8.319	−109.914	−111.681	1.767
20	2-Ethyl-7-methylnaphthalene	26.326	220.204	230.508	−10.304
21	1-Butylnaphthalene	27.927	240.078	246.321	−6.243
22	1-Propylnaphthalene	26.842	232.630	235.604	−2.974
23	2-Propylnaphthalene	26.842	230.999	235.604	−4.605
24	1,7-Dimethylnaphthalene	25.434	213.719	221.698	−7.979
25	2,3-Dimethylnaphthalene	25.434	215.016	221.698	−6.682
26	1,3-Dimethylnaphthalene	25.434	213.719	221.698	−7.979
27	1,4-Dimethylnaphthalene	25.434	216.899	221.698	−4.799
28	2-Methylnaphthalene	24.865	216.145	216.078	0.067
29	1-Ethylnaphthalene	25.757	225.978	224.888	1.090
30	1,2,4-Triethylbenzene	17.295	145.227	141.309	3.918
31	1,2,4,5-Tetramethylbenzene	15.188	119.453	120.498	−1.045
32	Pentylbenzene	17.628	152.925	144.598	8.327
33	*o*-Diethylbenzene	15.834	141.084	126.878	14.206
34	*p*-Diethylbenzene	15.834	137.863	126.878	10.985
35	1,2,4-Trimethylbenzene	14.619	116.943	114.878	2.065
36	1,3,5-Triethylbenzene	14.619	117.947	114.878	3.069
37	*m*-Ethyltoluene	14.942	126.440	118.068	8.372
38	*o*-Ethyltoluene	14.942	131.085	118.068	13.017
39	*o*-Xylol	14.050	122.089	109.258	12.831
40	*p*-Xylol	14.050	121.127	109.258	11.869
41	2,3-Dimethylhexane	3.270	17.698	2.784	14.914
42	2-Methylheptane	3.878	12.761	8.789	3.972
43	3-Methylheptane	3.878	13.724	8.789	4.935
44	3,3-Dimethylpentane	3.312	2.636	3.199	−0.563
45	2,3-Dimethylbutane	1.100	−4.100	−18.649	14.549
46	Hexane	2.316	−0.251	−6.639	6.388
47	Butane	0.146	−17.154	−28.072	10.918
48	2-Methylpropane	−0.462	−20.878	−34.077	13.199
49	Ethane	−2.024	−32.928	−49.505	16.577
50	Heptane	3.401	7.991	4.078	3.913

Table IX. Experimental and Theoretical Data for ΔG° (kJ/mol) Calculated with Eq. (4)

n	Molecule	D(a, P2)	$\Delta G^{\circ}_{exp.}$	$\Delta G^{\circ}_{theor.}$	Residue
Training set					
1	Bromomethane	1.380	−28.158	−26.281	−1.877
2	Chloromethane	−0.906	−62.886	−48.078	−14.808
3	Propane	−0.635	−23.472	−45.494	22.022
4	Pentane	1.679	−8.368	−23.430	15.062
5	2-Methylbutane	1.717	−14.811	−23.067	8.256
6	2-Methylpentane	2.874	−5.021	−12.035	7.014
7	3-Methylpentane	2.874	−2.134	−12.035	9.901
8	3-Methylhexane	4.031	4.602	−1.003	5.605
9	2,2,3-Trimethylbutane	4.434	4.268	2.839	1.429
10	Octane	5.150	16.401	9.666	6.735
11	4-Methylheptane	5.188	16.736	10.029	6.707
12	3-Ethylhexane	5.188	16.527	10.029	6.498
13	2,4-Dimethylhexane	5.226	11.715	10.391	1.324
14	2,5-Dimethylhexane	5.226	10.460	10.391	0.069
15	Ethylbenzene	17.098	130.583	123.590	6.993
16	*m*-Xylol	16.528	118.867	118.155	0.712
17	Propylbenzene	18.255	137.235	134.622	2.613
18	Cumol	18.517	136.984	137.121	−0.137
19	*p*-Ethyltoluol	17.409	126.692	126.556	0.136
20	1,2,3-Trimethylbenzene	16.839	124.558	121.121	3.437
21	Butylbenzene	19.412	144.683	145.654	−0.971
22	*m*-Diethylbenzene	18.290	136.691	134.956	1.735
23	1,2,3,4-Tetramethylbenzene	17.150	123.428	124.086	−0.658
24	1,2,3,5-Tetramethylbenzene	17.150	118.742	124.086	−5.344
25	Pentamethylbenzene	17.461	123.344	127.052	−3.708
26	Hexylbenzene	21.726	161.335	167.718	−6.383
27	1,3,5-Triethylbenzene	19.482	144.683	146.322	−1.639
28	Hexamethylbenzene	17.772	130.206	130.017	0.189
29	1-Phenylheptan	22.883	169.745	178.750	−9.005
30	1,2,4,5-Tetraethylbenzene	20.674	155.352	157.688	−2.336
31	1-Methylnaphthalene	25.985	217.694	208.328	9.366
32	2-Ethylnaphthalene	26.866	224.430	216.728	7.702
33	1,2-Dimethylnaphthalene	26.296	216.229	211.293	4.936
34	1,5-Dimethylnaphthalene	26.296	216.187	211.293	4.894
35	1,6-Dimethylnaphthalene	26.296	214.430	211.293	3.137
36	2,6-Dimethylnaphthalene	26.296	214.639	211.293	3.346
37	2,7-Dimethylnaphthalene	26.296	214.639	211.293	3.346
38	2-Ethyl-3-methylnaphthalene	27.177	224.011	219.694	4.317
39	2-Ethyl-6-methylnaphthalene	27.177	220.204	219.694	0.510
40	2-Butylnaphthalene	29.180	238.530	238.792	−0.262
41	Dimethyl ether	−8.068	−112.926	−116.367	3.441
42	Ethyl methyl ether	−8.821	−117.654	−123.547	5.893
43	Methyl-tert-butyl ether	−7.720	−125.436	−113.049	−12.387
44	Ditertbutyl ether	−7.372	−97.696	−109.731	12.035
45	Dipropyl ether	−7.260	−105.562	−108.663	3.101
46	Dibutyl ether	−4.946	−88.533	−86.599	−1.934
47	Diiodomethane	14.128	101.085	95.271	5.814
48	Triiodomethane	21.233	177.946	163.018	14.928
49	1-Iodopropane	6.470	27.949	22.252	5.697
50	2-Iodopropane	6.470	20.083	22.252	−2.169

Table IX. Continued

n	Molecule	D(a, P2)	$\Delta G^{\circ}_{exp.}$	$\Delta G^{\circ}_{theor.}$	Residue
51	Methylamine	8.497	32.259	41.580	−9.321
52	Ethylamine	9.378	37.279	49.980	−12.701
53	Sec-butylamine	11.730	40.627	72.407	−31.780
54	Tert-butyl amine	7.161	28.870	28.841	0.029
55	Trimethylamine	10.849	98.910	64.006	34.904
56	Triethylamine	13.492	110.290	89.207	21.083
57	Chloroform	−2.554	−68.534	−63.791	−4.743
58	Carbon tetrachloride	−3.378	−58.241	−71.648	13.407
59	1,2-Dichloroethane	−3.440	−73.848	−72.239	−1.609
60	1,1,2-Trichloroethane	−4.264	−77.488	−80.096	2.608
61	Hexachloroethane	−6.736	−56.819	−103.667	46.848
62	1-Chloropropane	−1.459	−50.668	−53.351	2.683
63	1,3-Dichloropropane	−2.283	−82.592	−61.207	−21.385
64	2,2-Dichloropropane	−2.283	−84.559	−61.207	−23.352
65	2-Chlorobutane	−0.302	−53.472	−42.319	−11.153
66	1-Chloro-2-methylpropane	−0.264	−49.664	−41.956	−7.708
67	1-Chloro-3-methylpropane	0.893	−43.681	−30.924	−12.757
68	2-Chloro-2-methylpropane	0.893	−56.484	−30.924	−25.560
69	*m*-Dichlorobenzene	14.258	78.576	96.511	−17.935
70	*p*-Dichlorobenzene	14.258	77.153	96.511	−19.358
71	Bromoethane	−0.330	−26.317	−42.586	16.269
72	1,2-Dibromoethane	1.132	−10.586	−28.645	18.059
73	1,2-Dibromopropane	2.289	−17.656	−17.613	−0.043
74	1-Bromobutane	1.984	−12.887	−20.522	7.635
75	1,2-Dibromobutane	3.446	−13.138	−6.581	−6.557
76	2,3-Dibromo-2-methylbutane	4.641	−13.347	4.813	−18.160
77	2-Bromo-2-methylpropane	2.022	−28.158	−20.159	−7.999
78	Hexachlorobenzene	10.962	44.183	65.084	−20.901
79	1,2,3-Trichloropropane	−3.107	−97.780	−69.064	−28.716
80	Pentachloroethane	−5.912	−66.651	−95.810	29.159
81	1,1-Dichloroethane	−3.440	−73.094	−72.239	−0.855
82	Dichloromethane	−1.730	−68.869	−55.935	−12.934
83	Dimethylamine	9.654	67.990	52.612	15.378
84	Diethylamine	11.416	72.090	69.413	2.677
85	Propylamine	10.535	39.790	61.012	−21.222
86	1,2-Diiodopropane	13.575	74.517	89.999	−15.482
87	1,4-Diiodobutane	14.732	82.090	101.031	−18.941
88	1,1-Diiodoethane	12.418	78.492	78.967	−0.475
89	Di-sec-butyl ether	−6.638	−104.056	−102.732	−1.324
90	Isopropyl-tertbutyl ether	−8.162	−128.825	−117.264	−11.561
91	Diisopropyl ether	−8.952	−121.880	−124.796	2.916
92	1,2,3,4-Tetraethylbenzene	20.674	155.938	157.688	−1.750
93	1,2,3,5-Tetraethylbenzene	20.674	154.557	157.688	−3.131
94	1,2,3-Triethylbenzene	19.482	151.544	146.322	5.222
95	3,3-Dimethylhexane	5.553	13.263	13.509	−0.246
96	Benzene	15.906	129.662	112.225	17.437
97	2,2-Dimethylhexane	5.553	10.711	13.509	−2.798
98	2,2-Dimethylpentane	4.396	0.084	2.477	−2.393
99	2,2-Dimethylbutane	3.239	−9.623	−8.555	−1.068
100	2,2-Dimethylpropane	2.082	−15.230	−19.587	4.357

Table IX. Continued

n	Molecule	D(a, P2)	$\Delta G^{\circ}_{exp.}$	$\Delta G^{\circ}_{theor.}$	Residue
Test set					
1	2,3-Dibromobutane	3.446	−11.924	−6.581	−5.343
2	1-Bromopentane	3.141	−5.732	−9.490	3.758
3	2-Bromobutane	1.984	−25.773	−20.522	−5.251
4	1-Bromopropane	0.827	−22.468	−31.554	9.086
5	2-Bromopropane	0.827	−27.238	−31.554	4.316
6	Chlorobenzene	15.082	99.161	104.368	−5.207
7	*o*-Dichlorobenzene	14.258	82.676	96.511	−13.835
8	2-Chloro-2-methylpropane	−0.264	−64.099	−41.956	−22.143
9	1-Chloropentane	0.855	−37.405	−31.287	−6.118
10	1-Chlorobutane	−0.302	−38.786	−42.319	3.533
11	2-Chloropropane	−1.459	−62.509	−53.351	−9.158
12	1,2-Dichloropropane	−2.283	−83.094	−61.207	−21.887
13	1,1,2,2-Tetrachloroethane	−5.088	−85.563	−87.953	2.390
14	Chloroethane	−2.616	−59.999	−64.383	4.384
15	Butylamine	11.692	49.204	72.044	−22.840
16	Iodethane	5.313	21.338	11.220	10.118
17	Iodmethane	7.023	15.648	27.525	−11.877
18	Diethyl ether	−9.574	−122.340	−130.727	8.387
19	Methyl propyl ether	−7.664	−109.914	−112.515	2.601
20	2-Ethyl-7-methylnaphthalene	27.177	220.204	219.694	0.510
21	1-Butylnaphthalene	29.180	240.078	238.792	1.286
22	1-Propylnaphthalene	28.023	232.630	227.760	4.870
23	2-Propylnaphthalene	28.023	230.999	227.760	3.239
24	1,7-Dimethylnaphthalene	26.296	213.719	211.293	2.426
25	2,3-Dimethylnaphthalene	26.296	215.016	211.293	3.723
26	1,3-Dimethylnaphthalene	26.296	213.719	211.293	2.426
27	1,4-Dimethylnaphthalene	26.296	216.899	211.293	5.606
28	2-Methylnaphthalene	25.985	216.145	208.328	7.817
29	1-Ethylnaphthalene	26.866	225.978	216.728	9.250
30	1,2,4-Triethylbenzene	19.482	145.227	146.322	−1.095
31	1,2,4,5-Tetramethylbenzene	17.150	119.453	124.086	−4.633
32	Pentylbenzene	20.569	152.925	156.686	−3.761
33	*o*-Diethylbenzene	18.290	141.084	134.956	6.128
34	*p*-Diethylbenzene	18.290	137.863	134.956	2.907
35	1,2,4-Trimethylbenzene	16.839	116.943	121.121	−4.178
36	1,3,5-Triethylbenzene	16.839	117.947	121.121	−3.174
37	*m*-Ethyltoluene	17.409	126.440	126.556	−0.116
38	*o*-Ethyltoluene	17.409	131.085	126.556	4.529
39	*o*-Xylol	16.528	122.089	118.155	3.934
40	*p*-Xylol	16.528	121.127	118.155	2.972
41	2,3-Dimethylhexane	5.226	17.698	10.391	7.307
42	2-Methylheptane	5.188	12.761	10.029	2.732
43	3-Methylheptane	5.188	13.724	10.029	3.695
44	3,3-Dimethylpentane	4.396	2.636	2.477	0.159
45	2,3-Dimethylbutane	2.912	−4.100	−11.673	7.573
46	Hexane	2.836	−0.251	−12.398	12.147
47	Butane	0.522	−17.154	−34.462	17.308
48	2-Methylpropane	0.560	−20.878	−34.099	13.221
49	Ethane	−1.792	−32.928	−56.526	23.598
50	Heptane	3.993	7.991	−1.366	9.357

Table X. Experimental and Theoretical Data for ΔG° (kJ/mol) Calculated with Eq. (5)

n	Molecule	D(a,S2)	$\Delta G^{\circ}_{\text{exp.}}$	$\Delta G^{\circ}_{\text{theor.}}$	Delta
Training set					
1	Bromomethane	−1.757	−28.158	−23.490	−4.668
2	Chloromethane	−4.127	−62.886	−45.320	−17.566
3	Propane	−4.603	−23.472	−49.704	26.232
4	Pentane	−1.854	−8.368	−24.383	16.015
5	2-Methylbutane	−1.992	−14.811	−25.654	10.843
6	2-Methylpentane	−0.482	−5.021	−11.746	6.725
7	3-Methylpentane	−0.551	−2.134	−12.381	10.247
8	3-Methylhexane	0.959	4.602	1.527	3.075
9	2,2,3-Trimethylbutane	0.645	4.268	−1.365	5.633
10	Octane	2.166	16.401	12.645	3.756
11	4-Methylheptan	2.469	16.736	15.436	1.300
12	3-Ethylhexane	2.211	16.527	13.060	3.467
13	2,4-Dimethylhexane	2.142	11.715	12.424	−0.709
14	2,5-Dimethylhexane	2.230	10.460	13.235	−2.775
15	Ethylbenzene	14.291	130.583	124.328	6.255
16	*m*-Xylol	14.003	118.867	121.676	−2.809
17	Propylbenzene	15.742	137.235	137.694	−0.459
18	Cumol	13.908	136.984	120.801	16.183
19	*p*-Ethyltoluol	14.729	126.692	128.363	−1.671
20	1,2,3-Trimethylbenzene	14.271	124.558	124.144	0.414
21	Butylbenzene	16.246	144.683	142.336	2.347
22	*m*-Diethylbenzene	15.309	136.691	133.705	2.986
23	1,2,3,4-Tetramethylbenzene	14.612	123.428	127.285	−3.857
24	1,2,3,5-Tetramethylbenzene	14.563	118.742	126.834	−8.092
25	Pentamethylbenzene	14.880	123.344	129.754	−6.410
26	Hexylbenzene	18.926	161.335	167.021	−5.686
27	1,3,5-Triethylbenzene	16.254	144.683	142.410	2.273
28	Hexamethylbenzene	15.246	130.206	133.125	−2.919
29	1-Phenylheptane	20.266	169.745	179.364	−9.619
30	1,2,4,5-Tetraethylbenzene	17.322	155.352	152.247	3.105
31	1-Methylnaphthalene	23.574	217.694	209.834	7.860
32	2-Ethylnaphthalene	24.251	224.430	216.070	8.360
33	1,2-Dimethylnaphthalene	24.281	216.229	216.346	−0.117
34	1,5-Dimethylnaphthalene	24.433	216.187	217.746	−1.559
35	1,6-Dimethylnaphthalene	24.258	214.430	216.134	−1.704
36	2,6-Dimethylnaphthalene	24.282	214.639	216.356	−1.717
37	2,7-Dimethylnaphthalene	24.282	214.639	216.356	−1.717
38	2-Ethyl-3-methylnaphthalene	24.838	224.011	221.477	2.534
39	2-Ethyl-6-methylnaphthalene	24.935	220.204	222.370	−2.166
40	2-Butylnaphthalene	26.206	238.530	234.077	4.453
41	Dimethyl ether	−11.744	−112.926	−115.480	2.554
42	Ethyl methyl ether	−12.273	−117.654	−120.353	2.699
43	Methyl-tert-butyl ether	−10.788	−125.436	−106.674	−18.762
44	Ditertbutyl ether	−11.101	−97.696	−109.557	11.861
45	Dipropyl ether	−11.375	−105.562	−112.081	6.519
46	Dibutyl ether	−8.587	−88.533	−86.401	−2.132
47	Diiodomethane	11.330	101.085	97.055	4.030
48	Triiodomethane	18.509	177.946	163.180	14.766
49	1-Iodopropane	2.576	27.949	16.422	11.527
50	2-Iodopropane	2.576	20.083	16.422	3.661

Table X. Continued

n	Molecule	D(a,S2)	$\Delta G^{\circ}_{exp.}$	$\Delta G^{\circ}_{theor.}$	Delta
51	Methylamine	4.331	32.259	32.587	−0.328
52	Ethylamine	4.893	37.279	37.763	−0.484
53	Sec-butylamine	6.054	40.627	48.457	−7.830
54	Tert-butyl amine	4.244	28.870	31.785	−2.915
55	Trimethylamine	9.901	98.910	83.892	15.018
56	Triethylamine	12.023	110.290	103.438	6.852
57	Chloroform	−6.325	−68.534	−65.566	−2.968
58	Carbon tetrachloride	−7.424	−58.241	−75.688	17.447
59	1,2-Dichloroethane	−5.410	−73.848	−57.138	−16.710
60	1,1,2-Trichloroethane	−6.509	−77.488	−67.260	−10.228
61	Hexachloroethane	−9.806	−56.819	−97.629	40.810
62	1-Chloropropane	−5.702	−50.668	−59.827	9.159
63	1,3-Dichloropropane	−6.801	−82.592	−69.950	−12.642
64	2,2-Dichloropropane	−6.801	−84.559	−69.950	−14.609
65	2-Chlorobutane	−4.293	−53.472	−46.849	−6.623
66	1-Chloro-2-methylpropane	−4.362	−49.664	−47.484	−2.180
67	1-Chloro-3-methylpropane	−3.091	−43.681	−35.777	−7.904
68	2-Chloro-2-methylpropane	−3.091	−56.484	−35.777	−20.707
69	*m*-Dichlorobenzene	11.002	78.576	94.033	−15.457
70	*p*-Dichlorobenzene	11.002	77.153	94.033	−16.880
71	Bromoethane	−1.941	−26.317	−25.185	−1.132
72	1,2-Dibromoethane	−0.670	−10.586	−13.477	2.891
73	1,2-Dibromopropane	−2.061	−17.656	−26.290	8.634
74	1-Bromobutane	−1.923	−12.887	−25.019	12.132
75	1,2-Dibromobutane	−0.652	−13.138	−13.312	0.174
76	2,3-Dibromo-2-methylbutane	0.550	−13.347	−2.240	−11.107
77	2-Bromo-2-methylpropane	−1.992	−28.158	−25.654	−2.504
78	Hexachlorobenzene	6.606	44.183	53.542	−9.359
79	1,2,3-Trichloropropane	−7.900	−97.780	−80.073	−17.707
80	Pentachloroethane	−8.707	−66.651	−87.506	20.855
81	1,1-Dichloroethane	−5.410	−73.094	−57.138	−15.956
82	Dichloromethane	−5.226	−68.869	−55.443	−13.426
83	Dimethylamine	6.526	67.990	52.805	15.185
84	Diethylamine	9.941	72.090	84.261	−12.171
85	Propylamine	6.524	39.790	52.787	−12.997
86	1,2-Diiodopropane	9.755	74.517	82.547	−8.030
87	1,4-Diiodobutane	11.164	82.090	95.526	−13.436
88	1,1-Diiodoethane	11.146	78.492	95.360	−16.868
89	Di-sec-butyl ether	−9.922	−104.056	−98.698	−5.358
90	Isopropyl-tertbutyl ether	−13.300	−128.825	−129.812	0.987
91	Diisopropyl ether	−11.392	−121.880	−112.238	−9.642
92	1,2,3,4-Tetraethylbenzene	17.818	155.938	156.816	−0.878
93	1,2,3,5-Tetraethylbenzene	17.521	154.557	154.080	0.477
94	1,2,3-Triethylbenzene	16.576	151.544	145.376	6.168
95	3,3-Dimethylhexane	2.224	13.263	13.179	0.084
96	Benzene	13.200	129.662	114.279	15.383
97	2,2-Dimethylhexane	2.142	10.711	12.424	−1.713
98	2,2-Dimethylpentane	0.802	0.084	0.081	0.003
99	2,2-Dimethylbutane	−0.519	−9.623	−12.087	2.464
100	2,2-Dimethylpropane	−2.130	−15.230	−26.925	11.695

Table X. Continued

n	Molecule	D(a,S2)	$\Delta G^{\circ}_{exp.}$	$\Delta G^{\circ}_{theor.}$	Residue
Test set					
1	2,3-Dibromobutane	−0.652	−11.924	−13.312	1.388
2	1-Bromopentane	−0.583	−5.732	−12.676	6.944
3	2-Bromobutane	−1.923	−25.773	−25.019	−0.754
4	1-Bromopropane	−3.332	−22.468	−37.997	15.529
5	2-Bromopropane	−3.332	−27.238	−37.997	10.759
6	Chlorobenzene	12.101	99.161	104.156	−4.995
7	*o*-Dichlorobenzene	11.002	82.676	94.033	−11.357
8	2-Chloro-2-methylpropane	−4.362	−64.099	−47.484	−16.615
9	1-Chloropentane	−2.953	−37.405	−34.506	−2.899
10	1-Chlorobutane	−4.293	−38.786	−46.849	8.063
11	2-Chloropropane	−5.702	−62.509	−59.827	−2.682
12	1,2-Dichloropropane	−6.801	−83.094	−69.950	−13.144
13	1,1,2,2-Tetrachloroethane	−7.608	−85.563	−77.383	−8.180
14	Chloroethane	−4.311	−59.999	−47.015	−12.984
15	Butylamine	7.028	49.204	57.429	−8.225
16	Iodoethane	3.967	21.338	29.234	−7.896
17	Iodomethane	4.151	15.648	30.929	−15.281
18	Diethyl ether	−12.871	−122.340	−125.861	3.521
19	Methyl propyl ether	−11.525	−109.914	−113.463	3.549
20	2-Ethyl-7-methylnaphthalene	24.935	220.204	222.370	−2.166
21	1-Butylnaphthalene	26.597	240.078	237.679	2.399
22	1-Propylnaphthalene	26.093	232.630	233.037	−0.407
23	2-Propylnaphthalene	25.702	230.999	229.435	1.564
24	1,7-Dimethylnaphthalene	24.258	213.719	216.134	−2.415
25	2,3-Dimethylnaphthalene	24.136	215.016	215.011	0.005
26	1,3-Dimethylnaphthalene	24.185	213.719	215.462	−1.743
27	1,4-Dimethylnaphthalene	24.234	216.899	215.913	0.986
28	2-Methylnaphthalene	23.598	216.145	210.055	6.090
29	1-Ethylnaphthalene	24.642	225.978	219.671	6.307
30	1,2,4-Triethylbenzene	16.352	145.227	143.312	1.915
31	1,2,4,5-Tetramethylbenzene	14.514	119.453	126.382	−6.929
32	Pentylbenzene	17.586	152.925	154.679	−1.754
33	*o*-Diethylbenzene	15.334	141.084	133.935	7.149
34	*p*-Diethylbenzene	15.382	137.863	134.378	3.485
35	1,2,4-Trimethylbenzene	14.295	116.943	124.365	−7.422
36	1,3,5-Triethylbenzene	14.295	117.947	124.365	−6.418
37	*m*-Ethyltoluene	14.656	126.440	127.690	−1.250
38	*o*-Ethyltoluene	14.632	131.085	127.469	3.616
39	*o*-Xylol	13.930	122.089	121.003	1.086
40	*p*-Xylol	14.076	121.127	122.348	−1.221
41	2,3-Dimethylhexane	2.312	17.698	13.990	3.708
42	2-Methylheptane	2.198	12.761	12.940	−0.179
43	3-Methylheptane	2.299	13.724	13.870	−0.146
44	3,3-Dimethylpentane	0.903	2.636	1.012	1.624
45	2,3-Dimethylbutane	−0.450	−4.100	−11.451	7.351
46	Hexane	−0.514	−0.251	−12.040	11.789
47	Butane	−3.194	−17.154	−36.726	19.572
48	2-Methylpropane	−3.263	−20.878	−37.361	16.483
49	Ethane	−3.212	−32.928	−36.892	3.964
50	Heptane	0.826	7.991	0.302	7.689

Table XI. Experimental and Theoretical Data for ΔG° (kJ/mol) Calculated with Eq. (6)

n	Molecule	D(a,NNC)	$\Delta G^\circ_{\text{exp.}}$	$\Delta G^\circ_{\text{theor.}}$	Residue
Training set					
1	Bromomethane	2.571	−28.158	−27.562	−0.596
2	Chloromethane	−0.753	−62.886	−60.679	−2.207
3	Propane	2.562	−23.472	−27.652	4.180
4	Pentane	4.254	−8.368	−10.794	2.426
5	2-Methylbutane	4.067	−14.811	−12.657	−2.154
6	2-Methylpentane	4.913	−5.021	−4.229	−0.792
7	3-Methylpentane	4.913	−2.134	−4.229	2.095
8	3-Methylhexane	5.759	4.602	4.200	0.402
9	2,2,3-Trimethylbutane	5.378	4.268	0.404	3.864
10	Octane	6.792	16.401	14.492	1.909
11	4-Methylheptane	6.605	16.736	12.629	4.107
12	3-Ethylhexane	6.605	16.527	12.629	3.898
13	2,4-Dimethylhexane	6.418	11.715	10.766	0.949
14	2,5-Dimethylhexane	6.418	10.460	10.766	−0.306
15	Ethylbenzene	17.944	130.583	125.599	4.984
16	*m*-Xylol	17.264	118.867	118.824	0.043
17	Propylbenzene	18.790	137.235	134.028	3.207
18	Cumol	18.603	136.984	132.165	4.819
19	*p*-Ethyltoluol	18.110	126.692	127.253	−0.561
20	1,2,3-Trimethylbenzene	17.430	124.558	120.478	4.080
21	Butylbenzene	19.636	144.683	142.456	2.227
22	*m*-Diethylbenzene	18.956	136.691	135.682	1.009
23	1,2,3,4-Tetramethylbenzene	17.596	123.428	122.132	1.296
24	1,2,3,5-Tetramethylbenzene	17.596	118.742	122.132	−3.390
25	Pentamethylbenzene	17.762	123.344	123.786	−0.442
26	Hexylbenzene	21.328	161.335	159.314	2.021
27	1,3,5-Triethylbenzene	19.968	144.683	145.764	−1.081
28	Hexamethylbenzene	17.928	130.206	125.440	4.766
29	1-Phenylheptane	22.174	169.745	167.743	2.002
30	1,2,4,5-Tetraethylbenzene	20.980	155.352	155.847	−0.495
31	1-Methylnaphthalene	27.002	217.694	215.844	1.850
32	2-Ethylnaphthalene	27.848	224.430	224.273	0.157
33	1,2-Dimethylnaphthalene	27.168	216.229	217.498	−1.269
34	1,5-Dimethylnaphthalene	27.168	216.187	217.498	−1.311
35	1,6-Dimethylnaphthalene	27.168	214.430	217.498	−3.068
36	2,6-Dimethylnaphthalene	27.168	214.639	217.498	−2.859
37	2,7-Dimethylnaphthalene	27.168	214.639	217.498	−2.859
38	2-Ethyl-3-methylnaphthalene	28.014	224.011	225.926	−1.915
39	2-Ethyl-6-methylnaphthalene	28.014	220.204	225.926	−5.722
40	2-Butylnaphthalene	29.540	238.530	241.130	−2.600
41	Dimethyl ether	−6.797	−112.926	−120.896	7.970
42	Ethyl methyl ether	−6.668	−117.654	−119.610	1.956
43	Methyl-tert-butyl ether	−6.435	−125.436	−117.289	−8.147
44	Ditertbutyl ether	−6.073	−97.696	−113.682	15.986
45	Dipropyl ether	−4.847	−105.562	−101.468	−4.094
46	Dibutyl ether	−3.155	−88.533	−84.610	−3.923
47	Diiodomethane	14.992	101.085	96.188	4.897
48	Triiodomethane	22.906	177.946	175.035	2.911
49	1-Iodopropane	8.262	27.949	29.137	−1.188
50	2-Iodopropane	7.244	20.083	18.995	1.088

Table XI. Continued

n	Molecule	D(a,NNC)	$\Delta G^{\circ}_{\text{exp.}}$	$\Delta G^{\circ}_{\text{theor.}}$	Residue
51	Methylamine	8.165	32.259	28.171	4.088
52	Ethylamine	8.294	37.279	29.456	7.823
53	Sec-Butylamine	9.799	40.627	44.450	−3.823
54	Tert-Butyl amine	8.527	28.870	31.778	−2.908
55	Trimethylamine	15.023	98.910	96.497	2.413
56	Triethylamine	15.410	110.290	100.353	9.937
57	Chloroform	−1.214	−68.534	−65.272	−3.262
58	Carbon tetrachloride	−0.495	−58.241	−58.109	−0.132
59	1,2-Dichloroethane	−2.964	−73.848	−82.707	8.859
60	1,1,2-Trichloroethane	−3.170	−77.488	−84.760	7.272
61	Hexachloroethane	−0.154	−56.819	−54.711	−2.108
62	1-Chloropropane	0.222	−50.668	−50.965	0.297
63	1,3-Dichloropropane	−2.118	−82.592	−74.279	−8.313
64	2,2-Dichloropropane	−3.143	−84.559	−84.491	−0.068
65	2-Chlorobutane	0.050	−53.472	−52.679	−0.793
66	1-Chloro-2-methylpropane	0.881	−49.664	−44.400	−5.264
67	1-Chloro-3-methylpropane	1.727	−43.681	−35.971	−7.710
68	2-Chloro-2-methylpropane	0.455	−56.484	−48.644	−7.840
69	*m*-Dichlorobenzene	14.300	78.576	89.294	−10.718
70	*p*-Dichlorobenzene	14.300	77.153	89.294	−12.141
71	Bromoethane	2.700	−26.317	−26.277	−0.040
72	1,2-Dibromoethane	3.684	−10.586	−16.473	5.887
73	1,2-Dibromopropane	3.512	−17.656	−18.187	0.531
74	1-Bromobutane	4.392	−12.887	−9.420	−3.467
75	1,2-Dibromobutane	4.358	−13.138	−9.758	−3.380
76	2,3-Dibromo-2-methylbutane	3.745	−13.347	−15.866	2.519
77	2-Bromo-2-methylpropane	2.933	−28.158	−23.956	−4.202
78	Hexachlorobenzene	9.036	44.183	36.849	7.334
79	1,2,3-Trichloropropane	−5.476	−97.780	−107.734	9.954
80	Pentachloroethane	−1.765	−66.651	−70.762	4.111
81	1,1-Dichloroethane	−0.830	−73.094	−61.446	−11.648
82	Dichloromethane	−1.088	−68.869	−64.017	−4.852
83	Dimethylamine	12.863	67.990	74.977	−6.987
84	Diethylamine	13.121	72.090	77.548	−5.458
85	Propylamine	9.140	39.790	37.885	1.905
86	1,2-Diiodopropane	12.944	74.517	75.784	−1.267
87	1,4-Diiodobutane	14.808	82.090	94.355	−12.265
88	1,1-Diiodoethane	13.116	78.492	77.498	0.994
89	Di-sec-butyl ether	−5.191	−104.056	−104.895	0.839
90	Isopropyl-tertbutyl ether	−6.478	−128.825	−117.717	−11.108
91	Diisopropyl ether	−6.883	−121.880	−121.752	−0.128
92	1,2,3,4-Tetraethylbenzene	20.980	155.938	155.847	0.091
93	1,2,3,5-Tetraethylbenzene	20.980	154.557	155.847	−1.290
94	1,2,3-Triethylbenzene	19.968	151.544	145.764	5.780
95	3,3-Dimethylhexane	6.411	13.263	10.696	2.567
96	Benzene	16.932	129.662	115.517	14.145
97	2,2-Dimethylhexane	6.411	10.711	10.696	0.015
98	2,2-Dimethylpentane	5.565	0.084	2.267	−2.183
99	2,2-Dimethylbutane	4.719	−9.623	−6.162	−3.461
100	2,2-Dimethylpropane	3.873	−15.230	−14.590	−0.640

Table XI. Continued

n	Molecule	D(a,NNC)	$\Delta G^{\circ}_{\text{exp.}}$	$\Delta G^{\circ}_{\text{theor.}}$	Residue
Test set					
1	2,3-Dibromobutane	3.340	−11.924	−19.901	7.977
2	1-Bromopentane	5.238	−5.732	−0.991	−4.741
3	2-Bromobutane	3.374	−25.773	−19.562	−6.211
4	1-Bromopropane	3.546	−22.468	−17.848	−4.620
5	2-Bromopropane	2.528	−27.238	−27.991	0.753
6	Chlorobenzene	15.616	99.161	102.405	−3.244
7	*o*-Dichlorobenzene	14.300	82.676	89.294	−6.618
8	2-Chloro-2-methylpropane	−0.391	−64.099	−57.073	−7.026
9	1-Chloropentane	1.914	−37.405	−34.108	−3.297
10	1-Chlorobutane	1.068	−38.786	−42.537	3.751
11	2-Chloropropane	−0.796	−62.509	−61.108	−1.401
12	1,2-Dichloropropane	−3.136	−83.094	−84.421	1.327
13	1,1,2,2-Tetrachloroethane	−3.376	−85.563	−86.812	1.249
14	Chloroethane	−0.624	−59.999	−59.394	−0.605
15	Butylamine	9.986	49.204	46.314	2.890
16	Iodoethane	7.416	21.338	20.709	0.629
17	Iodomethane	7.287	15.648	19.423	−3.775
18	Diethyl ether	−6.539	−122.340	−118.325	−4.015
19	Methyl propyl ether	−5.822	−109.914	−111.182	1.268
20	2-Ethyl-7-methylnaphthalene	28.014	220.204	225.926	−5.722
21	1-Butylnaphthalene	29.540	240.078	241.130	−1.052
22	1-Propylnaphthalene	28.694	232.630	232.701	−0.071
23	2-Propylnaphthalene	28.694	230.999	232.701	−1.702
24	1,7-Dimethylnaphthalene	27.168	213.719	217.498	−3.779
25	2,3-Dimethylnaphthalene	27.168	215.016	217.498	−2.482
26	1,3-Dimethylnaphthalene	27.168	213.719	217.498	−3.779
27	1,4-Dimethylnaphthalene	27.168	216.899	217.498	−0.599
28	2-Methylnaphthalene	27.002	216.145	215.844	0.301
29	1-Ethylnaphthalene	27.848	225.978	224.273	1.705
30	1,2,4-Triethylbenzene	19.968	145.227	145.764	−0.537
31	1,2,4,5-Tetramethylbenzene	17.596	119.453	122.132	−2.679
32	Pentylbenzene	20.482	152.925	150.885	2.040
33	*o*-Diethylbenzene	18.956	141.084	135.682	5.402
34	*p*-Diethylbenzene	18.956	137.863	135.682	2.181
35	1,2,4-Trimethylbenzene	17.430	116.943	120.478	−3.535
36	1,3,5-Triethylbenzene	17.430	117.947	120.478	−2.531
37	*m*-Ethyltoluene	18.110	126.440	127.253	−0.813
38	*o*-Ethyltoluene	18.110	131.085	127.253	3.832
39	*o*-Xylol	17.264	122.089	118.824	3.265
40	*p*-Xylol	17.264	121.127	118.824	2.303
41	2,3-Dimethylhexane	6.418	17.698	10.766	6.932
42	2-Methylheptane	6.605	12.761	12.629	0.132
43	3-Methylheptane	6.605	13.724	12.629	1.095
44	3,3-Dimethylpentane	5.565	2.636	2.267	0.369
45	2,3-Dimethylbutane	4.726	−4.100	−6.092	1.992
46	Hexane	5.100	−0.251	−2.366	2.115
47	Butane	3.408	−17.154	−19.223	2.069
48	2-Methylpropane	3.221	−20.878	−21.086	0.208
49	Ethane	1.716	−32.928	−36.080	3.152
50	Heptane	5.946	7.991	6.063	1.928

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