

Developing a Support Vector Machine Based QSPR Model to Predict Gas-to-Benzene Solvation Enthalpy of Organic Compounds

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Table S1 Comparison of experimental and predicted values of gas-to-benzene solvation enthalpy (ΔH_{Solv} in units of kJ mole^{-1}) at 298K for training and prediction sets

Number	Name	$\Delta H_{Solv}(\text{EXP})$	$\Delta H_{Solv}(\text{ERM})$	$\Delta H_{Solv}(\text{SVM})$
Training set				
1	Methane	-1.26	-1.12	-1.33
2	Propane	-13.39	-12.60	-13.32
3	2-Methylpropane	-15.48	-18.40	-15.64
4	Pentane	-22.13	-24.44	-21.63
5	Heptane	-31.00	-32.13	-30.57
6	Octane	-35.48	-33.44	-34.42
7	Decane	-43.85	-44.61	-43.78
8	Tetradecane	-61.63	-64.51	-60.26
9	Hexadecane	-70.08	-73.17	-70.15
10	2-Methylbutane	-20.50	-21.71	-20.57
11	3-Ethylpentane	-30.00	-31.49	-29.93
12	2,2-Dimethylpentane	-26.94	-28.29	-27.72
13	3,3-Diethylpentane	-36.86	-39.74	-37.49
14	2,2,4-Trimethylpentane	-29.16	-31.41	-30.69
15	2,2,5,5-Tetramethylhexane	-34.43	-37.94	-35.06
16	Cyclopentane	-25.65	-24.62	-25.58
17	Cycloheptane	-35.34	-32.55	-34.51
18	Cyclooctane	-39.68	-36.97	-38.01
19	Methylcyclohexane	-31.30	-33.29	-32.27
20	<i>cis</i> -1,2-Dimethylcyclohexane	-35.27	-37.17	-35.59
21	<i>cis</i> Decalin	-46.43	-47.93	-47.71
22	1-Butene	-18.53	-22.39	-19.26
23	<i>cis</i> 2-Butene	-20.95	-23.21	-20.04
24	<i>trans</i> 2-Butene	-19.23	-21.33	-20.14
25	2-Methylpropene	-19.10	-24.04	-19.03
26	1-Hexene	-27.91	-29.72	-28.68
27	1-Heptene	-32.47	-33.92	-32.16
28	1-Nonene	-41.21	-46.28	-40.12
29	1-Decene	-45.56	-51.52	-45.20
30	1-Tridecene	-59.07	-64.25	-59.00
31	1-Tetradecene	-63.43	-64.92	-63.58
32	<i>cis</i> 2-Octene	-35.98	-38.27	-35.96
33	<i>trans</i> 2-Octene	-35.81	-38.06	-35.79
34	<i>cis</i> 4-Octene	-35.44	-38.30	-35.98
35	<i>trans</i> 4-Octene	-35.31	-37.67	-35.47
36	1,3-Butadiene	-20.28	-23.71	-20.65
37	1,5-Hexadiene	-29.20	-31.39	-30.97
38	Cyclohexene	-31.51	-31.83	-31.58
39	1-Methylcyclohexene	-34.94	-35.91	-34.87
40	Norbornadiene	-33.66	-40.84	-34.36
41	Acetone	-30.08	-27.90	-30.01
42	2-Pentanone	-37.61	-35.85	-36.64
43	2-Hexanone	-42.17	-39.33	-41.78
44	3-Hexanone	-41.97	-39.55	-40.84
45	4-Heptanone	-45.81	-43.92	-45.74
46	2-Octanone	-50.84	-47.75	-49.61
47	5-Nonanone	-53.35	-51.93	-53.28

48	2-Decanone	-58.62	-56.39	-57.02
49	6-undecanone	-61.37	-61.41	-61.30
50	3,3-dimethyl-2-butanone	-37.66	-35.83	-38.07
51	2,2,4,4-tetramethyl-3-pentanone	-43.01	-45.21	-44.18
52	cyclopentanone	-43.72	-38.16	-42.52
53	cycloheptanone	-49.62	-46.00	-48.13
54	dimethyl ether	-21.10	-20.74	-21.17
55	dibutyl ether	-42.17	-46.27	-43.63
56	methyl butyl ether	-31.38	-33.24	-32.37
57	methyl heptyl ether	-44.81	-45.63	-45.71
58	methyl <i>tert</i> -amyl ether	-34.61	-35.37	-35.53
59	tetrahydrofuran	-31.80	-31.55	-31.73
60	1,4-dioxane	-39.03	-35.01	-37.99
61	2-methyltetrahydrofuran	-34.16	-35.28	-35.07
62	18-crown-6	-100.80	-90.07	-100.73
63	1-butanol	-35.14	-33.66	-34.74
64	1-hexanol	-49.66	-39.55	-48.43
65	1-octanol	-52.76	-47.10	-50.31
66	<i>tert</i> -butanol	-34.00	-31.33	-32.96
67	2-methyl-2-butanol	-33.47	-34.94	-34.63
68	2-ethoxyethanol	-39.43	-37.10	-38.11
69	1-fluorooctane	-47.61	-41.01	-47.54
70	1-chlorohexane	-41.97	-43.30	-43.49
71	1-chlorooctane	-50.38	-51.54	-52.75
72	1,1,2,2-tetrachloroethane	-47.72	-46.48	-47.79
73	phenol	-49.95	-45.07	-48.46
74	2,6-dimethylphenol	-52.59	-49.60	-50.76
75	1-naphthol	-69.20	-62.52	-67.18
76	dimethyl sulfoxide	-48.08	-41.45	-46.07
77	pyridine	-40.20	-38.91	-38.81
78	2-methylpyridine	-42.43	-44.62	-44.43
79	2,6-dimethylpyridine	-45.00	-46.00	-45.07
80	2-chloropyridine	-47.90	-48.86	-47.83
81	3-cyanopyridine	-54.10	-52.79	-53.60
82	4-cyanopyridine	-55.00	-53.35	-54.35
83	triethylamine	-37.06	-34.53	-35.77
84	benzene	-33.85	-35.01	-34.51
85	1,4-dimethylbenzene	-42.15	-42.62	-41.58
86	mesitylene	-44.77	-45.68	-44.18
87	phenanthrene	-74.04	-73.78	-73.97
88	biphenyl	-63.40	-64.58	-63.47
89	1,3-dichlorobenzene	-45.95	-53.85	-47.59
90	anisole	-46.58	-48.78	-48.46
91	γ -butyrolactone	-53.92	-47.34	-51.92
92	ethyl acetate	-34.74	-36.49	-36.29
93	difluorodichloromethane	-18.58	-15.84	-18.51
94	ethyl formate	-30.38	-36.91	-31.24
95	1-butanethiol	-35.79	-33.86	-35.23
96	methyl methacrylate	-38.44	-41.90	-40.02
97	benzotrile	-52.03	-51.04	-50.84
98	diiodomethane	-45.02	-46.56	-45.09
99	nitrobenzene	-52.72	-57.16	-52.08
100	trifluoromethylbenzene	-35.15	-40.74	-36.93

101	3-methylphenol	-51.04	-49.23	-53.14
102	ethyl benzoate	-58.78	-62.38	-58.85
103	acetonitrile	-31.23	-29.85	-31.16
104	2-nitropropane	-40.30	-41.52	-40.37
105	nitromethane	-35.01	-34.71	-34.94
106	fluorobenzene	-35.44	-37.93	-36.58
107	bromobenzene	-43.60	-48.94	-45.52
108	iodobenzene	-48.76	-50.39	-49.17
109	aniline	-50.54	-46.19	-48.08
110	carbon tetrachloride	-31.88	-28.28	-31.95
111	chloroform	-32.27	-33.01	-34.50
112	dimethoxymethane	-28.12	-30.12	-30.28
113	1,2-dimethoxyethane	-37.21	-33.84	-35.96
114	ethanol	-29.62	-29.56	-29.69
115	benzaldehyde	-48.95	-53.92	-50.34
116	4-chloronitrobenzene	-55.23	-60.29	-55.30
117	1,4-dibromobenzene	-54.54	-59.84	-54.61
118	4-nitrotoluene	-61.33	-65.61	-59.48
119	pyrrole	-42.10	-33.02	-41.49
120	n-methylpyrrole	-40.02	-36.52	-38.74
	prediction set			
121	ethane	-8.37	-6.69	-8.88
122	butane	-17.41	-19.90	-16.84
123	hexane	-26.65	-24.57	-25.23
124	nonane	-39.66	-45.11	-37.86
125	dodecane	-52.30	-57.97	-51.00
126	2,2-dimethylbutane	-22.88	-24.48	-23.33
127	2-methyloctane	-38.03	-44.04	-36.78
128	2,2,4,4-tetramethylpentane	-32.01	-33.18	-33.39
129	cyclohexane	-29.41	-26.40	-30.50
130	ethene	-9.00	-13.38	-9.54
131	1-pentene	-22.92	-26.16	-24.62
132	1-octene	-36.69	-39.85	-35.57
133	1-dodecene	-54.52	-58.59	-56.92
134	1-pentadecene	-67.82	-74.65	-69.40
135	cyclopentene	-26.27	-30.46	-28.22
136	2-butanone	-34.27	-31.84	-32.57
137	3-pentanone	-38.58	-35.86	-36.45
138	2-heptanone	-46.44	-40.13	-45.38
139	2-nonanone	-54.98	-51.83	-53.20
140	2-undecanone	-62.80	-55.10	-60.97
141	cyclohexanone	-46.16	-41.91	-44.39
142	diethyl ether	-26.36	-29.30	-27.11
143	methyl <i>tert</i> -butyl ether	-28.03	-30.31	-29.92
144	1,3-dioxane	-39.77	-35.16	-37.24
145	15-crown-5	-81.45	-76.07	-84.03
146	1-pentanol	-39.33	-35.86	-37.28
147	1-decanol	-65.00	-55.41	-62.37
148	1,1-difluoroethane	-18.13	-16.98	-19.43
149	chloroethane	-25.62	-28.10	-26.98
150	2,4-dimethylpyridine	-47.04	-42.77	-45.62
151	3-chloropyridine	-48.50	-53.95	-46.81
152	toluene	-37.66	-40.90	-39.42

153	naphthalene	-55.28	-50.06	-53.24
154	chlorotrifluoromethane	-5.02	-8.76	-5.68
155	1-nitropropane	-43.37	-40.54	-41.87
156	nitroethane	-38.29	-43.29	-36.03
157	chlorobenzene	-40.83	-46.01	-42.56
158	1-nitronaphthalene	-68.20	-75.74	-65.35
