Using COSMO-RS to Predict Hansen Solubility Parameters

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Table S1. Database of 195 HSP values obtained from literature.

Code	Molecule	MPa$^{1/2}$			Testing or Training	Reference
		δD	δP	δH		
1	1,2,3,5-Tetramethylbenzene	18.6	0.5	0.5	Testing	1
2	1,2,3-Trichloropropane	17.8	12.3	3.4	Testing	
3	1,2,4-Trichlorobenzene	20.2	4.2	3.2	Training	
4	1,2,4-Trimethylbenzene	18.0	1.0	1.0	Training	
5	1,2-Methylenedioxybenzene	19.0	2.8	5.9	Training	
6	1,3-Dichloro Propane	18.6	8.2	3.0	Training	
7	1,4-Butanediol	16.6	15.3	21.7	Testing	
8	1-Bromobutane	16.5	6.0	4.5	Testing	
9	1-Bromonaphthalene	20.3	3.1	4.1	Training	
10	1-Bromopropane	16.4	7.9	4.8	Training	
11	1-Butanol	16.0	5.7	15.8	Training	
12	1-Chloro-2-Ethyl Benzene	18.9	4.9	2.2	Training	
13	1-Chloro-4-Ethoxy Benzene	19.3	6.3	4.4	Testing	
14	1-Chloronaphthalene	19.9	4.9	2.5	Training	
15	1-Hexanol	15.9	5.8	12.5	Training	
16	1-Methyl Naphthalene	20.6	0.8	4.7	Training	
17	1-Octanol	16.0	5.0	11.9	Training	
18	1-Pentanol	15.9	5.9	13.9	Training	
19	1-Propanol	16.0	6.8	17.4	Testing	
20	2,3-Benzofuran (Cumaron)	18.7	5.1	5.7	Training	
21	2,5-Dichlorobenzotrifluoride	20.0	4.7	2.4	Testing	
22	2-Bromothiophene	20.1	5.2	4.6	Training	
23	2-Butanol	15.8	5.7	14.5	Training	
24	2-Chloroethyl Benzene	19.3	6.3	2.2	Training	
25	2-Pentanol	15.6	6.4	13.3	Testing	
26	2-Propanol	15.8	6.1	16.4	Training	
27	4-(Trifluoromethyl) Acetophenone	18.8	6.1	3.5	Testing	

Code	Molecule		MPa$^{1/2}$		Testing or	Reference
28	4-Chlorobenzotrichloride	20.3	5.5	3.5	Testing	
29	4-Fluoropropylphenone	19.6	7.1	3.5	Training	
30	Acrylonitrile	16.0	12.8	6.8	Training	
31	Aniline	19.4	5.1	10.2	Training	
32	Anisole	17.8	4.1	6.7	Training	
33	Benzaldehyde	19.4	7.4	5.3	Training	
34	Benzene	18.4	0.0	2.0	Training	
35	Benzonitrile	17.4	9.0	3.3	Training	
36	Benzotrichloride	20.2	6.6	3.2	Training	
37	Benzyl Benzoate	20.0	5.1	5.2	Training	
38	Benzyl Chloride	18.8	7.1	2.6	Training	
39	Benzylethyl Ether	18.4	3.8	3.8	Training	
40	Biphenyl	19.7	1.0	2.0	Testing	
41	1,1,2,2-Tetrachloroethane	18.8	5.1	5.3	Training	
42	Bis-(M-Phenoxyphenyl) Ether	19.6	3.1	5.1	Testing	
43	Bromide-2	18.2	2.1	0.0	Training	
44	Bromobenzene	20.5	5.5	4.1	Training	
45	Bromochloromethane	17.3	5.7	3.5	Testing	
46	Bromoform	21.4	4.1	6.1	Testing	
47	Butyl Benzoate	18.3	2.9	5.5	Training	
48	1,1,2-Trichlorotrifluoroethane	14.7	1.6	0.0	Training	
49	Chlorobenzene	19.0	4.3	2.0	Training	
50	1,1,1,2-Tetrachloroethane	18.0	4.4	4.2	Training	
51	1,1,1-Trichloroethane	16.8	4.3	2.0	Training	
52	Cyclohexane	16.8	0.0	0.2	Testing	
53	Cyclohexene	17.2	1.0	5.0	Training	
54	Cyclohexyl Benzene	18.7	0.0	1.0	Training	
55	Cyclohexylchloride	17.3	5.5	2.0	Training	
56	Cyclopentane	16.4	0.0	1.8	Testing	
57	Ddt	20.0	4.8	2.7	Testing	

Code	Molecule		MPa$^{1/2}$		Testing or	Reference
58	Decane	15.7	0.0	0.0	Training	
59	Dibromomethane	17.8	6.4	7.0	Testing	
60	Diphenyl Acetylene (G.C)	20.1	2.0	3.2	Testing	
61	Diphenyl Amine	20.0	3.3	5.9	Testing	
62	Diphenyl Ether	19.6	3.2	5.8	Training	
63	Diphenylmethane	19.5	1.0	1.0	Testing	
64	Dodecane	16.0	0.0	0.0	Training	
65	Ethanol	15.8	8.8	19.4	Testing	
66	Ethyl Benzene	17.8	0.6	1.4	Testing	
67	Ethyl Bromide	16.5	8.4	2.3	Training	
68	Ethyl Iodide	17.3	7.9	7.2	Training	
69	Ethylene Dibromide	19.2	3.5	8.6	Testing	
70	Ethylene Dichloride	19.0	7.4	4.1	Training	
71	Fluorene	20.0	1.7	1.7	Training	
72	Fluorobenzene	18.7	6.1	2.0	Training	
73	Heptane	15.3	0.0	0.0	Training	
74	Hexamethyl Benzene	19.2	1.6	0.0	Training	
75	Iodobenzene	19.9	5.6	4.5	Training	
76	Isopropyl Benzene (Cumene)	18.1	1.2	1.2	Training	
77	M-Dichlorobenze	19.7	5.1	2.7	Training	
78	Methyl Iodide	17.5	7.7	5.3	Training	
79	Mesitylene (1,3,5-Trimethylbenzene)	18.0	0.6	0.6	Training	
80	Methanol	15.1	12.3	22.3	Training	
81	Methyl Cyclohexane	16.0	0.0	1.0	Training	
82	Methylene Dichloride	18.2	6.3	6.1	Training	
83	Methylene Diiodide	17.8	3.9	5.5	Training	
84	Naphthalene	19.2	2.0	5.9	Training	
85	N-Butyl Amine	16.2	4.5	8.0	Testing	
86	N-Butylbenzene	17.4	0.1	1.1	Testing	
87	Nitrobenzene	20.0	8.6	4.1	Training	

Code	Molecule		MPa$^{1/2}$		Testing or	Reference
88	Nitroethane	16.0	15.5	4.5	Training	
89	N-Methyl-2-Pyrrolidone	18.0	12.3	7.2	Testing	
90	Nonane	15.7	0.0	0.0	Training	
91	N-Tetradecane	16.2	0.0	0.0	Training	
92	O-Bromotoluene	19.3	5.0	4.2	Testing	
93	O-Chlorostyrene	18.7	4.7	3.9	Testing	
94	Octane	15.5	0.0	0.0	Testing	
95	O-Dichlorobenzene	19.2	6.3	3.3	Training	
96	O-Xylene	17.8	1.0	3.1	Training	
97	Ozone	19.8	4.2	0.0	Testing	
98	P-Bromotoluene	19.3	6.8	4.1	Training	
99	P-Chlorostyrene	18.7	4.3	3.9	Testing	
100	P-Chlorotoluene	19.1	6.2	2.6	Training	
101	P-Dichlorobenzene	19.7	5.6	2.7	Testing	
102	Pentachloro Ethane	18.2	3.2	2.4	Training	
103	Pentane	14.5	0.0	0.0	Training	
104	Phenetole (Ethyl Phenyl Ether)	18.4	4.5	4.0	Training	
105	Phenyl Acetylene	18.8	2.8	4.0	Training	
106	Phosphorus Trichloride	18.4	3.6	0.0	Training	
107	Propyl Chloride	16.0	7.8	2.0	Testing	
108	Propylene Glycol	16.8	9.4	23.3	Training	
109	Pyridine	19.0	8.8	5.9	Testing	
110	Quinoline	19.8	5.6	5.7	Training	
111	Styrene	18.6	1.0	4.1	Testing	
112	Tetrachloroethylene	18.3	5.7	0.0	Training	
113	Tetrahydrofuran	16.8	5.7	8.0	Training	
114	Tetrahydrothiophene	18.9	7.5	5.8	Testing	
115	Thiophene	18.9	2.4	7.8	Training	
116	Toluene	18.0	1.4	2.0	Training	
117	Trinitrotoluene (TNT)	19.5	3.7	4.5	Training	

Code	Molecule		MPa$^{1/2}$		Testing or	Reference
118	A-Methyl Styrene	18.5	2.4	2.4	Training	
119	Aα-Dichloro Toluene	19.9	6.6	2.4	Training	
120	Chloroform	17.8	3.1	5.7	Testing	
121	Cis-Decahydronaphthalene	18.8	0.0	0.0	Testing	
122	2-Butoxyethanol	15.1	6.7	8.1	Training	2
123	4-Aminobenzoic Acid	17.2	13.2	15.6	Training	
124	Acrylic Acid	17.4	7.3	12.3	Training	
125	Benzoic Acid	17.1	8.6	10.8	Testing	
126	Benzyl Alcohol	18.0	6.2	12.4	Testing	
127	Bis(2-Chloroethyl) Ether	18.9	7.3	4.0	Training	
128	Butyl Acetate	16.0	6.5	3.8	Training	
129	Butyl Benzyl Phthalate	20.4	13.3	3.1	Training	
130	Dibutylphthalate	17.8	8.6	4.1	Training	
131	Diethyl Ether	14.5	2.9	5.1	Testing	
132	Dimethyl-Ethanolamine	16.1	9.2	15.3	Testing	
133	Dipropyleneglycol	16.5	10.6	17.7	Training	
134	Ethanolamine	17.0	15.5	21.2	Training	
135	Ethylbenzene	17.8	0.6	1.4	Training	
136	Ethylenecyanohydrin	17.2	18.8	17.6	Testing	
137	Formic Acid	14.3	11.9	16.6	Training	
138	Hexafluoro-I-Propanol	17.2	4.5	14.7	Training	
139	Hexamethylphosphoramide	18.5	8.6	11.3	Training	
140	Ibuprofen	16.4	6.4	8.9	Testing	
141	Lactose	24.2	11.2	34.9	Training	
142	Mannitol	19.0	10.3	33.5	Training	
143	N,N-Dimethylacetamide	16.8	11.5	10.2	Testing	
144	Piroxicam	16.8	21.4	6.6	Training	
145	Propylenecarbonate	20.0	18.0	4.1	Training	
146	Salicylic Acid	16.6	12.4	14.6	Training	
147	Sorbitol	19.0	10.3	33.5	Testing	

Code	Molecule		MPa$^{1/2}$		Testing or	Reference
148	Sucrose	24.7	11.3	35.1	Testing	
149	Tetrahydrofurfurylalcohol	17.8	8.2	10.2	Training	
150	Tricresyl Phosphate	19.0	12.3	4.5	Training	
151	Triethyl Phosphate	16.7	11.4	9.2	Training	
152	Trimethyl Phosphate	16.7	15.9	10.2	Training	
153	Urea	20.9	18.7	26.4	Training	
154	Γ - Butyrolactone	19.0	16.6	7.4	Testing	
155	Citric Acid	20.9	8.2	21.9	Training	
156	1,4-Dioxane	19.0	1.8	7.4	Testing	3
157	Isopropanol	15.8	6.1	16.4	Training	
158	Methyl Ethyl Ketone	16.0	9.0	5.1	Training	
159	Water	15.5	16.0	42.3	Training	
160	2-Methyl Propan-1-Ol	15.1	5.7	15.9	Testing	4
161	Butan-1-Ol	16.0	5.7	15.8	Training	
162	Cumene	18.1	1.2	1.2	Training	
163	Diethyl Malonate	16.1	7.7	8.3	Training	
164	Ethyl Acetate	15.8	5.3	7.2	Training	
165	Hexan-1-Ol	15.9	5.8	12.5	Training	
166	M-Cresol	18.0	5.1	12.9	Training	
167	N-Butyl Acetate	15.8	3.7	6.3	Testing	
168	N-Heptane	15.3	0.0	0.0	Training	
169	Octan-1-Ol	17.0	3.3	11.9	Training	
170	3-Methylbutyraldehyde	14.7	9.5	5.0	Training	5
171	Acetic Acid	14.5	8.0	13.5	Testing	
172	Acetophenone	19.6	8.6	3.7	Training	
173	Cyclohexanone	17.8	6.3	5.1	Training	
174	Diethylene Glycol	16.2	7.8	12.6	Testing	
175	Diethylphthalate	17.6	9.6	4.5	Training	
176	Dimethyl Sulfoxide	18.4	16.4	10.2	Training	
177	Ethylene Glycol	17.0	11.0	26.0	Testing	

Code	Molecule		MPa$^{1/2}$		Testing or	Reference
178	Glycerol	17.4	12.1	29.3	Testing	
179	Isooctane	14.1	0.0	0.0	Training	
180	Isopropyl Acetate	14.9	4.5	8.2	Training	
181	Methacrylic Acid	15.8	2.8	10.2	Training	
182	Propanol	16.0	6.8	17.4	Testing	
183	Propionic Acid	14.7	5.3	12.4	Testing	
184	Sulfolane	20.3	18.2	10.9	Training	
185	Xylene	17.6	1.0	3.1	Testing	
186	Acetone	7.6	5.1	3.4	Testing	6
187	Carbon Tetrachloride	8.7	0.0	0.3	Training	
188	Ethoxyethanol	7.9	4.5	7.0	Training	
189	Methyl Isobutyl Ketone	7.5	3.0	2.0	Testing	
190	N-Butanol	7.8	2.8	7.7	Training	
191	N-Hexane	7.3	0.0	0.0	Training	
192	N-Propanol	7.8	3.3	8.5	Training	
193	Acetonitrile	14.8	19.1	6.6	Training	7
194	Dichloromethane	18.2	6.3	6.2	Testing	
195	A-Endosulfan	15.4	16.0	5.1	Training	

Table S2. Data of COSMO-RS descriptors for the created database.

Code	$Area$ (A²)	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	kcal/mol			
							E_{int}	E_{MF}	E_{HB}	E_{vdW}
1	192.89	28.56	5.19	4.26	0.00	0.00	-8.28	1.65	0.00	-9.72
2	151.18	58.78	-19.53	-26.04	0.00	0.07	-5.47	2.63	0.00	-9.05
3	176.54	29.36	-12.30	-12.63	0.00	0.02	-9.11	1.49	0.00	-10.39
4	176.73	28.21	4.05	3.19	0.00	0.00	-7.45	1.65	0.00	-8.90
5	148.14	51.09	3.57	8.62	0.15	0.00	-5.79	2.05	-0.02	-7.04
6	133.99	49.13	1.14	1.30	0.00	0.00	-4.74	1.98	0.00	-7.66
7	138.25	95.47	38.68	118.41	7.27	3.30	-12.19	2.08	-8.79	-6.42
8	137.73	25.93	3.44	2.59	0.00	0.00	-5.46	1.49	0.00	-7.90
9	189.81	36.75	-8.38	-5.74	0.00	0.00	-9.95	1.99	0.00	-10.97
10	121.01	25.99	3.02	2.24	0.00	0.00	-4.72	1.46	0.00	-7.13
11	127.73	49.77	17.57	52.98	3.51	1.73	-8.32	1.17	-4.22	-6.22
12	173.77	28.51	-2.67	-2.05	0.00	0.00	-7.90	1.51	0.00	-9.21
13	187.47	45.10	1.41	8.26	0.33	0.00	-7.87	2.12	-0.01	-9.76
14	185.42	35.66	-8.23	-5.63	0.00	0.00	-8.91	1.93	0.00	-9.86
15	166.47	50.26	24.56	70.41	3.66	1.28	-9.01	1.64	-3.42	-8.18
16	184.63	37.07	-1.60	-1.10	0.00	0.00	-8.22	2.08	0.00	-9.31
17	205.67	53.00	18.40	55.99	3.59	1.72	-12.03	1.36	-4.11	-10.24
18	143.06	52.17	22.92	68.62	3.79	1.48	-8.56	1.48	-4.01	-6.97
19	106.87	48.42	24.38	71.61	3.70	1.29	-6.27	1.47	-3.58	-5.11
20	150.40	40.83	-5.15	-4.77	0.00	0.01	-6.29	1.93	0.00	-7.43
21	190.81	29.81	-13.73	-14.34	0.00	0.03	-7.66	1.70	0.00	-9.15
22	139.20	27.39	-9.04	-8.21	0.00	0.00	-7.97	1.41	0.00	-9.37
23	125.72	47.89	18.93	57.10	3.41	1.39	-7.55	1.21	-3.58	-6.13
24	174.19	47.94	2.05	2.07	0.00	0.00	-7.05	2.37	0.00	-9.21
25	141.06	44.16	14.67	46.64	2.72	1.24	-7.97	1.12	-3.08	-6.95
26	106.96	50.74	24.67	79.49	4.04	1.37	-6.95	1.33	-4.09	-5.14
27	198.22	56.63	12.75	37.82	1.36	0.00	-5.77	2.79	-0.09	-8.26

Code	$Area$ (A²)	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	kcal/mol			
							E_{int}	E_{MF}	E_{HB}	E_{vdW}
28	209.35	32.19	-12.56	-10.74	0.00	0.00	-10.93	1.71	0.00	-12.43
29	188.84	76.79	-18.88	-86.66	0.64	3.59	-8.23	2.73	-2.04	-8.72
30	98.28	45.51	10.43	23.41	0.85	0.01	-2.00	1.95	-0.22	-4.67
31	135.38	61.65	-15.56	-40.51	0.03	1.58	-4.45	2.30	-0.03	-6.51
32	150.75	43.41	8.27	15.53	0.41	0.00	-5.60	2.04	0.00	-7.42
33	144.94	51.69	20.26	47.89	1.56	0.00	-4.81	2.46	-0.02	-7.04
34	121.58	27.33	-0.48	-0.42	0.00	0.00	-4.84	1.51	0.00	-6.14
35	145.79	50.83	11.28	27.02	0.85	0.00	-4.84	2.53	-0.07	-7.09
36	189.92	30.08	-8.45	-5.62	0.00	0.00	-9.44	1.67	0.00	-10.90
37	250.75	69.37	13.16	30.94	0.92	0.00	-10.55	3.19	0.00	-12.37
38	160.11	44.65	-3.65	-3.14	0.00	0.00	-6.57	2.19	0.00	-8.55
39	187.14	47.46	23.77	63.01	2.21	0.00	-7.11	2.39	0.00	-9.29
40	199.40	44.33	-3.72	-2.63	0.00	0.00	-9.11	2.35	0.00	-10.10
41	150.26	42.59	-32.07	-60.19	0.00	1.68	-6.24	2.33	0.00	-9.52
42	388.60	100.10	-4.56	3.62	0.18	0.00	-18.62	4.31	-0.01	-19.25
43	89.65	13.85	-6.59	-6.57	0.00	0.00	-6.89	0.66	0.00	-7.56
44	145.92	30.52	-6.88	-5.12	0.00	0.00	-7.33	1.64	0.00	-8.76
45	103.61	33.09	-15.08	-21.57	0.00	0.21	-4.38	1.71	0.00	-7.04
46	132.47	29.56	-19.53	-34.58	0.00	1.10	-8.21	1.52	0.00	-10.67
47	230.10	54.08	21.64	44.37	1.37	0.00	-8.81	2.67	0.00	-11.27
48	149.37	7.84	-2.60	-1.00	0.00	0.00	-6.31	0.35	0.00	-7.62
49	141.01	29.33	-6.81	-5.11	0.00	0.00	-6.27	1.56	0.00	-7.63
50	149.37	31.72	-16.43	-22.29	0.00	0.27	-6.80	1.70	0.00	-9.45
51	133.06	22.20	-6.45	-4.96	0.00	0.00	-6.00	1.21	0.00	-8.15
52	131.73	5.74	0.31	0.06	0.00	0.00	-6.92	0.04	0.00	-6.75
53	129.87	15.78	5.46	5.26	0.01	0.00	-6.04	0.76	0.00	-6.59
54	210.06	29.16	2.65	1.47	0.00	0.00	-10.33	1.65	0.00	-10.61
55	151.49	25.26	7.50	5.73	0.00	0.00	-6.90	1.47	0.00	-8.16
56	120.06	5.94	0.21	0.04	0.00	0.00	-6.04	0.12	0.00	-6.14

Code	$Area$ (A²)	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	kcal/mol			
							E_{int}	E_{MF}	E_{HB}	E_{vdW}
57	309.52	59.33	-21.55	-19.60	0.00	0.04	-16.08	3.12	0.00	-17.84
58	235.07	10.98	0.60	0.11	0.00	0.00	-10.93	0.18	0.00	-12.06
59	108.97	33.72	-14.91	-21.40	0.00	0.22	-5.49	1.70	0.00	-8.13
60	233.38	50.72	-7.64	-5.18	0.00	0.00	-10.58	2.67	0.00	-11.88
61	214.36	63.68	-15.92	-37.14	0.00	1.31	-9.07	3.01	0.00	-10.72
62	211.32	51.50	-2.18	0.79	0.05	0.00	-9.50	2.42	0.00	-10.56
63	218.37	49.44	0.54	0.33	0.00	0.00	-9.67	2.68	0.00	-10.99
64	265.97	12.45	0.60	0.10	0.00	0.00	-12.53	0.16	0.00	-13.64
65	88.41	51.93	22.47	72.47	4.09	1.78	-6.95	1.19	-4.91	-4.18
66	158.98	27.96	1.83	1.13	0.00	0.00	-6.61	1.60	0.00	-8.01
67	103.35	26.36	2.50	1.90	0.00	0.00	-3.94	1.42	0.00	-6.31
68	110.81	26.33	1.50	0.84	0.00	0.00	-5.09	1.41	0.00	-7.45
69	126.35	47.10	-9.15	-11.44	0.00	0.00	-5.63	2.05	0.00	-8.63
70	117.20	45.45	-8.68	-10.44	0.00	0.00	-4.05	1.90	0.00	-6.90
71	205.08	45.16	-1.75	-1.32	0.00	0.00	-9.47	2.44	0.00	-10.35
72	129.23	29.37	-5.53	-4.36	0.00	0.00	-4.60	1.56	0.00	-5.95
73	176.99	8.62	0.45	0.08	0.00	0.00	-7.97	0.15	0.00	-9.06
74	216.90	28.75	8.24	7.55	0.01	0.00	-9.54	1.63	0.00	-10.96
75	154.16	31.86	-7.30	-5.30	0.00	0.00	-8.43	1.66	0.00	-9.88
76	175.48	28.89	1.83	1.11	0.00	0.00	-7.42	1.64	0.00	-8.84
77	160.11	29.94	-11.20	-9.87	0.00	0.00	-7.76	1.55	0.00	-9.10
78	91.86	25.49	-1.34	-1.81	0.00	0.00	-4.48	1.24	0.00	-6.67
79	179.20	28.00	4.09	3.22	0.00	0.00	-7.64	1.60	0.00	-9.03
80	67.86	52.56	21.65	70.52	4.15	1.91	-6.21	1.16	-5.21	-3.11
81	149.61	7.06	0.35	0.06	0.00	0.00	-7.78	0.10	0.00	-7.67
82	98.47	32.60	-15.38	-21.96	0.00	0.20	-3.36	1.72	0.00	-6.03
83	125.29	35.22	-13.94	-18.53	0.00	0.15	-7.92	1.65	0.00	-10.52
84	168.46	37.11	-3.49	-2.41	0.00	0.00	-7.46	2.03	0.00	-8.52
85	130.99	48.35	53.36	279.37	5.45	0.04	-3.64	2.22	-0.48	-6.32

Code	$Area$ (A²)	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	kcal/mol			
							E_{int}	E_{MF}	E_{HB}	E_{vdW}
86	195.01	28.34	2.00	1.14	0.00	0.00	-8.45	1.60	0.00	-9.84
87	149.31	52.14	6.20	12.43	0.24	0.00	-4.94	2.09	-0.02	-6.80
88	107.06	51.96	8.43	12.84	0.25	0.01	-1.95	1.71	-0.06	-4.54
89	139.50	63.78	68.74	195.85	6.87	0.00	-2.47	4.22	0.00	-6.67
90	216.94	10.15	0.60	0.11	0.00	0.00	-10.01	0.17	0.00	-11.13
91	301.14	13.36	0.68	0.12	0.00	0.00	-14.36	0.15	0.00	-15.46
92	161.45	29.76	-3.96	-2.81	0.00	0.00	-7.98	1.60	0.00	-9.38
93	170.71	33.68	-6.82	-4.84	0.00	0.00	-7.55	1.76	0.00	-9.10
94	193.88	9.28	0.42	0.07	0.00	0.00	-8.86	0.12	0.00	-9.92
95	157.55	28.65	-8.89	-7.10	0.00	0.00	-7.56	1.56	0.00	-8.91
96	157.35	28.43	2.92	2.25	0.00	0.00	-6.46	1.66	0.00	-7.92
97	63.97	17.74	-6.01	-10.78	0.00	0.00	1.41	0.71	0.00	-0.25
98	165.12	30.18	-4.73	-3.54	0.00	0.00	-8.14	1.67	0.00	-9.60
99	173.55	36.60	-7.84	-5.87	0.00	0.00	-7.52	1.94	0.00	-9.26
100	160.09	29.00	-4.72	-3.56	0.00	0.00	-7.19	1.58	0.00	-8.56
101	159.88	31.53	-11.95	-10.64	0.00	0.00	-7.63	1.67	0.00	-9.09
102	163.66	27.48	-19.04	-34.94	0.00	1.18	-8.15	1.47	0.00	-10.57
103	135.39	6.98	0.26	0.04	0.00	0.00	-5.87	0.10	0.00	-6.92
104	168.53	43.99	9.59	17.32	0.47	0.00	-6.41	2.13	0.00	-8.32
105	152.25	42.81	-11.40	-17.10	0.00	0.39	-5.89	2.09	0.00	-7.77
106	126.39	18.52	-9.51	-10.62	0.00	0.00	-6.74	0.83	0.00	-8.51
107	116.07	24.98	3.29	2.61	0.00	0.00	-4.04	1.35	0.00	-6.34
108	117.43	96.22	39.37	126.22	7.48	3.17	-11.08	2.10	-8.79	-5.34
109	117.50	46.34	29.49	114.56	3.36	0.00	-3.74	2.25	-0.03	-5.75
110	164.72	53.34	24.17	98.13	2.97	0.00	-6.63	2.54	-0.02	-8.17
111	154.46	35.07	-1.91	-1.15	0.00	0.00	-6.11	1.90	0.00	-7.80
112	147.48	10.61	-2.23	-0.87	0.00	0.00	-8.08	0.43	0.00	-9.45
113	112.03	35.30	37.80	102.74	3.45	0.00	-3.26	2.23	0.00	-5.47
114	124.02	31.17	17.76	28.26	0.68	0.00	-5.22	1.80	0.00	-7.00

Code	$Area$ (A²)	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	kcal/mol			
							E_{int}	E_{MF}	E_{HB}	E_{vdW}
115	114.22	30.34	-5.11	-5.09	0.00	0.00	-5.27	1.47	0.00	-6.73
116	140.78	27.54	1.29	0.90	0.00	0.00	-5.73	1.57	0.00	-7.09
117	217.02	100.01	-11.19	-24.45	0.05	0.40	-5.34	2.67	-0.04	-7.77
118	169.64	35.51	-0.69	-0.37	0.00	0.00	-6.82	1.94	0.00	-8.55
119	176.62	43.74	-14.41	-17.62	0.00	0.21	-7.78	2.27	0.00	-9.84
120	117.56	26.60	-20.66	-38.96	0.00	1.27	-5.01	1.55	0.00	-7.51
121	183.93	7.44	0.47	0.09	0.00	0.00	-10.38	0.07	0.00	-9.47
122	179.42	75.48	35.93	87.44	5.04	1.96	-9.84	2.38	-4.55	-8.62
123	166.11	125.61	-22.50	-93.22	3.98	6.45	-11.01	2.56	-5.69	-7.67
124	106.79	86.04	-15.10	-116.98	2.29	5.09	-7.38	1.78	-5.43	-4.67
125	152.25	86.57	-10.37	-88.66	2.03	4.10	-8.98	2.37	-4.09	-7.05
126	150.70	67.31	11.97	34.79	2.95	1.69	-8.74	2.14	-3.40	-7.28
127	165.83	75.21	12.72	37.62	1.54	0.00	-5.67	2.66	-0.09	-9.18
128	172.04	53.24	36.32	71.82	2.24	0.00	-4.42	2.84	0.00	-8.20
129	349.18	112.24	41.40	87.81	2.70	0.00	-12.77	5.47	-0.10	-16.78
130	332.93	85.76	41.94	75.99	1.93	0.00	-11.94	4.31	-0.02	-16.02
131	130.50	31.08	30.11	74.66	2.56	0.00	-3.79	1.72	0.00	-6.45
132	441.49	382.72	5.58	-156.86	18.68	20.31	-46.88	6.19	-32.97	-18.93
133	175.22	106.28	42.58	132.96	7.69	3.54	-14.33	2.13	-9.12	-8.28
134	103.06	95.17	77.56	384.19	9.79	1.59	-8.64	2.82	-7.81	-4.60
135	158.98	27.96	1.83	1.13	0.00	0.00	-6.61	1.60	0.00	-8.01
136	112.32	92.96	14.72	25.79	3.40	2.42	-6.13	2.01	-4.22	-4.86
137	72.53	85.68	-34.23	-187.30	1.58	6.26	-5.83	1.36	-5.39	-2.75
138	141.64	51.59	-45.60	-146.10	0.18	4.56	-2.97	2.28	-1.07	-5.14
139	211.15	74.65	90.32	298.47	9.08	0.00	-4.58	4.85	0.00	-10.38
140	253.61	80.86	17.29	20.41	1.96	1.50	-10.61	3.44	-1.73	-12.11
141	286.31	296.99	51.21	98.97	16.62	12.04	-32.93	4.14	-23.87	-11.84
142	198.26	169.80	29.85	57.03	8.54	6.38	-17.23	2.22	-12.24	-8.16
143	132.47	67.21	70.20	217.27	7.45	0.00	-1.34	4.07	-0.01	-6.35

Code	$Area$ (A²)	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	kcal/mol			
							E_{int}	E_{MF}	E_{HB}	E_{vdW}
144	318.01	174.99	32.15	18.01	7.53	5.28	-22.34	5.09	-10.45	-14.84
145	128.27	71.59	28.87	59.05	1.75	0.00	-3.09	2.67	-0.11	-5.63
146	158.97	88.12	-26.98	-145.33	1.28	5.28	-9.14	2.06	-3.99	-7.00
147	198.26	169.80	29.85	57.03	8.54	6.38	-17.23	2.22	-12.24	-8.16
148	319.37	330.71	39.51	73.98	17.51	14.83	-39.34	3.83	-28.73	-13.27
149	140.81	75.19	41.37	107.72	5.56	1.81	-8.92	2.37	-4.63	-6.65
150	385.96	100.68	25.63	62.86	2.28	0.00	-16.56	4.93	-0.03	-18.94
151	220.30	79.51	59.52	130.61	4.31	0.00	-5.47	4.01	0.00	-10.42
152	164.41	84.52	55.73	130.67	4.56	0.00	-2.90	3.65	-0.01	-7.49
153	91.06	123.03	16.88	88.88	8.10	5.32	-5.84	1.34	-4.41	-3.72
154	117.01	64.44	40.20	83.94	2.65	0.00	-2.10	3.23	-0.02	-5.30
155	0.00	-86.40	444.65	1343.23	0.59	9.89	-14.24	2.59	-11.58	-6.20
156	120.49	58.97	51.34	125.68	4.49	0.00	-2.92	2.97	0.00	-5.68
157	106.96	50.74	24.67	79.49	4.04	1.37	-6.95	1.33	-4.09	-5.14
158	120.96	46.32	36.95	82.20	2.72	0.00	-2.01	2.79	0.00	-5.75
159	43.07	74.87	12.66	71.65	5.70	3.85	-5.54	0.29	-5.84	-0.94
160	125.23	49.18	15.71	47.61	3.36	1.77	-8.24	1.11	-4.20	-6.10
161	127.73	49.77	17.57	52.98	3.51	1.73	-8.32	1.17	-4.22	-6.22
162	175.48	28.89	1.83	1.11	0.00	0.00	-7.42	1.64	0.00	-8.84
163	204.71	84.25	41.17	72.98	1.82	0.00	-4.90	3.59	-0.12	-9.32
164	132.60	50.60	33.70	67.00	2.06	0.00	-2.72	2.53	0.00	-6.20
165	166.47	50.26	24.56	70.41	3.66	1.28	-9.01	1.64	-3.42	-8.18
166	150.30	63.53	-19.69	-83.96	0.74	3.48	-7.43	2.20	-2.19	-7.23
167	172.04	53.24	36.32	71.82	2.24	0.00	-4.42	2.84	0.00	-8.20
168	176.99	8.62	0.45	0.08	0.00	0.00	-7.97	0.15	0.00	-9.06
169	205.67	53.00	18.40	55.99	3.59	1.72	-12.03	1.36	-4.11	-10.24
170	138.93	41.92	28.48	56.15	1.70	0.00	-3.14	2.56	0.00	-6.65
171	92.26	85.85	-4.33	-79.28	2.74	4.61	-6.73	1.70	-5.54	-3.84
172	161.69	55.92	24.48	59.80	2.04	0.00	-5.39	2.71	-0.01	-7.87

Code	$Area$ (A²)	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	kcal/mol			
							E_{int}	E_{MF}	E_{HB}	E_{vdW}
173	139.27	47.76	41.04	91.24	3.04	0.00	-3.86	3.04	0.00	-6.69
174	147.23	117.69	54.17	173.27	9.18	3.88	-14.09	2.43	-10.74	-6.72
175	261.63	88.69	42.65	80.10	2.06	0.00	-8.36	4.25	-0.02	-12.39
176	111.37	85.45	82.84	300.47	9.64	0.00	-1.05	4.17	-0.45	-5.71
177	99.06	99.34	39.33	131.13	7.92	3.65	-11.60	1.90	-10.05	-4.39
178	127.21	141.51	47.51	166.12	10.99	5.75	-17.75	2.13	-15.26	-5.56
179	179.50	10.67	0.50	0.08	0.00	0.00	-8.02	0.22	0.00	-9.19
180	147.57	48.62	32.27	64.15	1.94	0.00	-3.64	2.42	0.00	-7.01
181	123.23	77.48	-2.46	-64.75	2.09	3.86	-6.54	2.08	-4.07	-5.50
182	106.87	48.42	24.38	71.61	3.70	1.29	-6.27	1.47	-3.58	-5.11
183	111.05	82.89	-3.15	-78.03	2.63	4.49	-7.17	2.01	-5.28	-4.84
184	139.85	92.20	55.07	118.30	4.07	0.00	-2.76	3.90	-0.24	-6.41
185	160.33	27.50	2.77	2.06	0.00	0.00	-6.69	1.58	0.00	-8.07
186	102.65	47.73	35.81	82.29	2.77	0.00	-1.20	2.67	0.00	-4.82
187	134.22	9.93	-2.95	-1.20	0.00	0.00	-7.42	0.41	0.00	-8.78
188	138.95	63.88	29.00	66.66	3.93	1.62	-7.35	1.84	-3.55	-6.59
189	154.79	41.57	28.53	63.61	2.14	0.00	-4.22	2.40	0.00	-7.57
190	127.73	49.77	17.57	52.98	3.51	1.73	-8.32	1.17	-4.22	-6.22
191	152.37	7.55	0.29	0.05	0.00	0.00	-6.74	0.10	0.00	-7.79
192	106.87	48.42	24.38	71.61	3.70	1.29	-6.27	1.47	-3.58	-5.11
193	82.82	49.66	17.95	39.48	1.34	0.00	-1.11	1.97	-0.24	-3.80
194	98.47	32.60	-15.38	-21.96	0.00	0.20	-3.36	1.72	0.00	-6.03
195	280.75	73.28	5.06	13.44	0.30	0.06	-15.14	2.98	-0.09	-16.67

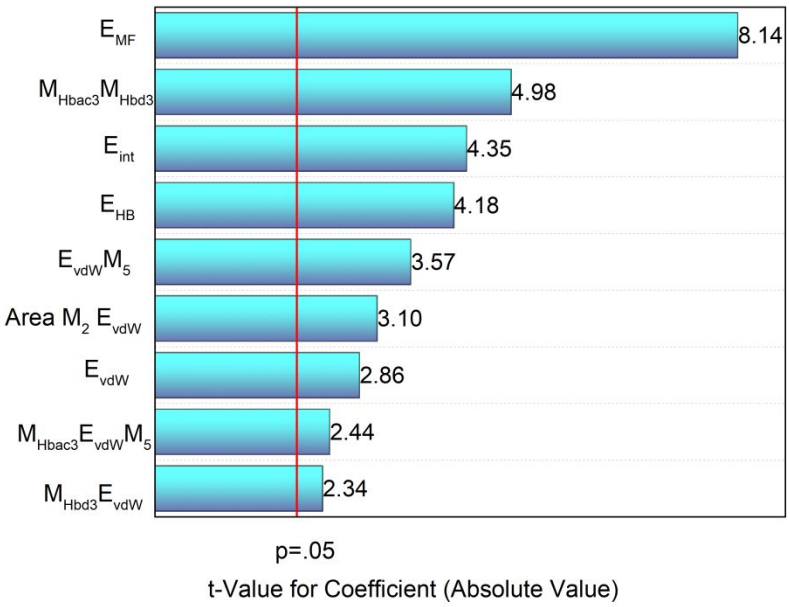

Figure S1. Pareto Chart of t-Values for the coefficients of δ_D model.

Table S3. Experimental and predicted HSP values ($MPa^{1/2}$) for the testing set after removing outliers.

Code	δD_{exp}	δD_{pred}	δP_{exp}	δP_{pred}	δH_{exp}	δH_{pred}
1	18.60	18.53	0.50	1.31	0.50	2.18
2	17.80	19.08	12.30	9.27	3.40	4.75
8	16.50	16.62	6.00	4.29	4.50	3.19
13	19.30	18.87	6.30	4.51	4.40	3.35
19	16.00	14.51	6.80	7.42	17.40	13.53
21	20.00	18.96	4.70	1.13	2.40	2.29
25	15.60	13.97	6.40	4.56	13.30	9.70
27	18.80	18.75	6.10	4.40	3.50	4.34
28	20.30	19.70	5.50	4.26	3.50	2.03
40	19.70	21.04	1.00	3.76	2.00	2.92
45	17.30	17.17	5.70	8.03	3.50	4.32
52	16.80	15.55	0.00	0.13	0.20	2.19
56	16.40	15.26	0.00	1.02	1.80	2.45
59	17.80	17.48	6.40	8.02	7.00	4.24
60	20.10	21.68	2.00	4.40	3.20	2.56
61	20.00	21.58	3.30	5.39	5.90	3.69
63	19.50	21.46	1.00	4.11	1.00	2.81
65	15.80	14.13	8.80	7.93	19.40	18.22
66	17.80	18.20	0.60	2.64	1.40	2.86
86	17.40	18.56	0.10	1.23	1.10	2.12
89	18.00	19.82	12.30	10.66	7.20	8.92

Code	δD_{exp}	δD_{pred}	δP_{exp}	δP_{pred}	δH_{exp}	δH_{pred}
92	19.30	18.65	5.00	3.80	4.20	2.91
93	18.70	18.80	4.70	3.42	3.90	2.93
94	15.50	15.14	0.00	-1.68	0.00	1.07
99	18.70	19.11	4.30	3.81	3.90	3.04
101	19.70	18.89	5.60	3.96	2.70	3.04
107	16.00	16.00	7.80	5.50	2.00	3.60
109	19.00	17.09	8.80	8.71	5.90	6.11
111	18.60	18.61	1.00	4.13	4.10	3.35
114	18.90	17.50	7.50	5.75	5.80	3.96
120	17.80	16.75	3.10	5.43	5.70	3.66
121	18.80	17.31	0.00	-1.73	0.00	1.18
125	17.10	18.31	8.60	8.02	10.80	13.15
126	18.00	16.96	6.20	7.19	12.40	11.46
131	14.50	15.40	2.90	5.46	5.10	4.30
136	17.20	15.68	18.80	13.53	17.60	18.06
140	16.40	18.06	6.40	6.61	8.90	4.99
143	16.80	18.42	11.50	12.21	10.20	9.79
154	19.00	18.70	16.60	12.43	7.40	7.24
160	15.10	13.95	5.70	5.31	15.90	13.26
167	15.80	16.97	3.70	6.29	6.30	5.00
182	16.00	14.51	6.80	7.42	17.40	13.53
185	17.60	18.17	1.00	2.49	3.10	2.80
194	18.20	16.88	6.30	8.34	6.20	4.40
R^2	0.68		0.77		0.90	
r	0.82		0.88		0.95	
MAE ($MPa^{1/2}$)	0.98		1.74		1.44	
MRE	0.06		0.93		0.62	

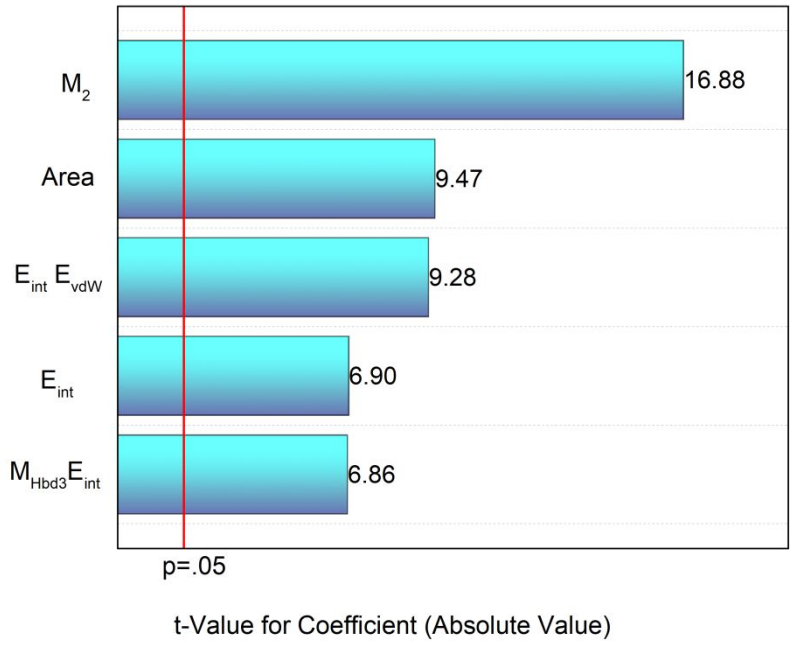

Figure S2. Pareto Chart of t-Values for the coefficients of δP model.

Table S4. Correlations between dependent and independent variables.

Dependent variables	Independent variables									
	Area	M_2	M_3	M_5	M_{Hbac_3}	M_{Hbd_3}	E_{int}	E_{MF}	E_{vdW}	E_{HB}
δD	0.264	0.198	-0.183	-0.119	-0.021	0.073	-0.210	0.278	-0.285	-0.032
δP	-0.073	0.516	0.406	0.295	0.518	0.318	-0.074	0.506	0.175	-0.346
δH	-0.121	0.669	0.320	0.217	0.760	0.678	-0.376	0.192	0.297	-0.740

Note: Values in red are the significants, $p < 0.05$

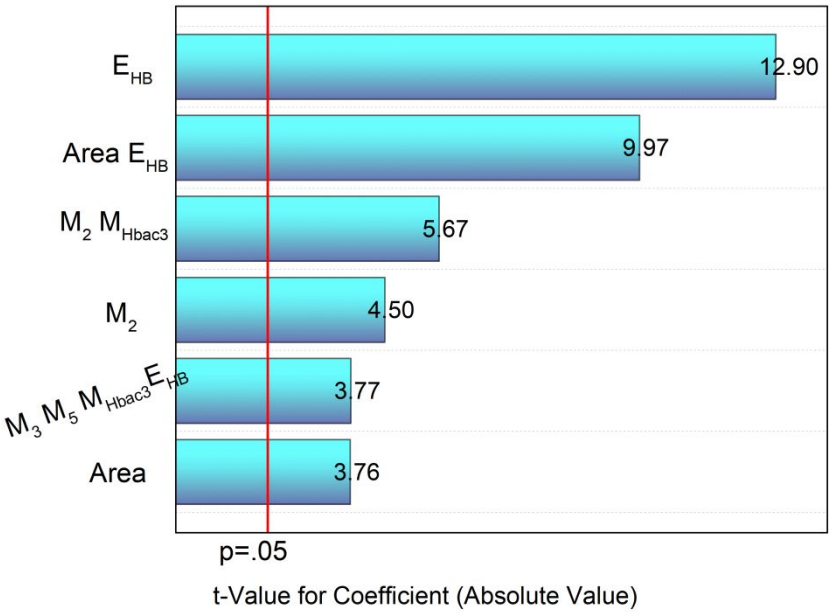

Figure S3. Pareto Chart of t-Values for the coefficients of δH model.

Table S5. HSP of different solutes predicted in this work in comparison to results estimate by the "Do it yourself (DIY) tool" and data from HSPiP database.

Source	Nicotine			Paracetamol			D-camphor			Caffeine		
	δD	δP	δH	δD	δP	δH	δD	δP	δH	δD	δP	δH
This work	18.1 2	5.2 3	5.7 7	19.1 9	9.46	20.7 9	18.7 4	4.31	4.3 1	19.0 9	13.1 9	12.4 5
*DIY tool ®	18.4 0	5.2 0	5.1 0	20.2 0	13.3 0	14.4 0	17.4 0	5.20	2.1 0	19.6 0	12.5 0	8.50
* HSPiP® database	18.5 0	7.8 0	6.5 0	17.8 0	10.5 0	13.9 0	17.8 0	10.3 0	5.2 0	19.5 0	10.1 0	13.0 0

* ® Steven Abbott and Hiroshi Yamamoto, 2008.

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