

Supplementary Material

A detailed listing of the prediction of vapor pressure (P^{vap}) at the normal boiling point (T_b) for all the 371 compounds considered in this study. These results are predicted using parameters listed in Table 2. The solvation energy components are also included. The 2nd column indicates the compound family: 1. alkane, 2. alcohol, 3. aldehyde, 4. ketone, 5. acid, 6. ester, 7. ether, 8. nitro compounds, 9. nitrile, 10. amine, 11. aromatic, 12. alkene, 13. alkyne, 14. F containing, 15. Cl containing, 16. multifunctional compounds.

id	type	Tb(K)	lnP ^{vap} (Pa)	$\Delta G^{cco}/RT$	$\Delta G^{dsp}/RT$	$\Delta G^{res}/RT$	$\Delta G^{cav}/RT$	ln(RT \bar{V})	$\Delta H^{vap}/RT$ (cal)	$\Delta H^{vap}/RT$ (exp)	name
1	1	231.1	12.25	-0.17	-8.22	0.26	3.32	17.05	8.37	9.76	propane
2	1	272.7	11.91	-0.17	-8.85	0.26	3.69	16.97	9.01	9.87	butane
3	1	309.2	11.76	-0.18	-9.35	0.27	4.13	16.90	9.37	10.04	pentane
4	1	341.9	11.47	-0.19	-9.83	0.28	4.38	16.83	9.91	10.11	hexane
5	1	371.6	11.30	-0.18	-10.28	0.28	4.72	16.76	10.28	10.30	heptane
6	1	398.8	11.16	-0.19	-10.66	0.29	5.03	16.69	10.57	10.46	octane
7	1	424.0	11.12	-0.22	-11.05	0.32	5.43	16.64	10.74	10.60	nonane
8	1	447.3	10.85	-0.22	-11.38	0.33	5.54	16.58	11.22	10.65	decane
9	1	469.1	10.87	-0.24	-11.64	0.35	5.88	16.52	11.24	10.83	undecane
10	1	489.5	10.61	-0.24	-11.97	0.35	6.00	16.47	11.73	10.91	dodecane
11	1	261.4	11.69	-0.21	-8.82	0.29	3.52	16.91	9.14	9.84	2-methylpropane
12	1	282.7	11.63	-0.27	-8.93	0.36	3.68	16.79	9.18	9.67	neopentane
13	1	301.0	11.47	-0.18	-9.38	0.27	3.89	16.87	9.65	9.91	2-methylbutane
14	1	322.9	11.51	-0.22	-9.38	0.30	4.02	16.78	9.53	9.84	2,2-dimethylbutane
15	1	331.1	11.19	-0.19	-9.81	0.28	4.10	16.81	10.12	9.94	2,3-dimethylbutane
16	1	354.0	11.56	-0.22	-9.67	0.30	4.39	16.75	9.57	9.84	2,2,3-trimethylbutane
17	1	333.4	11.30	-0.19	-9.79	0.28	4.21	16.80	10.03	10.05	2-methylpentane
18	1	336.4	11.30	-0.17	-9.84	0.27	4.22	16.82	10.04	10.10	3-methylpentane
19	1	363.2	11.18	-0.19	-10.21	0.29	4.56	16.73	10.33	10.18	2-methylhexane
20	1	365.0	11.20	-0.18	-10.33	0.28	4.68	16.76	10.34	10.23	3-methylhexane
21	1	352.3	11.27	-0.23	-9.89	0.32	4.35	16.72	10.03	10.02	2,2-dimethylpentane
22	1	362.9	11.17	-0.19	-10.29	0.28	4.59	16.77	10.31	10.09	2,3-dimethylpentane

23	1	353.6	10.87	-0.22	-10.33	0.31	4.40	16.72	10.66	10.07	2,4-dimethylpentane
24	1	359.2	11.48	-0.20	-9.74	0.29	4.37	16.75	9.73	9.95	3,3-dimethylpentane
25	1	392.1	11.02	-0.18	-10.76	0.28	4.98	16.70	10.72	10.37	3-methylheptane
26	1	372.4	10.92	-0.24	-10.38	0.32	4.56	16.65	10.58	9.95	2,2,4-trimethylpentane
27	1	386.6	10.93	-0.20	-10.60	0.29	4.73	16.71	10.68	10.14	2,3,4-trimethylpentane
28	1	383.0	11.36	-0.22	-10.15	0.31	4.71	16.70	9.99	10.04	2,2,3-trimethylpentane
29	1	415.6	10.81	-0.19	-11.09	0.30	5.17	16.63	11.12	10.48	4-methyloctane
30	1	240.4	12.61	-1.09	-7.90	1.20	3.11	17.29	8.17	9.97	cyclopropane
31	1	322.4	12.04	-0.14	-9.26	0.22	4.09	17.13	9.14	10.14	cyclopentane
32	1	353.9	11.79	-0.09	-9.76	0.18	4.42	17.04	9.55	10.16	cyclohexane
33	1	391.9	11.69	-0.10	-10.07	0.19	4.68	16.99	9.77	10.26	cycloheptane
34	1	424.3	11.61	-0.11	-10.43	0.20	5.01	16.94	9.94	10.29	cyclooctane
35	1	345.0	11.56	-0.16	-9.78	0.23	4.27	16.99	9.80	10.17	methylcyclopentane
36	1	374.1	11.23	-0.13	-10.14	0.22	4.38	16.91	10.28	10.05	methylcyclohexane
37	1	402.9	11.13	-0.15	-10.40	0.23	4.59	16.85	10.47	10.02	cis-1,2-dimethylcyclohexane
38	2	337.9	12.24	-5.80	-3.83	1.37	2.51	18.00	9.42	12.52	methanol
39	2	351.4	12.63	-5.23	-5.16	2.27	3.09	17.66	9.09	13.37	ethanol
40	2	370.4	12.33	-4.91	-6.31	2.53	3.58	17.44	9.61	13.53	1-propanol
41	2	390.8	12.08	-4.68	-7.23	2.73	3.98	17.27	10.03	13.25	1-butanol
42	2	411.0	11.83	-4.47	-8.07	2.83	4.40	17.14	10.45	12.94	1-pentanol
43	2	430.6	11.66	-4.31	-8.80	2.93	4.82	17.02	10.78	12.80	1-hexanol
44	2	449.5	11.40	-4.14	-9.37	2.97	5.02	16.92	11.10	12.65	1-heptanol
45	2	468.4	11.43	-4.00	-9.87	3.00	5.47	16.83	11.04	12.15	1-octanol
46	2	486.3	11.18	-3.87	-10.52	3.01	5.80	16.76	11.54	12.02	1-nonanol
47	2	504.1	11.04	-3.75	-10.88	3.02	5.97	16.68	11.67	11.91	1-decanol
48	2	537.0	10.80	-3.56	-11.63	3.02	6.42	16.55	12.04	11.43	1-dodecanol
49	2	355.4	12.29	-5.07	-6.35	2.80	3.52	17.39	9.47	13.33	2-propanol
50	2	380.8	12.40	-4.20	-7.25	2.68	3.92	17.25	9.36	13.22	2-methyl-1-propanol
51	2	372.7	12.47	-4.19	-7.40	2.89	3.96	17.22	9.08	13.21	2-butanol

52	2	384.7	12.03	-3.86	-8.31	2.82	4.29	17.09	9.72	12.93	3-methyl-2-butanol
53	2	375.2	11.51	-4.24	-8.60	2.90	4.39	17.06	10.69	12.69	tert-pentanol
54	2	401.9	12.26	-3.91	-8.07	2.75	4.35	17.13	9.55	13.27	2-methyl-1-butanol
55	2	404.4	11.70	-4.55	-8.00	2.77	4.36	17.13	10.60	13.12	3-methyl-1-butanol
56	2	392.2	11.86	-4.28	-8.24	2.95	4.35	17.09	10.14	13.07	2-pentanol
57	2	388.5	11.77	-4.16	-8.44	2.92	4.36	17.10	10.23	12.88	3-pentanol
58	2	421.2	11.87	-4.02	-8.88	2.94	4.82	17.01	10.23	12.56	2-methyl-1-pentanol
59	2	404.9	11.40	-4.02	-8.89	2.86	4.48	16.96	10.76	12.20	4-methyl-2-pentanol
60	2	394.1	11.73	-3.72	-8.92	2.87	4.55	16.97	10.10	11.56	3-methyl-3-pentanol
61	2	432.4	11.34	-4.01	-9.58	3.01	5.04	16.88	10.99	11.83	2-heptanol
62	2	434.0	11.88	-4.12	-8.83	2.83	4.80	17.20	10.33	12.60	cyclohexanol
335	2	568.8	10.63	-3.36	-12.22	3.00	6.78	16.43	12.29	11.04	1-tetradecanol
336	2	583.4	10.54	-3.30	-12.58	2.99	7.04	16.39	12.45	10.95	1-pentadecanol
337	2	597.2	10.48	-3.24	-12.83	3.00	7.22	16.34	12.57	10.84	1-hexadecanol
338	2	610.5	10.34	-3.18	-12.87	2.97	7.16	16.27	12.76	10.57	1-heptadecanol
339	2	355.6	12.11	-4.76	-7.08	3.07	3.72	17.17	9.47	13.19	tert-butanol
340	2	386.3	12.51	-3.67	-7.24	2.76	3.64	17.01	8.59	12.88	2,2-dimethyl-1-propanol
63	3	294.0	11.69	-8.42	-5.34	5.37	2.50	17.58	9.05	10.46	acetaldehyde
64	3	321.2	11.63	-7.26	-6.58	5.01	3.08	17.38	9.61	10.55	propanal
65	3	348.0	11.52	-6.67	-7.51	4.97	3.51	17.22	9.93	10.50	butyraldehyde
66	3	376.2	11.62	-6.23	-8.12	4.96	3.93	17.08	9.71	10.93	valeraldehyde
67	3	401.5	11.29	-5.83	-8.85	4.72	4.25	16.99	10.49	10.96	hexanal
68	3	426.0	11.30	-5.50	-9.30	4.59	4.62	16.89	10.55	10.97	heptanal
69	3	447.2	11.20	-5.27	-9.97	4.52	5.10	16.82	10.71	11.17	octanal
70	3	468.2	11.05	-5.06	-10.28	4.40	5.25	16.73	11.02	11.23	nonanal
71	4	329.4	11.54	-8.34	-6.12	5.69	2.93	17.38	9.35	10.80	acetone
72	4	352.8	11.48	-7.32	-7.17	5.32	3.44	17.22	9.75	10.75	2-butanone
73	4	375.5	11.38	-6.82	-7.97	5.19	3.90	17.08	10.07	10.75	2-pentanone
74	4	400.7	11.17	-6.49	-8.65	5.12	4.20	16.98	10.49	10.89	methylbutylketone
75	4	424.2	11.04	-6.13	-9.14	5.00	4.44	16.87	10.74	10.87	2-heptanone
76	4	446.2	10.91	-5.87	-9.63	4.87	4.74	16.79	10.99	10.99	2-octanone
77	4	467.2	10.79	-5.61	-10.17	4.75	5.09	16.72	11.27	11.12	2-nonanone

78	4	367.6	11.28	-6.66	-8.01	5.12	3.76	17.07	10.08	10.68	methylisopropylketone
79	4	389.2	11.09	-5.97	-8.62	4.72	4.02	16.94	10.48	10.68	4-methyl-2-pentanone
80	4	390.6	11.06	-6.35	-8.63	5.03	4.06	16.96	10.44	10.77	3-methyl-2-pentanone
81	4	379.5	11.22	-6.14	-8.31	4.80	3.94	16.94	10.01	10.57	3,3-dimethyl-2-butanone
82	4	418.0	10.92	-6.22	-9.10	5.01	4.37	16.87	10.84	11.06	5-methyl-2-hexanone
83	4	375.1	11.41	-6.37	-8.07	4.88	3.88	17.09	10.06	10.74	3-pentanone
84	4	396.7	11.28	-5.91	-8.77	4.69	4.30	16.97	10.35	10.80	3-hexanone
85	4	386.6	11.12	-5.76	-8.69	4.57	4.05	16.94	10.36	10.89	ethylisopropylketone
86	4	417.2	11.14	-5.55	-9.34	4.57	4.59	16.87	10.59	10.79	4-heptanone
87	4	461.6	10.88	-5.15	-10.32	4.37	5.27	16.72	11.10	11.05	5-nonanone
88	4	397.6	10.56	-5.38	-9.49	4.32	4.28	16.83	11.16	10.76	2,4-dimethyl-3-pentanone
89	4	441.4	10.36	-4.42	-10.47	3.76	4.81	16.68	11.74	10.78	diisobutylketone
90	4	403.8	11.89	-6.95	-7.58	5.39	3.70	17.32	9.30	10.85	cyclopentanone
91	4	428.6	11.44	-6.51	-8.26	5.00	4.01	17.21	9.91	10.69	cyclohexanone
92	5	391.1	11.20	-6.37	-4.85	1.95	2.74	17.74	10.80	7.36	aceticacid
93	5	414.3	11.64	-5.70	-5.67	2.46	3.05	17.50	10.32	9.12	propionicacid
94	5	436.4	11.75	-5.35	-6.48	2.68	3.56	17.33	10.31	9.92	butyricacid
95	5	459.0	11.63	-5.19	-7.15	2.96	3.82	17.19	10.54	11.04	valericacid
96	5	478.9	11.57	-4.98	-7.80	3.10	4.18	17.08	10.68	11.50	hexanoicacid
97	5	512.9	11.31	-4.69	-8.90	3.28	4.75	16.87	11.13	13.16	octanoicacid
98	5	427.7	11.42	-5.14	-8.68	2.80	5.13	17.31	11.23	9.67	isobutyricacid
99	5	450.2	11.64	-4.92	-7.06	2.74	3.71	17.17	10.38	12.45	2-methylbutanoicacid
341	5	543.2	11.20	-4.44	-9.99	3.36	5.54	16.73	11.41	13.00	decanoicacid
342	5	571.9	10.82	-4.28	-10.79	3.43	5.88	16.58	11.99	12.73	lauricacid
343	5	437.0	11.73	-4.79	-6.64	2.53	3.50	17.13	10.06	12.91	pivalicacid
100	6	304.9	11.76	-7.03	-6.18	4.63	2.84	17.51	9.54	11.10	methylformate

101	6	327.5	11.59	-6.63	-7.18	4.85	3.27	17.28	9.86	11.02	ethylformate
102	6	330.1	11.81	-6.79	-7.09	5.00	3.38	17.31	9.55	11.10	methylacetate
103	6	350.2	11.49	-6.45	-7.95	5.09	3.68	17.12	10.01	11.06	ethylacetate
104	6	374.7	11.39	-6.06	-8.62	4.97	4.10	17.00	10.23	10.94	propylacetate
105	6	399.3	11.24	-5.72	-9.19	4.84	4.42	16.90	10.52	11.08	butylacetate
106	6	421.2	10.98	-5.40	-9.82	4.69	4.70	16.82	11.00	10.99	pentylacetate
107	6	444.7	10.99	-5.21	-10.19	4.59	5.06	16.74	11.02	11.17	hexylacetate
108	6	465.6	10.91	-4.96	-10.50	4.46	5.26	16.66	11.18	11.32	heptylacetate
109	6	484.5	10.78	-4.79	-10.96	4.36	5.57	16.59	11.46	11.40	octylacetate
110	6	447.2	10.79	-4.85	-10.23	4.20	4.80	16.88	11.24	11.03	cyclohexylacetate
111	6	361.7	11.05	-5.92	-8.78	4.84	3.94	16.97	10.62	10.90	isopropylacetate
112	6	389.8	11.03	-5.61	-9.30	4.78	4.27	16.89	10.75	10.97	isobutylacetate
113	6	415.2	10.99	-5.46	-9.74	4.72	4.66	16.80	10.92	10.65	isopentylacetate
114	6	352.6	11.66	-5.99	-8.02	4.70	3.82	17.15	9.97	11.09	methylpropionate
115	6	372.3	11.44	-5.66	-8.71	4.70	4.13	17.00	10.23	10.88	ethylpropionate
116	6	395.7	11.25	-5.30	-9.34	4.52	4.47	16.90	10.55	10.78	propylpropionate
117	6	375.9	11.57	-5.57	-8.70	4.58	4.23	17.02	10.14	11.00	methylbutyrate
118	6	394.7	11.11	-5.34	-9.40	4.56	4.39	16.90	10.77	11.00	ethylbutyrate
119	6	459.7	10.83	-4.61	-10.77	4.16	5.39	16.66	11.33	11.39	butylvalerate
120	6	365.5	11.35								2-
											methylpropanoicacid
121	7	248.3	12.55	-5.34	-8.75	4.42	4.03	16.99	10.32	10.92	methylester
122	7	307.6	11.98	-5.30	-6.83	4.27	3.11	17.30	8.21	10.32	dimethylether
123	7	363.2	11.44	-3.66	-8.71	3.36	3.99	17.00	9.30	10.47	diethylether
124	7	414.2	11.14	-3.10	-9.90	3.00	4.63	16.81	10.19	10.49	dipropylether
125	7	332.2	11.51	-2.83	-10.77	2.80	5.27	16.67	10.80	10.72	dibutylether
126	7	331.7	11.64	-3.56	-9.33	3.30	4.19	16.90	9.95	10.21	methylsec-butylether
127	7	328.4	11.85	-2.91	-9.29	2.74	4.19	16.89	9.75	10.19	methylisobutylether
128	7	359.5	11.66	-3.57	-8.78	3.26	4.03	16.90	9.30	10.23	methyltert-butylether
129	7	326.2	11.37	-3.12	-9.34	2.94	4.34	16.84	9.64	10.25	methyltert-amylether
130	7	312.2	11.99	-3.21	-9.39	2.98	4.12	16.86	10.11	10.44	ethylisopropylether
131	7	337.0	11.60	-3.81	-8.63	3.46	3.93	17.02	9.26	10.38	methylpropylether
				-3.27	-9.27	3.11	4.15	16.89	9.86	9.85	ethylpropylether

132	7	343.3	11.75	-3.54	-9.23	3.30	4.29	16.93	9.70	10.44	methylbutylether
133	7	365.4	11.45	-3.01	-9.83	2.93	4.55	16.81	10.18	10.40	ethylbutylether
134	7	341.5	10.70	-3.04	-10.04	2.87	4.17	16.74	11.03	10.26	diisopropylether
135	7	283.6	12.76	-6.23	-6.10	4.51	2.90	17.68	8.06	10.95	ethyleneoxide
136	7	339.1	12.38	-4.39	-8.15	3.79	3.83	17.30	8.80	10.58	tetrahydrofuran
138	8	374.4	10.77	-8.88	-4.47	3.93	2.42	17.77	10.60	11.17	nitromethane
139	8	387.2	11.19	-8.11	-5.57	4.50	2.87	17.50	10.12	11.28	nitroethane
140	8	404.3	11.27	-7.63	-6.50	4.75	3.35	17.31	9.92	11.18	1-nitropropane
141	8	425.9	11.14	-7.20	-7.25	4.78	3.65	17.16	10.19	10.91	1-nitrobutane
142	8	393.4	11.16	-7.44	-6.57	4.66	3.22	17.29	10.09	10.95	2-nitropropane
137	9	298.9	10.22	-8.78	-3.05	2.89	1.21	17.95	10.27	10.84	hydrogencyanide
143	9	354.8	11.56	-9.41	-4.22	5.33	2.11	17.75	8.58	10.23	acetonitrile
144	9	370.5	11.55	-8.54	-5.36	5.35	2.61	17.48	9.07	10.23	propionitrile
145	9	390.8	11.40	-8.05	-6.34	5.42	3.07	17.30	9.45	10.63	butyronitrile
146	9	414.5	11.29	-7.61	-7.12	5.35	3.51	17.17	9.81	10.83	valeronitrile
147	9	436.8	11.17	-7.21	-7.78	5.25	3.86	17.05	10.11	10.47	n-hexanoicacidnitrile
148	9	376.8	11.25	-8.10	-6.32	5.42	3.00	17.25	9.48	10.83	isobutyronitrile
149	10	239.7	10.70	-8.12	-3.37	1.51	2.47	18.20	9.67	11.70	ammonia
150	10	266.8	12.43	-5.90	-5.20	2.74	3.08	17.72	8.79	11.76	methylamine
151	10	289.7	11.97	-5.48	-6.52	3.13	3.42	17.42	9.61	11.36	ethylamine
152	10	321.0	11.91	-4.95	-7.47	3.23	3.85	17.25	9.96	11.06	propylamine
153	10	350.6	11.73	-4.54	-8.24	3.21	4.18	17.12	10.34	10.92	butylamine
154	10	377.7	11.65	-4.27	-8.89	3.24	4.55	17.01	10.53	11.03	1-aminopentane
155	10	405.9	11.56	-3.98	-9.40	3.17	4.84	16.92	10.72	11.03	hexylamine
156	10	430.1	11.48	-3.78	-9.89	3.16	5.15	16.84	10.84	11.03	heptylamine
157	10	280.0	12.96	-4.17	-6.56	3.03	3.30	17.36	8.30	11.43	dimethylamine
158	10	328.6	12.42	-3.04	-8.60	2.94	4.09	17.04	8.85	10.63	diethylamine
159	10	382.0	11.82	-2.65	-9.82	2.66	4.78	16.84	9.80	11.08	dipropylamine
160	10	432.0	11.41	-2.39	-10.67	2.47	5.30	16.70	10.48	11.06	dibutylamine
161	10	276.0	12.62	-2.98	-7.95	3.05	3.46	17.05	8.09	10.08	trimethylamine
162	10	361.9	11.34	-1.81	-10.01	1.97	4.39	16.80	10.18	10.25	triethylamine
163	10	429.7	10.28	-0.32	-11.34	0.39	4.96	16.59	11.83	10.14	tripropylamine
164	10	304.9	12.03	-4.59	-7.54	3.35	3.63	17.18	9.56	11.07	isopropylamine

191	11	435.2	11.47	-1.84	-9.55	1.84	4.13	16.90	10.11	10.65	1-ethyl-4-methylbenzene
192	11	456.6	11.08	-1.78	-10.27	1.78	4.48	16.86	10.77	10.60	1,2-diethylbenzene
344	11	470.0	11.71	-1.67	-9.68	1.72	4.46	16.88	9.77	10.84	1,2,4,5-tetramethylbenzene
345	11	504.6	11.80	-1.56	-9.83	1.62	4.72	16.85	9.63	10.97	pentamethylbenzene
193	12	225.5	12.33	-1.61	-7.69	1.65	2.86	17.12	8.34	9.84	propylene
194	12	266.9	11.98	-1.30	-8.48	1.40	3.33	17.03	8.96	9.97	1-butene
195	12	303.1	11.73	-1.20	-9.02	1.30	3.72	16.94	9.43	10.05	1-pentene
196	12	336.6	11.49	-1.12	-9.50	1.24	4.01	16.86	9.89	10.16	1-hexene
197	12	366.8	11.31	-1.06	-9.97	1.18	4.37	16.79	10.25	10.27	1-heptene
198	12	394.4	11.18	-1.00	-10.40	1.14	4.72	16.72	10.56	10.44	1-octene
199	12	420.0	11.06	-0.95	-10.80	1.09	5.06	16.66	10.84	10.52	1-nonene
200	12	293.2	11.50	-1.13	-9.06	1.24	3.55	16.90	9.62	9.92	3-methyl-1-butene
201	12	327.0	11.28	-0.97	-9.52	1.09	3.85	16.83	10.02	10.08	4-methyl-1-pentene
202	13	249.9	12.18	-4.31	-6.54	3.04	2.63	17.37	9.18	10.63	propyne
203	13	281.2	11.97	-3.65	-7.61	2.97	3.07	17.18	9.35	10.61	1-butyne
204	13	313.3	11.73	-3.36	-8.41	2.92	3.52	17.06	9.78	10.48	1-pentyne
205	13	344.5	11.55	-3.12	-9.07	2.84	3.94	16.96	10.04	10.81	1-hexyne
206	13	372.9	11.37	-2.91	-9.58	2.73	4.26	16.87	10.34	10.54	1-heptyne
207	13	399.4	11.22	-2.75	-9.99	2.62	4.55	16.79	10.61	10.69	1-octyne
208	13	423.9	11.10	-2.61	-10.45	2.53	4.91	16.72	10.87	10.99	1-nonyne
209	14	194.8	11.57	-6.60	-5.02	3.31	2.32	17.55	9.03	10.72	methylfluoride[R41]
210	14	235.5	11.67	-5.55	-6.43	3.50	2.83	17.32	9.16	10.26	fluoroethane[R161]
235	14	267.2	11.94	-2.45	-7.95	2.70	2.94	16.70	8.88	10.45	perfluorocyclobutane
236	14	221.5	10.71	-7.22	-4.88	2.95	2.28	17.57	10.76	10.92	difluoromethane[R32]
237	14	191.1	11.35	-6.23	-5.61	3.76	2.13	17.30	9.18	10.52	fluoroform[R23]
211	15	248.9	11.76	-4.68	-5.89	2.71	2.09	17.54	9.42	10.40	methylchloride
212	15	285.4	11.66	-4.25	-6.96	2.93	2.60	17.32	9.57	10.42	ethylchloride
213	15	319.7	11.54	-3.76	-7.82	2.84	3.08	17.19	9.70	10.23	1-chloropropane
214	15	351.6	11.40	-3.45	-8.46	2.75	3.48	17.07	9.97	10.46	butylchloride
215	15	381.5	11.27	-3.19	-9.00	2.65	3.85	16.97	10.22	10.39	1-chloropentane

241	16	243.4	11.72	-1.16	-7.27	1.31	1.81	17.03	8.56	10.05	dichlorodifluoromethane[R12]
242	16	320.8	11.56	-1.16	-7.67	1.27	2.24	16.88	8.89	10.17	1,1,2-trichloro-1,2,2-trifluoroethane[R113]
243	16	276.2	11.60								1,1-dichlorotetrafluoroethane[R114a]
244	16	276.9	11.71	-1.14	-7.58	1.24	2.24	16.84	8.75	10.04	1,2-dichlorotetrafluoroethane[R114]
245	16	234.0	12.07	-1.05	-7.49	1.20	2.22	16.83	8.56	10.01	chloropentafluoroethane[R115]
246	16	357.9	11.58	-0.92	-7.23	1.16	2.28	16.78	8.01	9.94	fluorobenzene
247	16	353.4	10.49	-2.84	-8.32	2.31	3.24	17.19	9.77	10.54	hexafluorobenzene
248	16	404.9	11.55	-4.80	-8.43	3.67	3.09	16.97	11.45	10.80	chlorobenzene
249	16	452.6	11.31	-2.38	-8.46	2.12	3.08	17.20	9.81	10.52	benzylchloride
250	16	318.3	11.57	-3.83	-8.68	3.14	3.54	17.14	10.54	10.78	3-chloro-1-propene
251	16	453.6	11.14	-4.24	-7.32	3.09	2.78	17.26	9.87	10.98	o-dichlorobenzene
252	16	446.2	11.42	-2.69	-8.45	2.23	2.88	17.17	10.30	10.59	m-dichlorobenzene
253	16	486.2	11.19	-2.11	-8.48	1.97	2.90	17.13	9.96	10.51	1,2,4-trichlorobenzene
254	16	532.5	11.61	-2.03	-8.71	1.95	2.87	17.11	10.35	10.91	1-chloronaphthalene
255	16	268.7	12.13	-2.14	-8.89	2.03	3.54	17.06	9.91	11.15	1,3-butadiene
256	16	299.1	11.86	-2.18	-7.72	2.08	2.83	17.11	8.77	10.08	1,4-pentadiene
257	16	332.6	11.69	-1.74	-8.59	1.87	3.35	16.99	9.37	9.85	1,5-hexadiene
258	16	470.5	12.67	-1.72	-9.19	1.86	3.83	16.91	9.65	9.92	1,2-ethanediol
259	16	487.6	11.52	-6.18	-5.04	2.01	3.95	17.93	9.89	13.59	1,3-propanediol
260	16	501.2	12.05	-7.71	-5.93	2.98	4.48	17.70	11.64	14.37	1,4-butanediol
261	16	413.6	10.85	-6.74	-6.68	3.29	4.68	17.50	10.50	15.11	2,4-pentanedione
262	16	452.5	10.22	-8.17	-7.57	5.74	3.66	17.20	11.26	10.44	dimethylmalonate
263	16	469.4	11.36	-10.43	-8.02	7.32	4.22	17.13	11.96	12.80	dimethylsuccinate
264	16	315.0	10.31	-7.22	-8.69	5.70	4.56	17.01	10.94	12.09	dimethoxymethane
265	16	357.8	12.30	-10.08	-7.95	7.28	3.89	17.17	11.39	10.83	1,2-dimethoxyethane
				-4.87	-8.36	4.24	4.21	17.08	9.28	10.97	

266	16	252.0	10.26	-6.35	-5.74	3.18	1.70	17.46	11.43	11.16	cyanogen
267	16	559.2	9.99	-11.18	-5.47	6.14	3.06	17.45	11.73	11.15	glutaronitrile
268	16	568.2	10.36	-11.00	-6.12	6.76	3.43	17.29	11.00	11.84	adipodinitrile
269	16	390.4	11.75	-7.60	-6.25	3.85	4.16	17.59	10.33	12.23	ethylenediamine
270	16	410.2	11.29	-7.67	-6.95	4.25	4.30	17.36	10.56	12.26	1,3-diaminopropane
271	16	537.4	10.84	-3.12	-10.34	3.02	4.41	16.87	11.50	10.97	diphenylmethane
272	16	477.9	11.22	-5.64	-8.04	3.57	4.04	17.30	11.55	12.34	benzylalcohol
273	16	492.1	11.55	-4.60	-8.75	3.37	4.36	17.16	10.96	12.45	2-phenylethanol
274	16	508.2	11.06	-5.13	-9.04	3.78	4.44	17.02	11.55	13.03	3-phenyl-1-propanol
275	16	397.5	13.07	-5.48	-6.69	3.80	4.01	17.44	8.37	11.74	2-methoxy-ethanol
276	16	444.5	11.62	-5.11	-9.05	3.85	4.95	16.99	10.92	11.74	2-butoxy-ethanol
277	16	494.2	10.83	-7.86	-4.98	2.85	3.10	17.73	11.20	13.11	ethylenecyanohydrin
278	16	443.2	11.89	-7.27	-5.49	2.76	4.09	17.80	10.53	13.52	ethanolamine
279	16	460.7	12.01	-6.98	-6.14	3.43	4.16	17.54	9.84	14.41	3-amino-1-propanol
280	16	370.2	12.33	-5.57	-5.86	3.06	3.18	17.53	9.52	12.96	allyl alcohol
281	16	386.8	10.20	-7.76	-5.34	2.70	2.91	17.69	12.63	13.16	2-propyn-1-ol
282	16	401.8	12.12	-5.20	-6.10	2.75	3.06	17.61	10.09	12.47	2-chloroethanol
283	16	434.2	11.13	-6.63	-6.82	3.60	3.53	17.45	11.57	13.16	3-chloro-1-propanol
284	16	426.7	11.92	-3.52	-8.70	3.04	3.95	17.16	9.79	11.08	anisole
285	16	443.2	11.58	-3.30	-9.26	3.03	4.10	17.02	10.18	11.14	ethoxybenzene
286	16	374.5	12.06	-5.33	-8.18	4.28	3.96	17.32	9.80	11.04	1,4-dioxane
287	16	304.5	11.83	-3.17	-7.81	2.61	2.85	17.35	9.66	10.74	furan
288	16	434.9	11.57	-6.59	-6.94	4.62	3.04	17.44	10.01	11.53	furfural
289	16	475.3	11.43	-5.70	-8.31	4.41	3.87	17.16	10.27	11.16	acetophenone
290	16	414.2	11.44	-5.75	-5.27	2.24	2.64	17.58	10.49	8.24	acrylic acid
291	16	451.9	11.31	-5.76	-7.91	4.33	3.38	17.27	10.32	11.03	benzaldehyde
292	16	325.8	11.76	-7.14	-5.95	4.77	2.59	17.48	9.25	10.56	acrolein
293	16	487.2	11.12	-5.57	-9.24	4.74	4.25	16.95	11.04	11.37	benzylacetate
294	16	345.7	11.53	-5.42	-7.53	4.03	3.26	17.18	10.14	10.98	vinylacetate
295	16	377.2	11.43	-5.95	-8.20	4.81	3.70	17.07	10.34	10.70	allylacetate
296	16	484.0	11.13	-6.50	-7.40	4.37	3.36	17.30	10.33	10.95	nitrobenzene
297	16	464.2	11.13	-6.54	-7.27	4.53	3.15	17.27	10.15	10.79	benzonitrile
298	16	506.7	10.94	-7.01	-7.72	4.93	3.54	17.21	10.90	11.37	benzylcyanide

299	16	350.5	11.07	-8.48	-5.15	5.01	2.17	17.52	9.64	10.68	acrylonitrile
300	16	391.7	11.02	-7.84	-5.93	4.71	2.70	17.38	10.44	10.86	allyl cyanide
301	16	457.2	12.56	-4.44	-7.54	3.35	3.81	17.39	9.11	11.65	aniline
302	16	457.7	11.87	-4.35	-8.45	3.46	4.02	17.20	10.24	11.52	alpha-aminotoluene
303	16	326.5	12.12	-5.02	-6.90	3.16	3.52	17.36	9.75	11.30	3-amino-1-propene
304	16	418.3	11.94	-2.33	-8.83	2.31	3.71	17.08	9.54	10.66	styrene
305	16	416.0	11.84	-2.96	-8.46	2.70	3.44	17.12	9.71	10.33	phenylacetylene
306	16	444.8	11.88	-2.29	-9.20	2.27	4.11	17.00	9.65	10.67	3-methylstyrene
307	16	445.9	11.91	-2.31	-8.99	2.28	3.95	16.98	9.57	10.65	p-methylstyrene
308	16	388.4	12.03	-5.08	-7.43	3.95	3.19	17.39	9.35	10.91	pyridine
309	16	481.2	11.79	-8.75	-5.83	5.82	2.89	17.66	9.49	10.93	pyridazine
310	16	396.9	11.86	-6.17	-6.93	4.41	3.06	17.49	9.84	13.27	pyrimidine
311	16	510.3	11.90	-4.23	-8.54	3.57	3.89	17.21	9.79	11.03	quinoline
312	16	403.0	12.74	-4.81	-6.46	3.29	3.14	17.58	8.86	11.67	pyrrole
313	16	401.2	12.17	-5.09	-8.00	3.70	4.22	17.35	9.97	11.42	morpholine
314	16	517.8	11.99	-2.08	-9.32	2.10	4.24	17.05	9.55	10.80	1-methylnaphthalene
315	16	531.5	11.57	-2.03	-10.00	2.06	4.58	16.96	10.22	11.03	1-ethylnaphthalene
316	16	451.1	11.80	-1.80	-9.46	1.83	4.17	17.07	9.74	10.54	indane
317	16	375.2	10.70								1',1',1'-
318	16	432.3	11.66	-3.50	-8.63	2.51	3.37	16.95	10.70	10.49	trifluorotoluene
319	16	435.7	11.44	-2.07	-8.78	1.94	3.47	17.10	9.72	10.67	o-chlorotoluene
320	16	472.7	11.44	-2.44	-8.66	2.08	3.37	17.08	9.93	10.75	p-chlorotoluene
321	16	495.6	11.16	-4.66	-8.79	3.91	3.91	17.07	10.46	11.16	methylbenzoate
322	16	505.0	11.25	-6.11	-7.82	4.33	3.60	17.16	10.24	11.30	o-nitrotoluene
323	16	473.5	12.51	-6.27	-7.77	4.42	3.69	17.18	10.09	11.22	m-nitrotoluene
324	16	475.4	12.19	-4.04	-8.03	3.23	4.09	17.24	8.98	11.45	o-methylaniline
325	16	482.0	12.26	-4.18	-7.86	2.94	4.00	17.29	9.84	12.20	3-methylphenol
326	16	501.7	11.99	-3.54	-7.84	2.90	3.46	17.28	9.16	11.60	o-chloroaniline
327	16	469.0	12.41	-4.60	-7.29	3.33	3.27	17.28	9.41	11.06	m-chloroaniline
328	16	466.7	11.79	-3.83	-8.27	3.11	4.18	17.23	9.11	11.62	n-methylaniline
329	16	447.5	9.87	-3.48	-9.01	2.93	4.29	17.07	9.79	11.00	n,n-dimethylaniline
330	16	402.6	12.01	-6.00	-8.38	3.67	3.33	17.26	12.97	10.79	o-chlorophenol
	16			-4.52	-8.09	3.78	3.63	17.22	9.46	10.91	2-methylpyridine

331	16	417.3	12.10	-5.00	-7.87	4.09	3.62	17.26	9.23	10.88	3-methylpyridine
332	16	418.5	11.93	-5.21	-7.87	4.25	3.50	17.26	9.45	10.87	4-methylpyridine
333	16	373.2	10.29	-6.46	-2.32	-2.15	2.30	18.92	11.35	13.16	water
334	16	425.0	9.27	-8.62	-4.12	2.23	2.17	17.61	12.24	12.28	aminiacetonitrile
346	16	447.2	11.44	-2.14	-8.48	2.04	2.88	17.14	9.95	10.69	p-dichlorobenzene
347	16	491.8	11.02								1,2,3-
348	16	481.6	11.34	-2.57	-8.59	2.20	2.86	17.12	10.57	11.28	trichlorobenzene
349	16	491.5	9.82	-1.31	-8.75	1.52	2.79	17.09	10.12	10.79	trichlorobenzene
350	16	540.2	11.15	-10.04	-4.37	4.12	2.33	17.79	12.56	12.03	malonicacidnitrile
351	16	528.2	11.58	-9.32	-4.84	4.99	2.70	17.62	10.55	12.14	1,2-dicyanoethane
352	16	553.7	10.68	-2.28	-9.90	2.30	4.47	17.00	10.31	11.09	biphenyl
353	16	455.0	11.89	-2.62	-10.84	2.64	4.71	16.79	11.77	11.06	1,2-diphenylethane
354	16	530.0	11.38	-4.36	-7.44	2.67	3.59	17.43	10.42	12.29	phenol
355	16	462.5	10.46	-7.51	-6.75	4.13	4.11	17.40	11.19	13.40	levulinicacid
356	16	491.1	11.91	-7.19	-5.35	2.72	2.58	17.69	12.23	12.94	chloroaceticacid
357	16	389.2	12.47	-2.32	-9.17	2.35	3.93	17.13	9.72	10.57	naphthalene
358	16	516.4	11.94	-5.20	-7.09	4.16	3.11	17.48	8.96	10.62	pyrazine
359	16	514.3	11.95	-4.38	-8.46	3.70	3.86	17.23	9.66	11.03	isoquinoline
360	16	511.7	12.11	-2.16	-9.29	2.15	4.22	17.03	9.59	10.76	2-methylnaphthalene
361	16	473.6	12.51	-5.48	-7.42	4.24	3.58	17.18	8.95	10.91	p-nitrotoluene
362	16	464.2	12.41	-4.00	-7.98	3.25	4.01	17.23	8.97	11.62	p-methylaniline
363	16	475.1	11.88	-3.88	-8.16	3.02	4.14	17.28	9.45	12.00	2-methylphenol
364	16	503.7	11.76	-4.25	-7.95	2.80	3.99	17.29	10.41	12.24	4-methylphenol
365	16	558.0	9.84	-4.80	-7.52	3.42	3.35	17.31	9.83	11.63	p-chloroaniline
366	16	487.0	11.80	-7.39	-5.93	3.33	2.67	17.16	12.16	13.12	2-nitroaniline
367	16	493.1	11.56	-4.19	-7.55	2.97	3.25	17.31	10.09	11.32	m-chlorophenol
368	16	478.2	11.80	-4.28	-7.64	2.80	3.33	17.35	10.69	11.48	p-chlorophenol
369	16	474.2	11.04	-4.49	-8.39	3.31	4.14	17.23	10.13	12.65	guaiacol
370	16	494.3	9.70	-7.52	-7.04	5.13	3.09	17.37	10.71	11.54	3-cyanopyridine
371	16	514.0	10.01	-8.81	-4.29	1.78	3.08	17.93	12.62	12.70	acetamide
				-8.28	-4.41	2.35	2.66	17.69	12.13	12.57	acrylamide