

Table S1. List of compounds collected from the DIPPR database and used to develop the QSPR models for critical temperature, critical pressure and acentric factor.

	Compound name
1	1,1,1,2,3,3-hexafluoropropane
2	1,1,1,2-tetrafluoroethane
3	1,1,1-trichloroethane ⁽³⁾
4	1,1,1-trifluoroethane ⁽³⁾
5	1,1,2-trichlorotrifluoroethane
6	1,1-dichloro-1-fluoroethane ⁽³⁾
7	1,1-dichloroethane ⁽²⁾
8	1,1-difluoroethane ⁽²⁾
9	1,1-difluoroethylene ⁽²⁾
10	1,2,3-trimethylbenzene ^{(2) (3)}
11	1,2,4,5-tetramethylbenzene ⁽³⁾
12	1,2,4-trimethylbenzene ⁽³⁾
13	1,2-dibromotetrafluoroethane
14	1,2-dichlorotetrafluoroethane ⁽³⁾
15	1,2-dimethoxyethane ^{(2) (3)}
16	1,3-butadiene ⁽¹⁾
17	1,4-dioxane ⁽³⁾
18	1,6-hexane diamine
19	1-butanol ^{(2) (3)}
20	1-butene ⁽¹⁾
21	1-chloro-1,1-difluoroethane ^{(2) (3)}
22	1-decanol
23	1-dodecanol
24	1-heptanol
25	1-heptene ⁽¹⁾
26	1-hexanol ^{(2) (3)}
27	1-hexene ⁽¹⁾
28	1-methyl-2-pyrrolidinone
29	1-methylnaphthalene
30	1-nonanol ⁽³⁾
31	1-nonene ⁽¹⁾
32	1-octanol ⁽²⁾
33	1-octene ⁽¹⁾
34	1-pentanamine ⁽³⁾
35	1-pentanol
36	1-pentene ⁽¹⁾
37	1-propanol
38	2-(2-butoxyethoxy) ethanol ⁽³⁾
39	2,2,3,3-tetramethylhexane ⁽¹⁾
40	2,2,3,3-tetramethylpentane ⁽¹⁾
41	2,2,3,4-tetramethylpentane ⁽¹⁾
42	2,2,3-trimethylbutane ⁽¹⁾
43	2,2,3-trimethylpentane ⁽¹⁾
44	2,2,4,4-tetramethylpentane ⁽¹⁾
45	2,2,4-trimethylpentane ⁽¹⁾
46	2,2,5,5-tetramethylhexane ⁽¹⁾
47	2,2-dichloro-1,1,1-trifluoroethane ⁽³⁾
48	2,2-dimethylbutane ⁽¹⁾
49	2,2-dimethylheptane ⁽¹⁾
50	2,2-dimethylhexane ⁽¹⁾

51	2,2-dimethylpentane ⁽¹⁾
52	2,3,3,4-tetramethylpentane ⁽¹⁾
53	2,3,3-trimethylpentane ⁽¹⁾
54	2,3,4-trimethylpentane ⁽¹⁾
55	2,3-dimethylbutane ⁽¹⁾
56	2,3-dimethylhexane ⁽¹⁾
57	2,3-dimethylpentane ⁽¹⁾
58	2,4-dimethylhexane ⁽¹⁾
59	2,4-dimethylpentane ⁽¹⁾
60	2,5-dimethylhexane ⁽¹⁾
61	2-butanol ^{(2) (3)}
62	2-butoxyethanol ⁽²⁾
63	2-chloro-1,1,1,2-tetrafluoroethane
64	2-ethoxyethylacetate ⁽²⁾
65	2-heptanol ⁽²⁾
66	2-heptanone
67	2-hexanol ⁽²⁾
68	2-hexanone ⁽³⁾
69	2-methyl 1-butene ⁽¹⁾
70	2-methyl 1-pentanol
71	2-methyl 3-ethylpentane ⁽¹⁾
72	2-methyl-1-butanol
73	2-methyl-1-propanol ^{(2) (3)}
74	2-methyl-2-butanol ⁽²⁾
75	2-methyl-2-propanol ⁽²⁾
76	2-methyleptane ⁽¹⁾
77	2-methylhexane ⁽¹⁾
78	2-methylnaphthalene ^{(2) (3)}
79	2-methyloctane ⁽¹⁾
80	2-methylpentane ⁽¹⁾
81	2-methylpyridine ⁽²⁾
82	2-nonanol ⁽³⁾
83	2-octanol ^{(2) (3)}
84	2-pentanol ^{(2) (3)}
85	2-pentanone ⁽³⁾
86	2-propanol, 1,1'-iminobis ^{(2) (3)}
87	3,3,5-trimethylheptane ⁽¹⁾
88	3,3-dimethylhexane ⁽¹⁾
89	3,3-dimethylpentane ⁽¹⁾
90	3,4-dimethylhexane ⁽¹⁾
91	3-ethylhexane ⁽¹⁾
92	3-ethylpentane ⁽¹⁾
93	3-hexanone
94	3-methyl 1-butanol ⁽³⁾
95	3-methyl 1-butene ⁽¹⁾
96	3-methyl 1-pentanol ^{(2) (3)}
97	3-methyl 2-butanol
98	3-methyl 3-ethylpentane ⁽¹⁾
99	3-methyleptane ⁽¹⁾
100	3-methylhexane ⁽¹⁾
101	3-methylpentane ⁽¹⁾
102	3-pentanone ⁽³⁾
103	4-methyleptane ⁽¹⁾
104	5-nonanone ⁽³⁾
105	acetal ⁽³⁾
106	acetamide

107	acetic acid
108	acetone
109	acetonitrile ^{(2) (3)}
110	acetophenone ⁽²⁾
111	anisole
112	benzenamine,3-methyl-
113	benzene
114	benzene, penthyl- ⁽²⁾
115	benzene,1-ethyl-3methyl-
116	biphenyl ⁽³⁾
117	bromobenzene ⁽³⁾
118	bromoethane
119	bromotrifluoromethane ^{(2) (3)}
120	butanal
121	carbon tetrafluoride ⁽³⁾
122	chlorodifluoromethane ⁽³⁾
123	chloropentafluoroethane
124	chlorotrifluoromethane ^{(2) (3)}
125	chlorotrimethylsilane ^{(2) (3)}
126	cis 2-butene ⁽¹⁾
127	cis 2-pentene ⁽¹⁾
128	cumene ⁽³⁾
129	cyclobutane ⁽¹⁾
130	cyclohexane,1,1-dimethyl- ⁽¹⁾
131	cyclohexane,1,3-dimethyl-,cis- ⁽¹⁾
132	cyclohexane,1,3-dimethyl-,trans ⁽¹⁾
133	cyclohexane,1,4-dimethyl-,cis- ⁽¹⁾
134	cyclohexane,ethyl- ⁽¹⁾
135	cyclohexane,propyl- ⁽¹⁾
136	cyclohexene,1,2-dimethyl-,cis- ⁽¹⁾
137	cyclohexene,1,2-dimethyl-,trans- ⁽¹⁾
138	cycloheptane ⁽¹⁾
139	cyclohexane ⁽¹⁾
140	cyclohexanol
141	cyclooctane ⁽¹⁾
142	cyclopentane ⁽¹⁾
143	cyclopentane,1,1-dimethyl- ⁽¹⁾
144	cyclopentane,1,2-dimethyl-,cis- ⁽¹⁾
145	cyclopentane,1,2-dimethyl-,trans ⁽¹⁾
146	cyclopentane,1,3-dimethyl-,cis- ⁽¹⁾
147	cyclopentane,1,3-dimethyl-,trans- ⁽¹⁾
148	cyclopentene ⁽¹⁾
149	cyclopropane ⁽¹⁾
150	decafluorobutane ⁽²⁾
151	decanal ⁽²⁾
152	dibenzothiophene ⁽²⁾
153	dichlorodifluoromethane ⁽²⁾
154	dichlorodimethylsilane ^{(2) (3)}
155	dichlorofluoromethane
156	dichloromethane
157	diethylamine ⁽²⁾
158	diethylene glycol monopropylether ⁽²⁾
159	diethylether ⁽²⁾
160	difluoromethane ⁽³⁾
161	diisopropylamine ^{(2) (3)}
162	diisopropylether ⁽²⁾

163	dimethylether
164	di-n-butylamine ⁽³⁾
165	di-n-octylamine ⁽²⁾
166	di-n-propylether
167	ethane,2-(difluoromethoxy)-1,1,1-trifluoro- ⁽³⁾
168	ethanethioic acid, s-ethyl ester ⁽²⁾
169	ethanol ⁽³⁾
170	ethene, 2-chloro-1,1-difluoroethene ⁽²⁾
171	ether, bis(difloromethyl) ⁽²⁾
172	ethyl acetate ^{(2) (3)}
173	ethyl chloride ⁽²⁾
174	ethyl fluoride ⁽²⁾
175	ethyl formate
176	ethyl propionate
177	ethyl-3-ethoxypropionate
178	ethylamine
179	ethylbenzene ⁽³⁾
180	ethylcyclopentane ⁽¹⁾
181	ethylene ⁽¹⁾
182	ethylene glycol monopropyl ether ^{(2) (3)}
183	ethyne ^{(2) (3)}
184	fluorobenzene
185	formic acid,propilester
186	furan ⁽³⁾
187	heptanal ^{(2) (3)}
188	hexafluorobenzene ⁽²⁾
189	hexafluoroethane
190	hexanal ^{(2) (3)}
191	hexane,2,2,5-trimethyl- ⁽¹⁾
192	hydrazine ⁽³⁾
193	indane
194	iodobenzene ^{(2) (3)}
195	isobutane ⁽¹⁾
196	isobutylacetate ⁽³⁾
197	isobutylbenzene
198	isobutyric acid ^{(2) (3)}
199	isopentane ⁽¹⁾
200	isopropanol ⁽³⁾
201	isopropyl acetate ⁽²⁾
202	isopropylamine
203	isovaleric acid ^{(2) (3)}
204	m-cresol ⁽³⁾
205	mesitylene ^{(2) (3)}
206	methanamine,n-methyl-
207	methanethiol ^{(2) (3)}
208	methanol
209	methoxyacetone ^{(2) (3)}
210	methyl acetate ⁽²⁾
211	methyl chloride
212	methyl ethylether ⁽³⁾
213	methyl formate ^{(2) (3)}
214	methyl isobutylketone ⁽²⁾
215	methyl isopropylether
216	methyl isopropylketone ⁽²⁾
217	methyl n-butylether ^{(2) (3)}
218	methyl n-butyrate

219	methyl n-pentylether
220	methyl n-propylether
221	methyl propionate ⁽³⁾
222	methyl tert-butylether ^{(2) (3)}
223	methylacetylene ⁽²⁾
224	methylamine ⁽²⁾
225	methylcyclopentane ⁽¹⁾
226	methylcyclohexane ⁽¹⁾
227	methylethylketone ⁽²⁾
228	methylfluoride
229	methylisobutyrate
230	m-xylene
231	n,n-dimethylaniline ⁽³⁾
232	naphthalene
233	n-butane ⁽¹⁾
234	n-butylacetate ⁽³⁾
235	n-butylamine ⁽²⁾
236	n-butylbenzene ⁽²⁾
237	n-butyric acid ⁽²⁾
238	n-decane ⁽¹⁾
239	n-decanoic acid
240	neopentane ⁽¹⁾
241	n-heptane ⁽¹⁾
242	n-heptanoic acid ⁽²⁾
243	n-hexane ⁽¹⁾
244	n-hexanoic acid ⁽²⁾
245	nitrogen trifluoride
246	nitromethane ^{(2) (3)}
247	n-methylaniline ⁽²⁾
248	n-nonane ⁽¹⁾
249	n-nonanoic acid ⁽³⁾
250	n-octane ⁽¹⁾
251	n-octanoic acid
252	n-pentane ⁽¹⁾
253	n-pentanoic acid ⁽³⁾
254	n-pentylacetate
255	n-propyl n-butyrate ⁽²⁾
256	n-propyl propionate
257	n-propylacetate
258	n-propylamine
259	n-propylbenzene
260	n-propylchloride ⁽³⁾
261	o-cresol ⁽²⁾
262	octafluorocyclobutane
263	octafluoropropane ⁽³⁾
264	octamethylcyclotetrasiloxane ⁽³⁾
265	octanal
266	octane,3-methyl- ⁽¹⁾
267	octane,4-methyl- ⁽¹⁾
268	oxirane ⁽³⁾
269	o-xylene ⁽²⁾
270	p-cresol
271	p-cymene
272	p-diethylbenzene ⁽³⁾
273	pentafluoroethane
274	pentanal ⁽²⁾

275	pentane,3,3-diethyl- ⁽¹⁾
276	pentane,dodecafluoro-
277	perfluoro n-decane ⁽²⁾ ⁽³⁾
278	perfluoromethylcyclopentane ⁽²⁾
279	perfluoro-n-heptane
280	phenol
281	piperidine ⁽²⁾ ⁽³⁾
282	propadiene ⁽¹⁾
283	propane ⁽¹⁾
284	propane,1,1,2,2,3-pentafluoro- ⁽³⁾
285	propanoic acid,butylester ⁽²⁾ ⁽³⁾
286	propionic acid
287	propionitrile ⁽³⁾
288	propylene ⁽¹⁾
289	propylene glycol monomethyletheracetate ⁽²⁾
290	p-xylene ⁽²⁾
291	pyridine ⁽²⁾ ⁽³⁾
292	pyrrolidine ⁽³⁾
293	tetrachloromethane ⁽³⁾
294	tetrafluoroethylene ⁽²⁾ ⁽³⁾
295	tetrahydrofuran ⁽²⁾ ⁽³⁾
296	thiobismethane ⁽²⁾ ⁽³⁾
297	thiophene ⁽²⁾
298	toluene ⁽³⁾
299	trans 2-pentene ⁽¹⁾
300	trans-1,4-dimethylcyclohexane ⁽¹⁾
301	trichlorofluoromethane
302	triethylamine
303	trifluoroiodomethane
304	trifluoromethane
305	trimethylamine ⁽²⁾ ⁽³⁾
306	vinyl fluoride ⁽²⁾ ⁽³⁾

⁽¹⁾ compound in the validation set of the models for the critical temperature

⁽²⁾ compound in the validation set of the models for the critical pressure

⁽³⁾ compound in the validation set of the models for the acentric factor