Supplementary Material to "CombiFF optimization of a GROMOS-compatible force field for (halo)alkanes: Bypassing the use of charge groups."

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S1 Van der Waals radii

Table S1: Van-der-Waals radii associated with the employed atom types used in the calculation of Coulomb integrals.

atom type	vdW radius [nm]
CH0	0.170
CX4	0.170
CH1	0.220
CX3	0.220
CH2	0.220
CX2	0.220
CH3	0.220
CX1	0.220
F	0.147
Cl	0.175
Br	0.185
I	0.198

S2 Calibration Set

S2.1 Molecular properties

Table S2: List of molecules used in the force-field optimization and their associated experimental values at a given pressure P and temperature T: the liquid density ρ, heat of vaporization ΔH_{vap}, melting point, boiling point, critical point, and the static dielectric permittivity ϵ^0.

	class	smiles	P [bar]	T [K]	ρ [kg m^{-3}]	ΔH_{vap} [kJ mol^{-1}]	m.p. [K]	b.p. [K]	c.p. [K]	ϵ^0 [-]
1	Alk	CCC	1.00	230.00	582.13	18.8	85.5	231.1	369.8	1.7
2	Alk	CC(C)C	19.85	260.00	597.94	-	113.8	261.4	407.8	1.7
3	Alk	CC(C)C	1.00	265.00	-	22.4	113.8	261.4	407.8	1.7

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	class	smiles	P [bar]	T [K]	ρ [kg m^{-3}]	ΔH_{vap} [kJ mol^{-1}]	m.p. [K]	b.p. [K]	c.p. [K]	ϵ^0 [-]
4	Alk	CCCC	1.00	273.15	601	-	134.9	272.6	425.1	1.8
5	Alk	CCCC	9.93	300.00	572.45	-	134.9	272.6	425.1	1.8
6	Alk	CCCC	1.00	264.00	-	23.1	134.9	272.6	425.1	1.8
7	Alk	CC(C)(C)C	0.99	282.01	603.71	23.65	256.8	282.6	433.8	1.8
8	Alk	CC(C)(C)C	1.76	298.15	585.96	-	256.8	282.6	433.8	1.8
9	Alk	CCC(C)C	0.92	298.15	616.05	25.46	113.3	301	460.4	1.8
10	Alk	CCCCC	1.01	298.15	621.14	26.61	143.5	309.2	469.7	1.8
11	Alk	CCC(C)(C)C	1.01	298.15	644.43	28.78	174.2	322.9	489	1.9
12	Alk	CC(C)C(C)C	1.01	298.15	658.56	30.03	145.1	331.1	500	1.9
13	Alk	CCC(C)CC	1.01	298.15	659.94	30.87	110.3	336.4	504.4	1.9
14	Alk	CCCC(C)C	1.01	298.15	648.45	30.43	119.5	333.4	497.7	1.9
15	Alk	CCCCCC	1.00	298.15	656.1	31.76	177.9	341.9	507.6	1.9
16	Alk	CCCCCCC	0.06	298.15	681.95	36.5	182.6	371.6	540.2	1.9
17	Alk	CCCCCCCC	1.01	298.15	698.86	41.03	216.4	398.8	568.7	1.9
18	Br	CCBr	1.00	298.15	1451.2	-	154.8	311.5	503.8	9.0
19	Br	CCBr	1.00	305.00	-	27.6	154.8	311.5	503.8	9.0
20	Br	CC(Br)Br	1.00	298.15	2091.75	-	210.2	381.1	635.8	5.0
21	Br	BrCCBr	1.00	298.15	2169.52	41.7	282.9	404.5	650.1	5.0
22	Br	BrCC(Br)Br	1.00	298.15	2610.1	-	243.9	462.1	671.9	6.8
23	Br	CC(C)Br	1.00	298.15	1301.37	30.2	184.2	332.6	532.5	9.5
24	Br	CCCBr	1.00	298.15	1345.5	31.9	163.1	344.1	536.9	8.1
25	Br	CC(Br)CBr	1.00	298.15	1924.95	41.7	217.8	413.2	654.7	4.6
26	Br	BrCCCBr	1.00	298.15	1971.19	-	238.2	440.4	654.7	9.5
27	Br	CC(Br)(Br)CBr	1.00	293.15	2298.54	-	-	464.1	686.8	6.0
28	Br	CC(Br)C(Br)Br	1.00	293.15	2354.8	-	-	474.1	686.8	6.0
29	Br	BrCC(Br)CBr	1.00	298.15	2411.04	-	287.1	495.3	686.8	6.0
30	Br	CC(C)(C)Br	1.00	298.15	1212.5	31.8	256.4	346.4	557.6	11.0
31	Br	CC(C)CBr	1.00	298.15	1257.09	34.9	155.3	364.7	557.6	7.7
32	Br	CCC(C)Br	1.00	298.15	1253.6	34.8	-	364.4	557.6	8.7
33	Br	CCCCBr	1.00	298.15	1268.6	36.6	160.7	374.8	557.6	7.3
34	Br	CC(CBr)CBr	1.00	298.15	1799.5	-	-	448.1	672.7	6.6
35	Br	CCC(Br)CBr	1.00	298.15	1787	45.6	207.8	439.5	672.7	4.7
36	Br	CC(Br)CCBr	1.00	293.15	1796	-	-	448.1	672.7	9.1
37	Br	CC(C)(Br)C(Br)Br	1.00	294.15	2175.3	-	-	503.1	701.1	6.8
38	Br	CC(Br)(CBr)CBr	1.00	298.15	2180.3	-	-	493.1	701.1	6.8
39	Br	CC(C)(C)CBr	0.03	298.15	1193.46	-	-	379.1	581	7.5
40	Br	CCC(C)(C)Br	0.03	298.15	1209.52	-	-	381.1	581	9.2
41	Br	CCC(C)CBr	1.00	298.15	1214.4	-	-	393.6	581	7.5
42	Br	CCC(Br)CC	1.00	298.15	1205.1	-	146.9	391.8	581	8.4
43	Br	CC(C)CCBr	1.00	298.15	1200.7	-	161.2	393.6	581	6.3
44	Br	CCCC(C)Br	1.00	298.15	1200.5	38.5	177.7	390.6	581	7.5
45	Br	CCCCCBr	1.00	298.15	1211.4	40.9	185.2	402.7	581	6.3
46	Br	CC(C)(C)C(Br)Br	1.00	293.15	1669.5	-	-	453.1	689.9	7.5
47	Br	CCC(C)(Br)CC	1.00	293.15	1179.2	-	-	403.1	602.9	5.8
48	Br	CCCC(Br)CC	1.00	298.15	1157.16	-	-	414.4	602.9	5.8
49	Br	CCCCCCBr	1.00	298.15	1168.8	45.6	188.2	428.4	602.9	5.8
50	Br	CCCCCCCBr	1.00	298.15	1134.8	50.4	217.1	452.1	623.5	5.3
51	Br	CCCCCCCCBr	1.00	298.15	1107.7	55.1	218.2	473.9	643	5.1
52	Cl	CCCl	1.00	285.45	906.2	24.9	134.8	285.4	460.4	9.4

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	class	smiles	P [bar]	T [K]	ρ [kg m^{-3}]	ΔH_{vap} [kJ mol^{-1}]	m.p. [K]	b.p. [K]	c.p. [K]	ϵ^0 [-]
53	Cl	CCCl	1.39	298.15	889.97	-	134.8	285.4	460.4	9.4
54	Cl	CC(Cl)Cl	1.00	298.15	1168.07	30.6	176.2	330.4	523	10.1
55	Cl	ClCCCl	1.00	298.15	1245.58	34.4	237.6	356.6	561.6	10.4
56	Cl	CC(Cl)(Cl)Cl	1.00	298.15	1329.32	32.4	243.2	347.2	545	7.2
57	Cl	ClCC(Cl)Cl	1.00	298.15	1432.75	40.1	236.8	387	551.3	7.2
58	Cl	CC(C)Cl	1.00	298.15	855.63	-	156.1	308.9	496.5	8.6
59	Cl	CC(Cl)CCl	1.00	298.15	1153	36.2	172.6	369.5	573.3	8.4
60	Cl	ClCCCCl	1.00	298.15	1180	40.6	173.7	393.6	573.3	10.3
61	Cl	CC(C)(C)Cl	1.00	298.15	836.3	28.6	247.6	323.8	530.2	9.7
62	Cl	CC(C)CCl	1.00	298.15	871.35	31.7	142.8	342	530.2	7.0
63	Cl	CCC(C)Cl	1.01	298.15	867.47	31.5	141.8	341.2	520.6	8.6
64	Cl	CCCCCl	1.01	298.15	880.4	33.5	150.1	351.6	530.2	7.3
65	Cl	CC(Cl)C(C)Cl	1.00	298.15	1106.3	-	-	391.1	599.9	8.1
66	Cl	CCC(Cl)CCl	1.00	298.15	1111.8	40.1	-	397.1	599.9	7.7
67	Cl	ClCCCCCl	1.00	298.15	-	46.4	234.4	427.1	599.9	9.3
68	Cl	CCC(C)(C)Cl	1.00	298.15	859.65	-	200.6	358.8	560.5	12.3
69	Cl	CCC(C)CCl	1.00	298.15	875	-	-	373.7	560.5	8.3
70	Cl	CC(C)CCCl	1.00	298.15	870	36.2	168.8	371.7	560.5	6.1
71	Cl	CCCC(C)Cl	1.00	298.15	866	36	-	369.7	560.5	8.3
72	Cl	CCCCCCl	1.00	298.00	877.8	38.2	174.2	381.5	560.5	6.7
73	Cl	ClCCCCCCl	1.00	298.15	1095.6	51.3	200.3	453.1	624.5	9.9
74	Cl	CCCCCCCl	1.00	298.15	873.54	42	179.2	408.2	588	6.1
75	Cl	CC(CCl)C(C)(C)Cl	1.00	298.15	1064	-	-	-	-	8.6
76	Cl	CC(Cl)CCC(C)Cl	1.00	298.15	1044.1	-	-	-	-	8.6
77	Cl	ClCCCCCCCl	1.01	298.15	1063.7	-	-	477.1	647.4	8.6
78	Cl	CCCCCCCCl	1.00	298.15	871.5	47	203.8	433.6	613.5	5.5
79	Cl	CCCCCCCCCl	1.00	298.15	869.35	51.4	215.3	456.6	637.1	5.0
80	F	CCF	1.00	236.05	817.6	20.7	129.9	235.4	375.3	6.1
81	F	CCF	9.09	298.15	707.47	-	129.9	235.4	375.3	6.1
82	F	CC(F)F	1.00	249.66	1009	22.7	154.6	247.3	386.4	6.1
83	F	CC(F)F	6.25	298.15	907	-	154.6	247.3	386.4	6.1
84	F	CC(F)(F)F	1.00	220.16	1182.86	19.2	161.6	225.8	345.9	10.6
85	F	CC(C)F	1.00	263.75	769.2	-	-	263.8	421.1	6.1
86	F	CCCF	1.00	270.65	781.8	-	114.2	269.9	421.1	6.1
87	F	CCC(F)F	0.62	276.30	-	25.12	-	281.1	430.4	6.1
88	F	FCCCF	1.00	298.15	1005.7	-	-	314.4	430.4	6.1
89	F	CC(C)(C)F	1.00	285.25	752.7	-	-	285.2	460.3	6.1
90	F	CC(C)(C)F	1.39	298.15	735.3	-	-	285.2	460.3	6.1
91	F	CCC(C)F	1.00	298.15	756.56	-	151.8	298.2	460.3	6.1
92	F	CCCCF	1.00	298.15	770.82	-	139.2	305.6	460.3	6.1
93	F	FCCCCF	1.00	298.15	976.7	-	-	350.9	463.6	6.1
94	F	CCCC(F)(F)F	1.38	298.15	1010	-	-	289.9	406.6	6.1
95	F	CCC(C)(C)F	1.00	298.15	773.73	-	-	317.9	494.6	3.9
96	F	CCC(C)CF	0.34	298.15	791.47	-	-	329.1	494.6	3.9
97	F	CCCCCF	1.00	298.15	784.9	30.93	153.2	335.9	494.6	3.9
98	F	CCCCC(C)F	1.00	293.15	791.4	-	-	359.4	525.4	6.1
99	F	CCCCCCF	1.00	298.15	795.79	35.57	170.2	364.6	525.4	6.1
100	F	CC(C)CC(C)(F)F	1.00	293.15	888.2	-	-	-	-	6.1
101	F	FCCCCCCF	1.00	298.15	940.7	-	-	-	-	6.1

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	class	smiles	P [bar]	T [K]	ρ [kg m^{-3}]	ΔH_{vap} [kJ mol^{-1}]	m.p. [K]	b.p. [K]	c.p. [K]	ϵ^0 [-]
102	F	CCCCCCCF	1.00	298.15	800.88	40.8	200.2	391.1	553.5	6.1
103	F	CCCCCCCCF	1.00	298.15	806.69	-	209.2	415.4	579.2	3.9
104	I	CCI	1.00	298.15	1924.04	31.7	162.2	345.4	562.2	7.8
105	I	CC(C)I	1.00	298.15	1694.54	34.1	182.8	362.6	583.8	8.2
106	I	CCCI	1.00	298.15	1737.25	36.01	171.8	375.6	602.3	7.1
107	I	ICCCI	1.00	298.15	2565.1	-	253.2	496.1	775.2	6.5
108	I	ICCCI	0.01	368.52	-	53.5	253.2	496.1	775.2	6.5
109	I	CC(C)(C)I	0.06	298.15	1536.03	35.71	239.6	373.2	596.8	6.7
110	I	CC(C)CI	0.02	298.15	1595.11	38.8	-	393.6	625	6.5
111	I	CCC(C)I	1.00	298.15	1589	38.5	-	393.1	623.3	6.5
112	I	CCCCI	1.00	298.15	1606.74	40.3	169.7	403.7	638.8	6.3
113	I	ICCCCI	1.00	298.15	2349.57	59	279.1	477.2	806.4	6.5
114	I	CC(C)(C)CI	1.00	293.15	1494	-	-	407.1	670.9	6.8
115	I	CCC(C)(C)I	0.01	298.15	1486.59	-	-	402.1	670.9	8.2
116	I	CC(C)C(C)I	1.00	293.15	1524	-	-	413.1	670.9	6.8
117	I	CCC(I)CC	1.00	298.15	1505.48	-	-	418.1	670.9	7.4
118	I	CC(C)CCI	1.00	298.15	1495.15	42.2	-	421.4	659.1	5.6
119	I	CCCC(C)I	1.00	293.15	1500.9	-	-	416.1	670.9	6.8
120	I	CCCCCI	1.00	298.15	1507.35	44.4	187.6	430.1	671.4	5.8
121	I	ICCCCCI	1.00	298.15	2173.44	-	282.1	500.1	843.6	6.5
122	I	CCCC(C)CI	1.00	293.15	1443	-	-	441.1	697.2	5.3
123	I	CCCCC(C)I	1.00	293.15	1419.3	-	-	442.1	697.2	5.3
124	I	CCCCCCI	1.00	298.15	1431.81	-	199.1	454.5	704.4	5.3
125	I	CCCCCCI	1.00	346.00	-	46.2	199.1	454.5	704.4	5.3
126	I	ICCCCCCI	1.00	298.15	2034.2	-	282.6	522.5	831.8	6.5
127	I	CCCCCCCI	1.00	298.15	1371.9	-	224.9	477.1	736.7	4.9
128	I	CCCCCCCI	0.01	356.73	-	48.44	224.9	477.1	736.7	4.9
129	I	CCCCCCCCI	1.00	298.15	1326.65	-	227.4	498.3	764.8	4.7
130	I	CCCCCCCCI	0.01	373.66	-	50.92	227.4	498.3	764.8	4.7
131	Mix	CC(Cl)Br	1.00	283.15	1667	-	-	356.1	-	7.4
132	Mix	ClCCBr	1.01	298.15	1727.01	-	256.4	380.1	-	7.4
133	Mix	ClCCBr	1.00	308.00	-	37.6	256.4	380.1	-	7.4
134	Mix	FCCBr	1.00	298.15	1704.4	-	-	344.6	-	7.4
135	Mix	FCCCl	0.33	298.15	1167.53	-	-	326.1	497.1	7.4
136	Mix	ClCCI	1.00	288.43	2133.57	-	-	413.1	-	7.4
137	Mix	CC(F)(F)Cl	1.07	264.56	1188.76	22.7	142.7	263.1	410.3	7.4
138	Mix	CC(F)(F)Cl	3.61	298.15	1107.72	19.74	142.7	263.1	410.3	7.4
139	Mix	CC(F)(Cl)Cl	1.00	298.15	1233.66	26.04	169.7	304.9	478.9	7.4
140	Mix	FC(Cl)CCl	1.00	298.14	1369.2	-	213.2	346.9	523.6	7.4
141	Mix	FC(F)(Br)CBr	1.00	293.15	2223.8	-	211.8	365.6	-	7.4
142	Mix	FC(F)(Cl)CCl	1.00	298.14	1406.6	-	171.9	319.8	479.1	7.4
143	Mix	FC(F)C(F)Br	1.00	283.15	1874	-	-	-	-	7.4
144	Mix	FC(F)(F)CCl	1.00	284.60	1353.9	-	167.7	279.2	426.2	7.4
145	Mix	FC(Cl)(Cl)CCl	1.00	298.14	1482.6	-	168.4	361.1	535	7.4
146	Mix	FC(Cl)C(Cl)Cl	1.00	298.14	1529.8	-	-	375.1	555.6	7.4
147	Mix	FC(F)(F)CI	1.00	298.15	2130	-	-	327.6	-	7.4
148	Mix	CC(C)(Cl)Br	1.00	293.15	1495	-	-	368.1	-	7.4
149	Mix	CC(Br)CCl	1.00	293.15	1537	-	-	390.1	-	7.4
150	Mix	CC(Cl)CBr	1.00	293.15	1531	-	-	391.1	-	7.4

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	class	smiles	P [bar]	T [K]	ρ [kg m^{-3}]	ΔH_{vap} [kJ mol^{-1}]	m.p. [K]	b.p. [K]	c.p. [K]	ϵ^0 [-]
151	Mix	ClCCCBr	1.00	293.15	1596.9	-	214.3	416.4	-	7.4
152	Mix	CC(C)(F)Cl	1.00	293.15	998.2	-	-	-	515.4	7.4
153	Mix	CC(F)CCl	1.00	293.15	1086	-	-	-	-	7.4
154	Mix	ClCCCI	1.00	293.15	1904	-	-	444.1	-	7.4
155	Mix	ClC(Cl)CCBr	1.00	293.15	1708.4	-	-	-	-	7.4
156	Mix	ClCC(Br)CBr	1.00	287.15	2093	-	-	469.1	-	7.4
157	Mix	CC(F)(Cl)CCl	0.07	298.15	1255.25	-	-	361.8	536.5	7.4
158	Mix	ClC(Cl)(Br)CCBr	1.00	293.15	2077.2	-	-	-	-	7.3
159	Mix	ClCCCCBr	1.01	298.15	1485.12	-	-	448.1	-	7.4
160	Mix	CC(Cl)C(Cl)CBr	1.00	293.15	1598.5	-	-	-	-	7.4
161	Mix	CCC(F)(F)C(C)Cl	1.00	293.15	1108.5	-	-	-	-	7.4
162	Mix	CC(C)(C)C(C)(Cl)Br	1.00	293.15	1250	-	-	-	-	7.4

S2.2 Molecular Structures

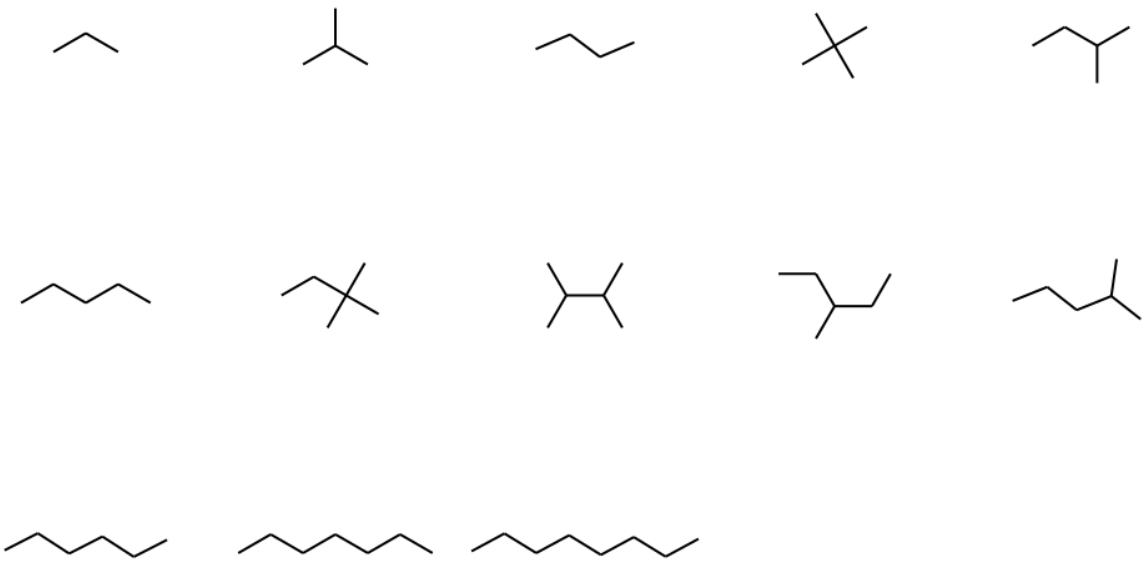


Figure S1: Chemical structures of the molecules listed in Table S2 belonging to the alkane family.

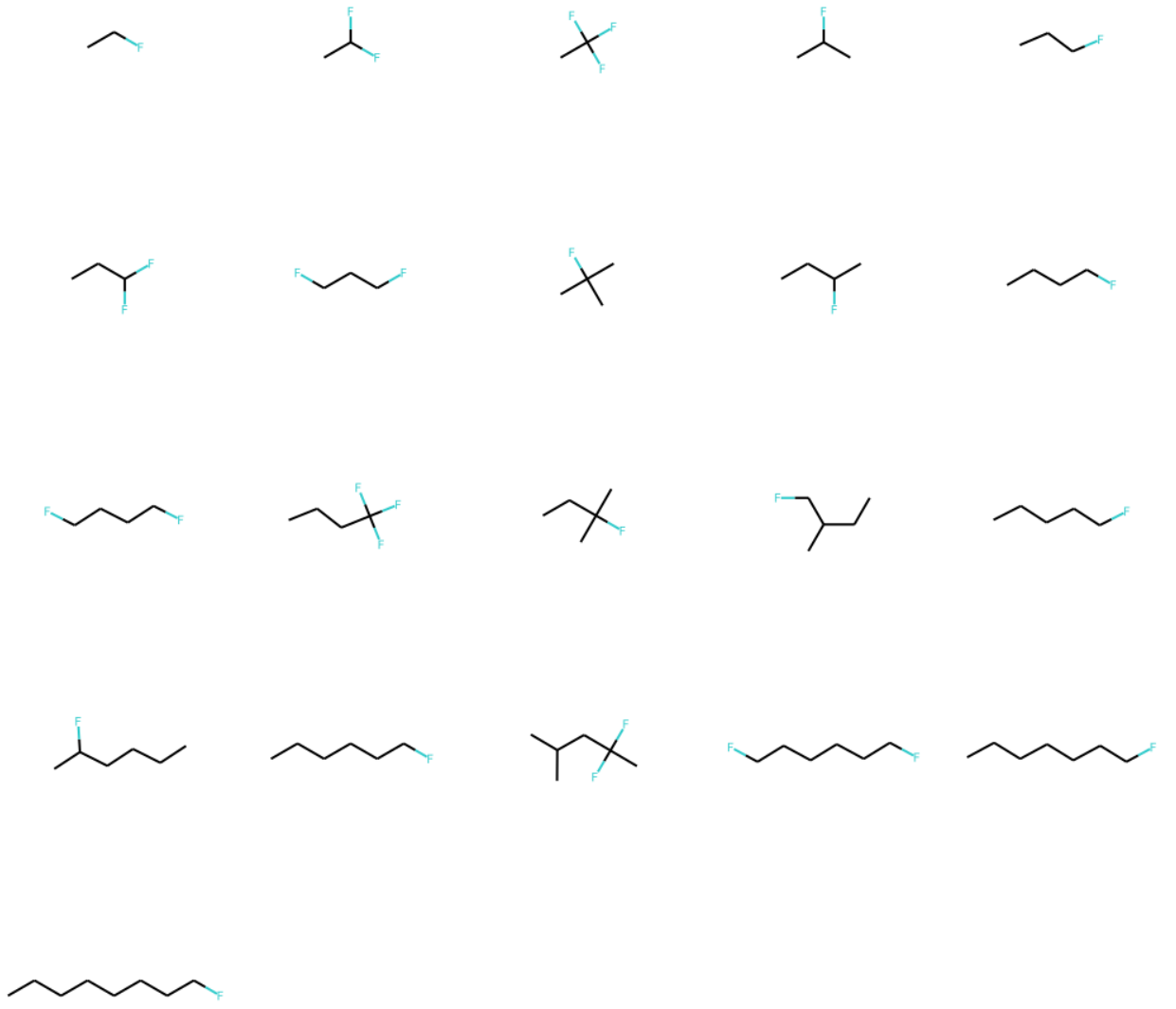


Figure S2: Chemical structures of the molecules listed in Table S2 belonging to the fluoroalkane family.

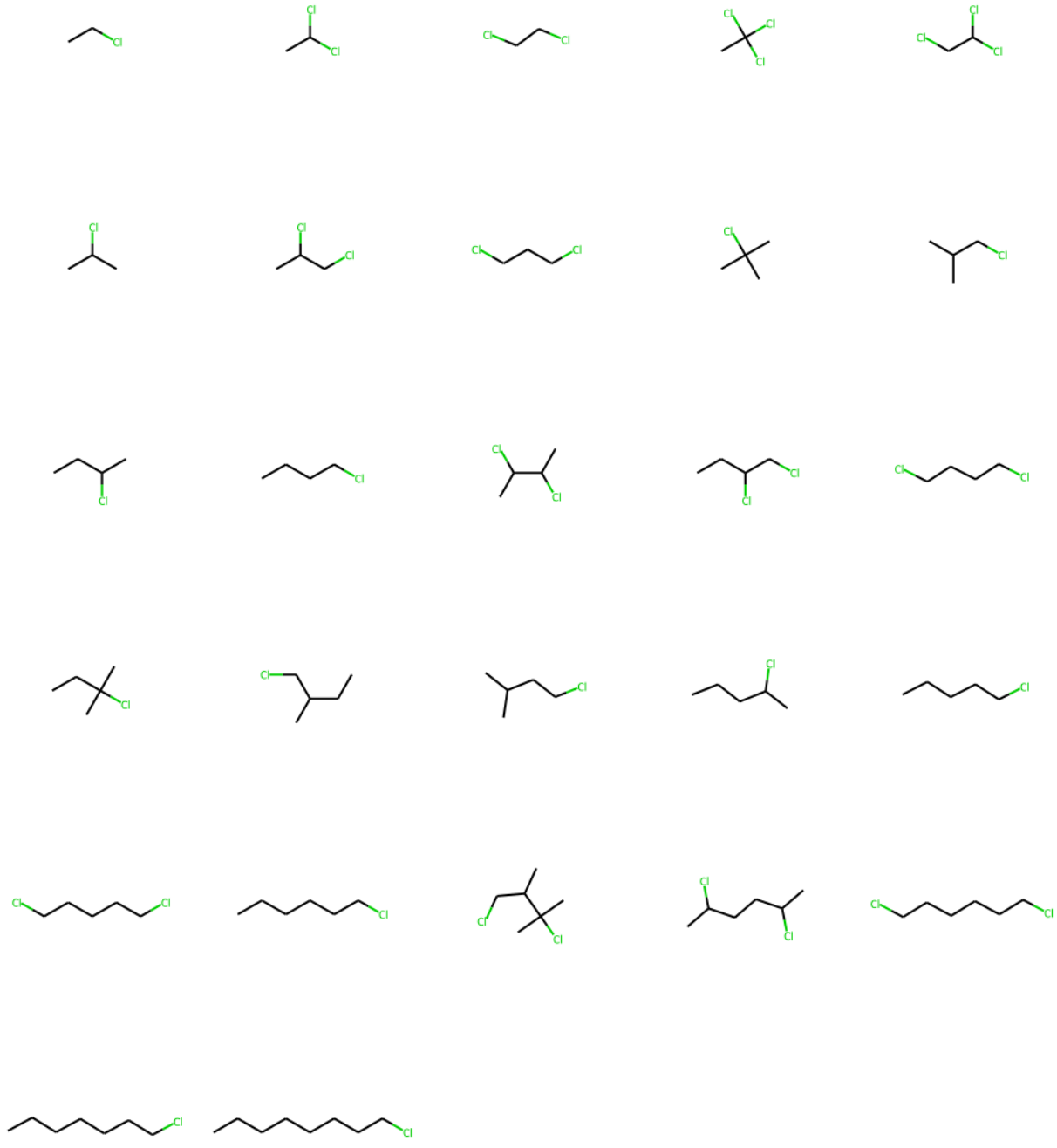


Figure S3: Chemical structures of the molecules listed in Table S2 belonging to the chloroalkane family.

Figure S4: Chemical structures of the molecules listed in Table S2 belonging to the bromoalkane family.

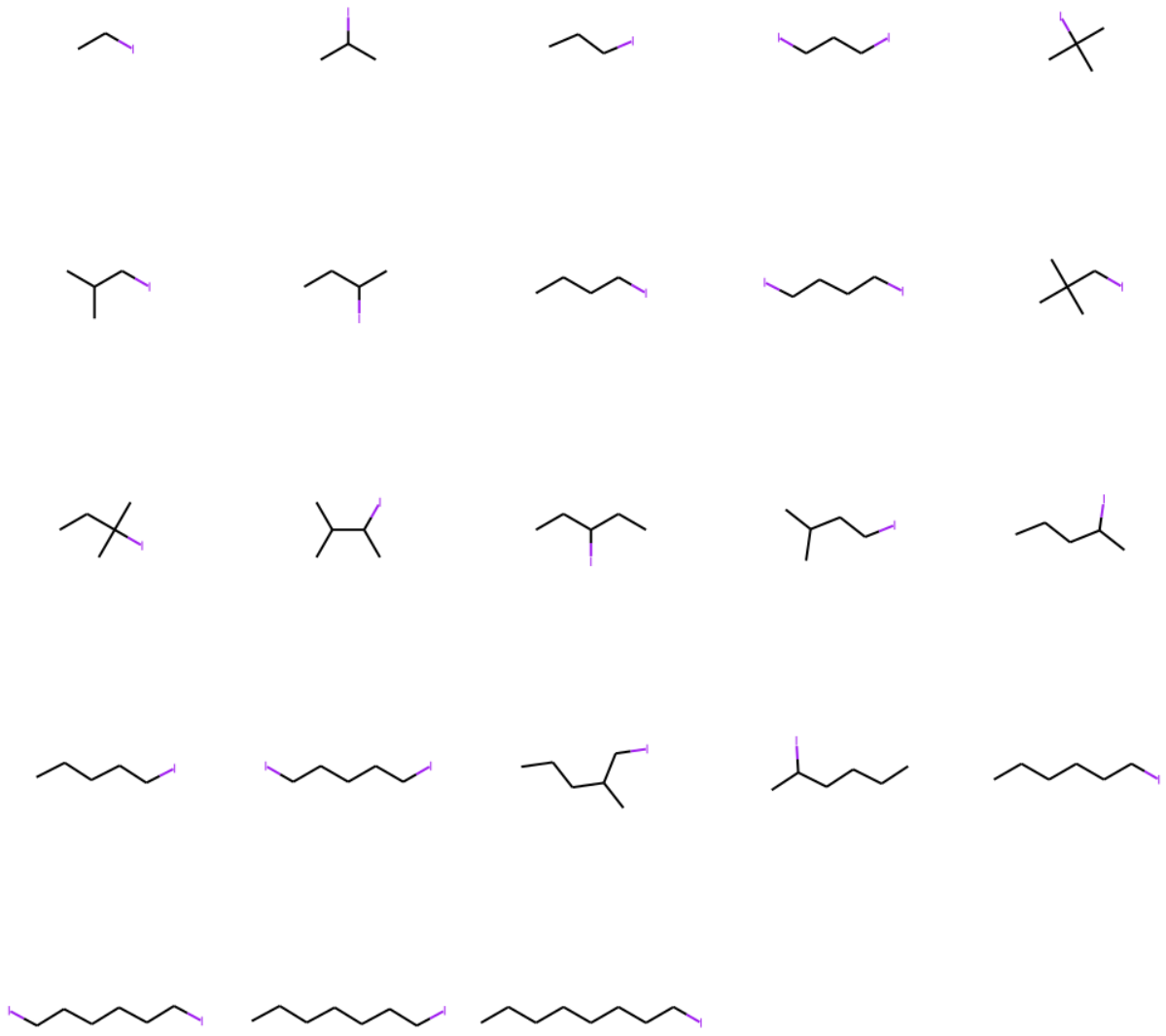


Figure S5: Chemical structures of the molecules listed in Table S2 belonging to the iodoalkane family.

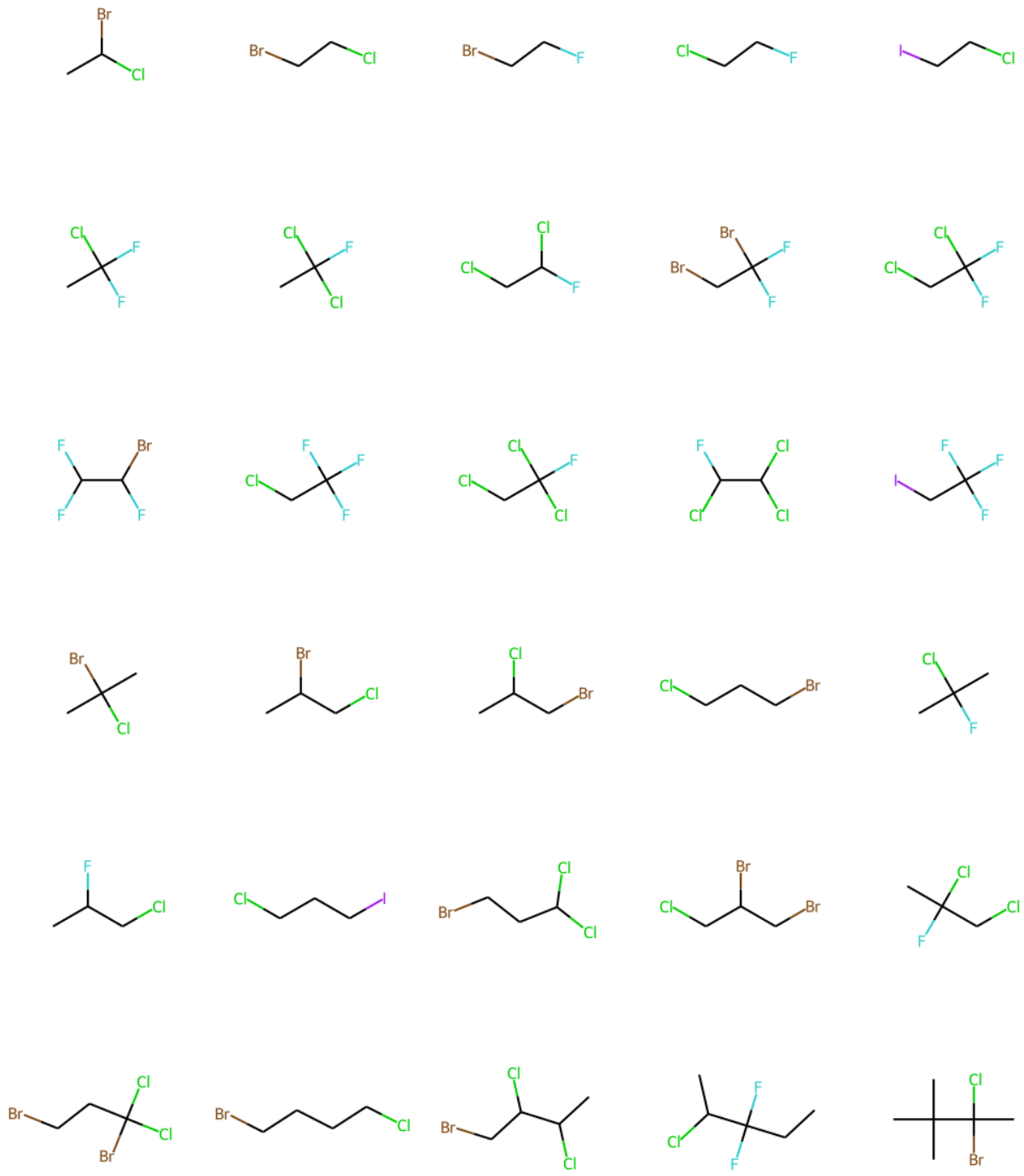


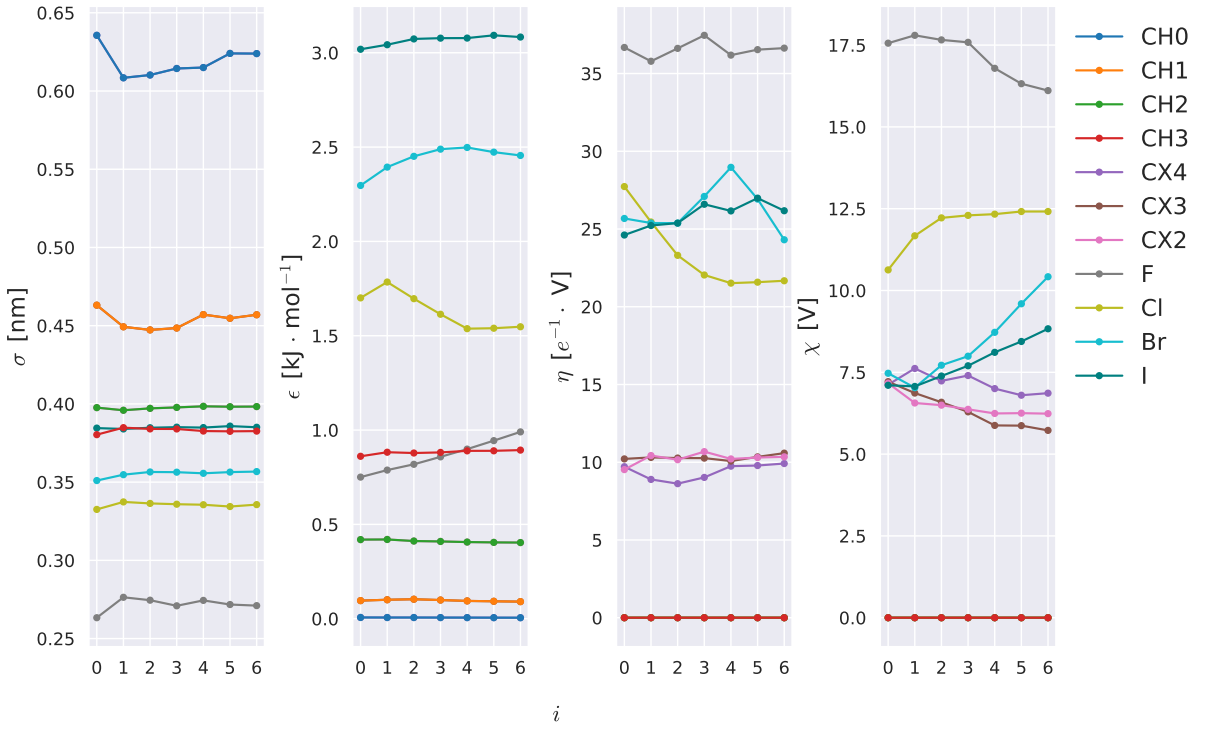
Figure S6: Chemical structures of the molecules listed in Table S2 belonging to the haloalkane family with multiple types of halogen atoms.

S3 Preliminary comparison against QM calculations

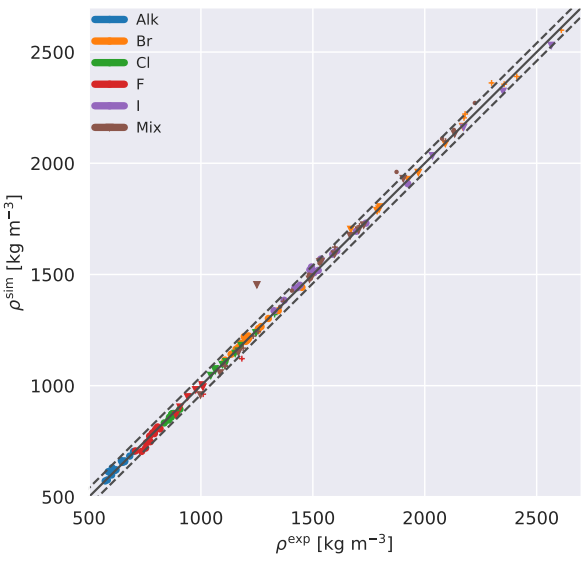
Table S3: Electronegativity χ (in V) and hardness η (in e^{-1} V) parameters optimized against DDEC charges. In the EEM-G scheme, charge groups were emulated by constraining the hardness of the CHn atom type to 10^{10}, and the corresponding electronegativities to 0. In all of the schemes, the parameters were constrained to the range (6, 60) in the corresponding units. In the SQE-M scheme, the bond hardness of all bond types was additionally constrained to 10 e^{-1} V.

	atom	EEM-G		EEM-M		SQE-M	
		χ	η	χ	η	χ	η
0	CH0	0.00	1E10	6.00	22.92	6.00	21.62
1	CX4	7.42	18.22	7.81	13.61	7.21	16.07
2	CH1	0.00	1E10	6.00	30.77	6.50	20.62
3	CX3	6.00	25.46	6.80	18.48	6.10	21.97
4	CH2	0.00	1E10	8.58	60.00	8.43	60.00
5	CX2	6.86	30.03	7.27	21.58	6.05	31.12
6	CH3	0.00	1E10	10.87	57.24	10.90	34.07
7	CX1	6.00	45.97	6.00	36.44	6.00	38.80
8	CH4	0.00	1E10	8.64	14.40	8.64	14.40
9	F	26.56	52.35	23.50	50.36	32.43	60.00
10	Cl	15.85	29.36	15.31	33.40	16.29	17.07
11	Br	15.86	33.67	13.25	24.55	14.11	8.28
12	I	14.06	29.24	12.55	23.68	12.92	6.00

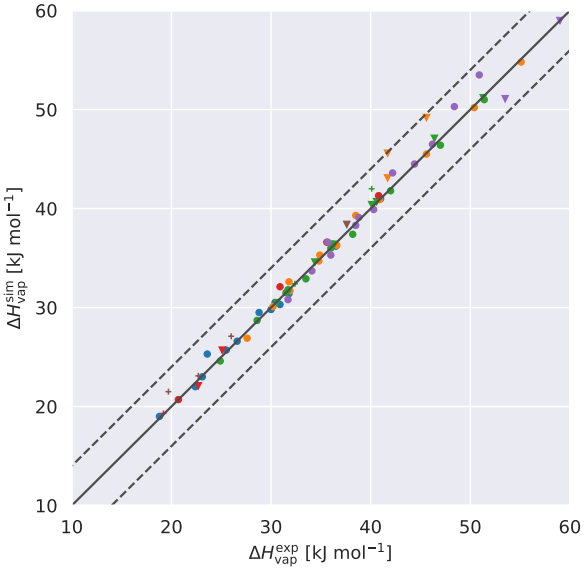
S4 Parameter evolution and final observables



(a) Evolution of the nonbonded parameters (LJ collision diameter σ, LJ well depth ϵ, electrostatic hardness η and electronegativity χ) as a function of the iteration of the optimization. Different colors correspond to different atom types. Note that the CHn and CX$(4-n)$ atom types share the same LJ parameters.

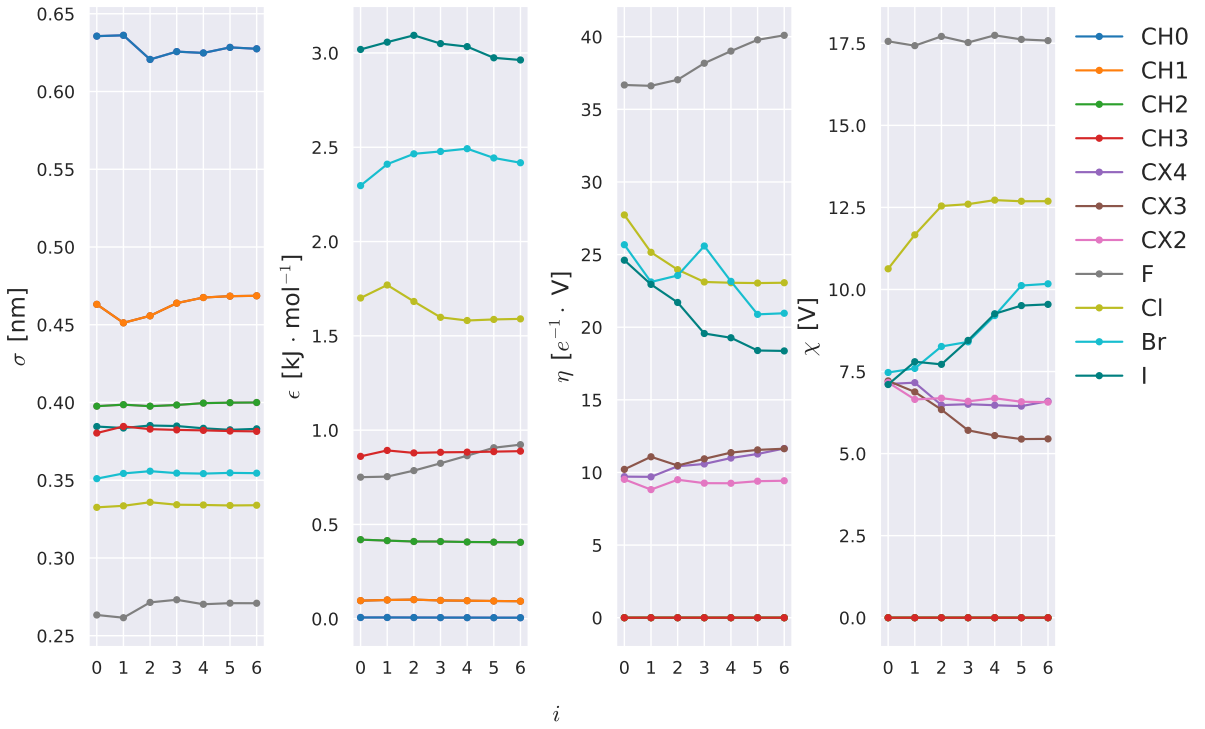


(b) Comparison between experimental and simulated densities from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 40 kg m^{-3}.

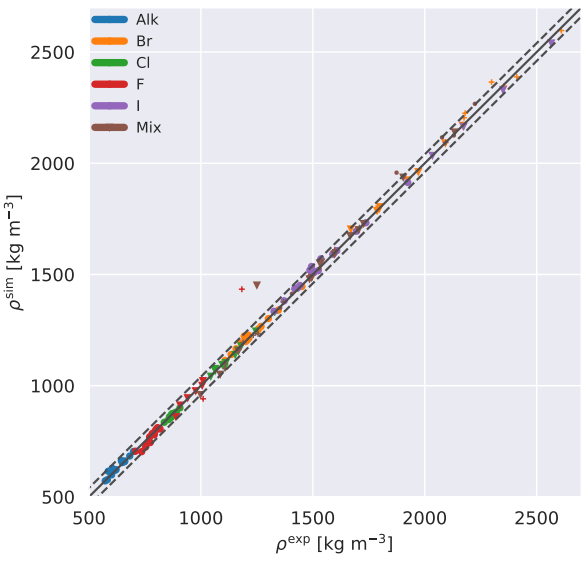


(c) Comparison between experimental and simulated heats of vaporization from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 4 kJ mol^{-1}.

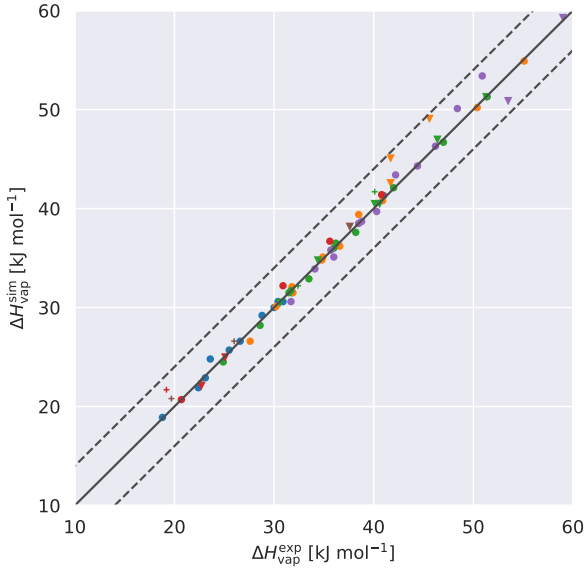
Figure S7: Parameter evolution and comparison of final observables from the **CG/EEM-G** optimization scheme. Different colors in (b) and (c) correspond to different families of molecules, as described in the Main text.



(a) Evolution of the nonbonded parameters (LJ collision diameter σ, LJ well depth ϵ, electrostatic hardness η and electronegativity χ) as a function of the iteration of the optimization. Different colors correspond to different atom types. Note that the CHn and CX$(4-n)$ atom types share the same LJ parameters.

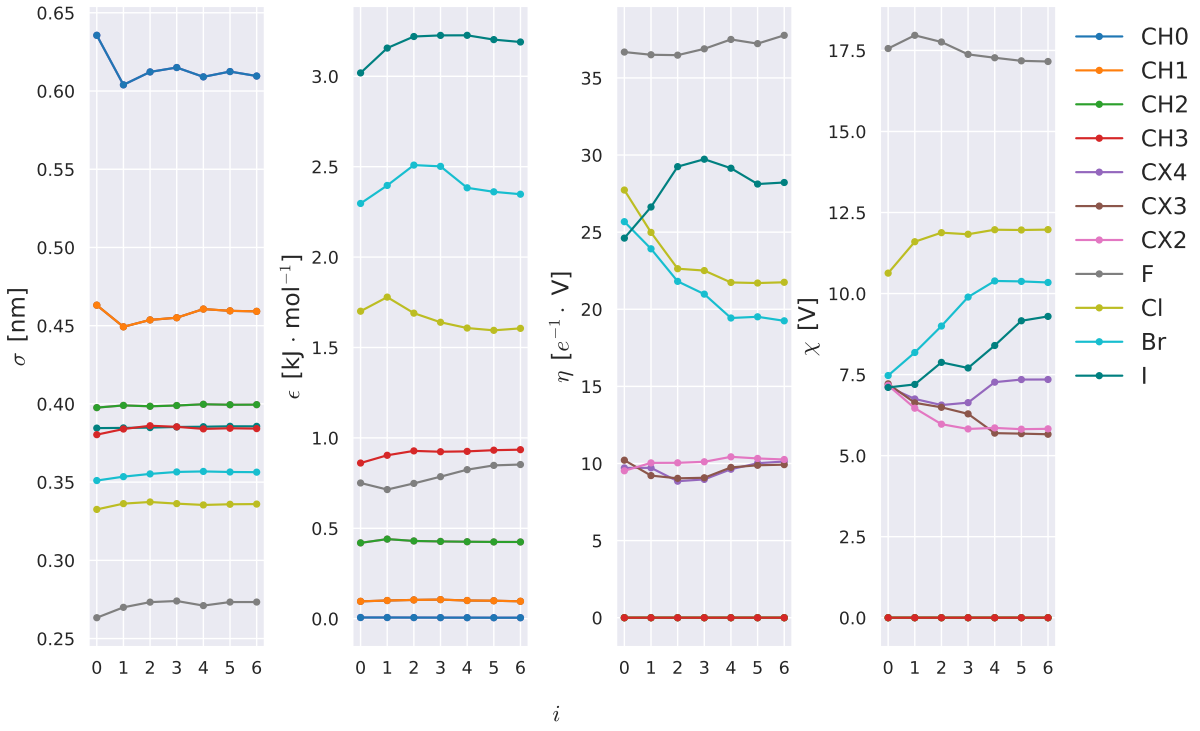


(b) Comparison between experimental and simulated densities from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 40 kg m^{-3}.

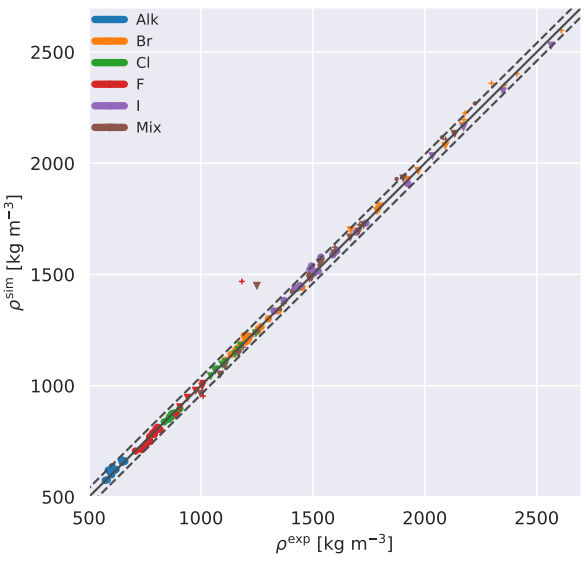


(c) Comparison between experimental and simulated heats of vaporization from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 4 kJ mol^{-1}.

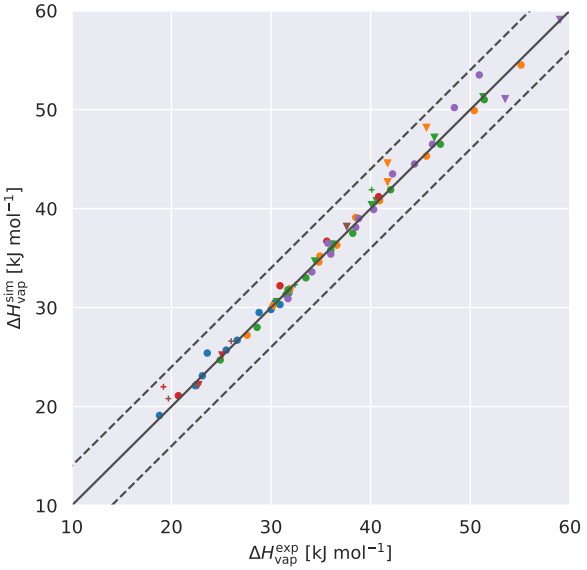
Figure S8: Parameter evolution and comparison of final observables from the **AT/EEM-G** optimization scheme. Different colors in (b) and (c) correspond to different families of molecules, as described in the Main text.



(a) Evolution of the nonbonded parameters (LJ collision diameter σ, LJ well depth ϵ, electrostatic hardness η and electronegativity χ) as a function of the iteration of the optimization. Different colors correspond to different atom types. Note that the CHn and CX$(4-n)$ atom types share the same LJ parameters.

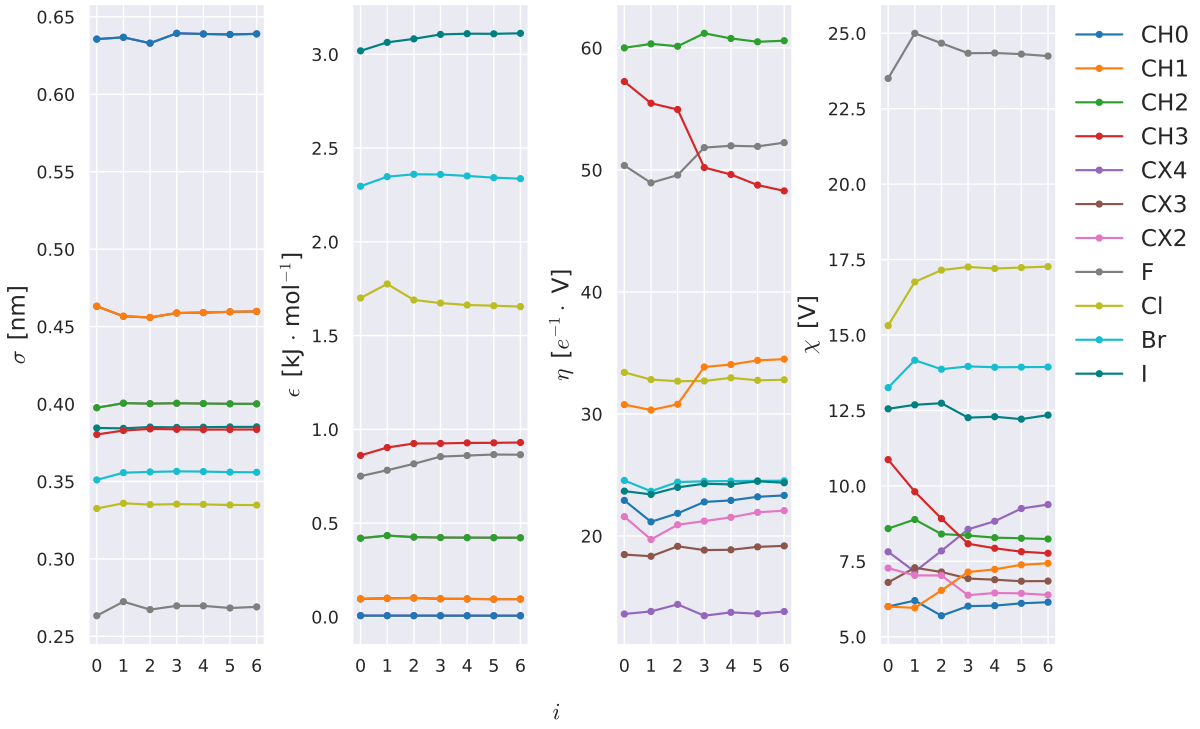


(b) Comparison between experimental and simulated densities from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 40 kg m^{-3}.

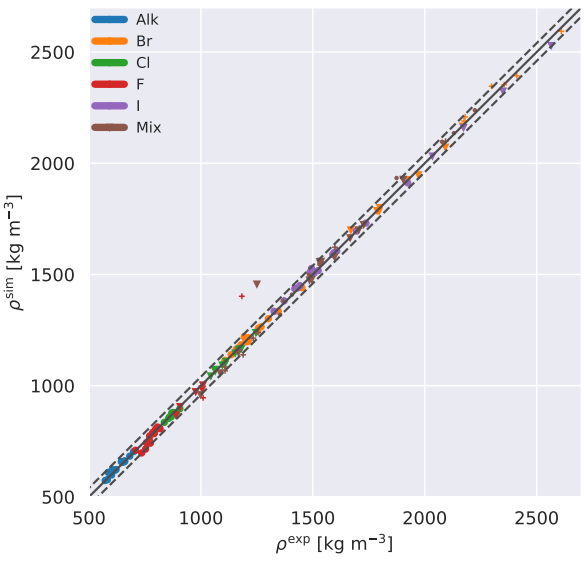


(c) Comparison between experimental and simulated heats of vaporization from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 4 kJ mol^{-1}.

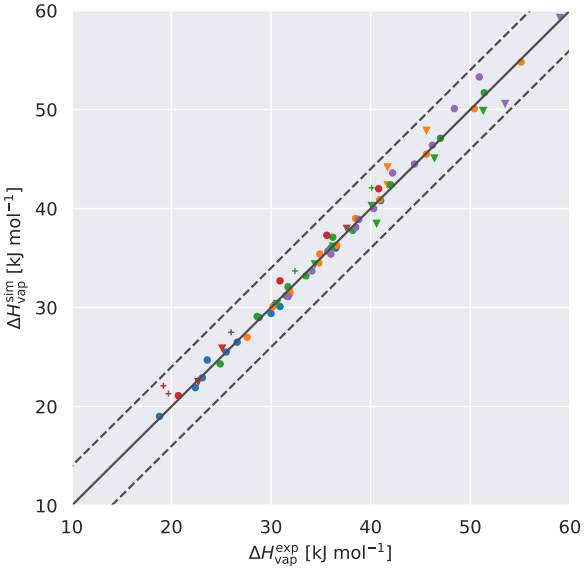
Figure S9: Parameter evolution and comparison of final observables from the **SH/EEM-G** optimization scheme. Different colors in (b) and (c) correspond to different families of molecules, as described in the Main text.



(a) Evolution of the nonbonded parameters (LJ collision diameter σ, LJ well depth ϵ, electrostatic hardness η and electronegativity χ) as a function of the iteration of the optimization. Different colors correspond to different atom types. Note that the CHn and CX$(4-n)$ atom types share the same LJ parameters.

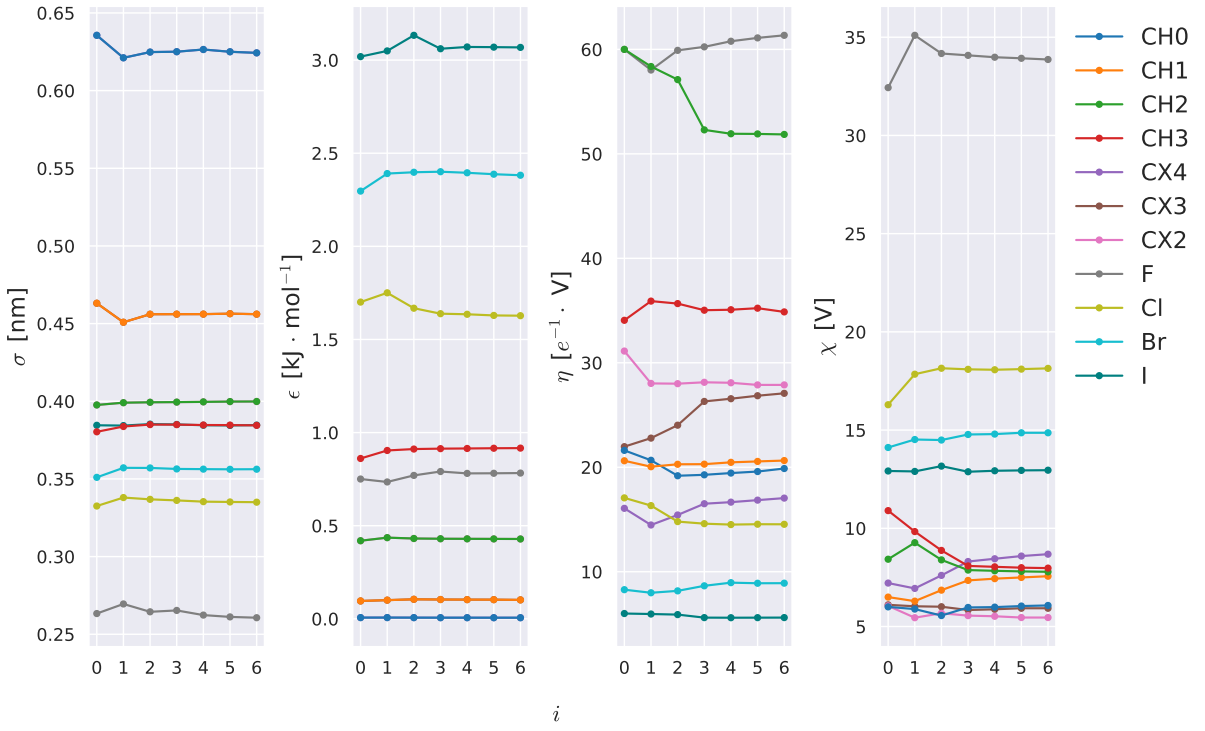


(b) Comparison between experimental and simulated densities from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 40 kg m^{-3}.

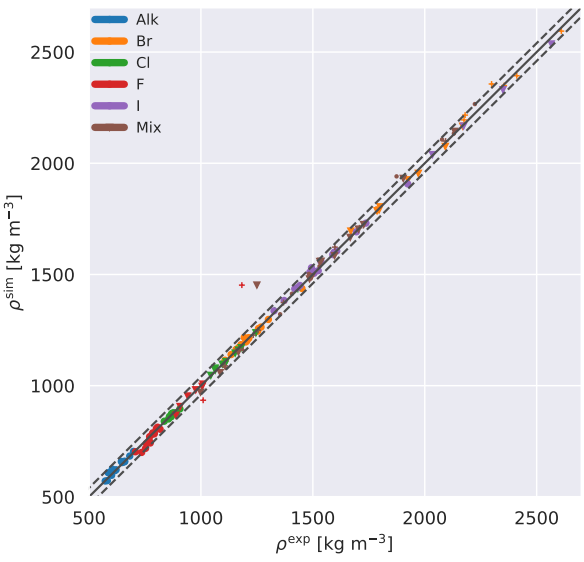


(c) Comparison between experimental and simulated heats of vaporization from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 4 kJ mol^{-1}.

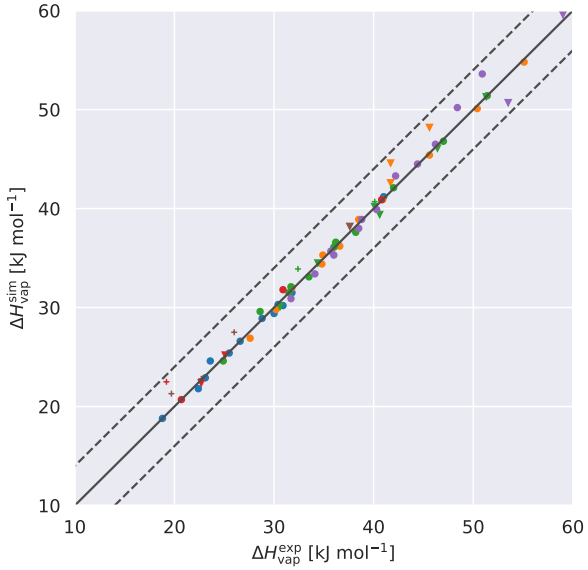
Figure S10: Parameter evolution and comparison of final observables from the **SH/EEM-M** optimization scheme. Different colors in (b) and (c) correspond to different families of molecules, as described in the Main text.



(a) Evolution of the nonbonded parameters (LJ collision diameter σ, LJ well depth ϵ, electrostatic hardness η and electronegativity χ) as a function of the iteration of the optimization. Different colors correspond to different atom types. Note that the CHn and CX$(4-n)$ atom types share the same LJ parameters.



(b) Comparison between experimental and simulated densities from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 40 kg m^{-3}.



(c) Comparison between experimental and simulated heats of vaporization from the optimized force field (4th iteration). The dashed lines mark a deviation of ± 4 kJ mol^{-1}.

Figure S11: Parameter evolution and comparison of final observables from the **SH/SQE-M** optimization scheme. Different colors in (b) and (c) correspond to different families of molecules, as described in the Main text.

S5 Final parameters

Table S4: Final parameters in the **CG/EEM-G** scheme. The optimized parameters are the LJ collision radius σ (in nm), the LJ well depth ϵ (in kJ mol^{-1}), the hardness η (in $e^{-1}V$) and electronegativity χ (in V).

atom type	σ	ϵ	η	χ
CH0	0.62	0.01	0.00	0.00
CX4	0.62	0.01	9.92	6.86
CH1	0.46	0.09	0.00	0.00
CX3	0.46	0.09	10.58	5.73
CH2	0.40	0.40	0.00	0.00
CX2	0.40	0.40	10.35	6.24
CH3	0.38	0.89	0.00	0.00
CX1	0.38	0.89	10.44	6.91
F	0.27	0.99	36.63	16.11
Cl	0.34	1.55	21.67	12.41
Br	0.36	2.46	24.31	10.42
I	0.39	3.08	26.17	8.83

Table S5: Final parameters in the **AT/EEM-G** scheme. The optimized parameters are the LJ collision radius σ (in nm), the LJ well depth ϵ (in kJ mol^{-1}), the hardness η (in $e^{-1}V$) and electronegativity χ (in V).

atom type	σ	ϵ	η	χ
CH0	0.63	0.01	0.00	0.00
CX4	0.63	0.01	11.65	6.60
CH1	0.47	0.09	0.00	0.00
CX3	0.47	0.09	11.64	5.45
CH2	0.40	0.41	0.00	0.00
CX2	0.40	0.41	9.43	6.57
CH3	0.38	0.89	0.00	0.00
CX1	0.38	0.89	9.22	8.17
F	0.27	0.92	40.10	17.58
Cl	0.33	1.59	23.06	12.69
Br	0.35	2.42	20.96	10.17
I	0.38	2.96	18.37	9.55

Table S6: Final parameters in the **SH/EEM-G** scheme. The optimized parameters are the LJ collision radius σ (in nm), the LJ well depth ϵ (in kJ mol^{-1}), the hardness η (in $e^{-1}V$) and electronegativity χ (in V).

atom type	σ	ϵ	η	χ
CH0	0.61	0.01	0.00	0.00
CX4	0.61	0.01	10.13	7.35
CH1	0.46	0.10	0.00	0.00
CX3	0.46	0.10	9.92	5.66
CH2	0.40	0.42	0.00	0.00
CX2	0.40	0.42	10.26	5.83
CH3	0.38	0.93	0.00	0.00
CX1	0.38	0.93	10.24	7.07
F	0.27	0.85	37.76	17.16
Cl	0.34	1.61	21.75	11.97
Br	0.36	2.35	19.25	10.34
I	0.39	3.19	28.22	9.29

Table S7: Final parameters in the **SH/EEM-M** scheme. The optimized parameters are the LJ collision radius σ (in nm), the LJ well depth ϵ (in kJ mol^{-1}), the hardness η (in $e^{-1}V$) and electronegativity χ (in V).

atom type	σ	ϵ	η	χ
CH0	0.64	0.01	23.32	6.14
CX4	0.64	0.01	13.81	9.38
CH1	0.46	0.09	34.49	7.43
CX3	0.46	0.09	19.19	6.84
CH2	0.40	0.42	60.58	8.24
CX2	0.40	0.42	22.08	6.39
CH3	0.38	0.93	48.28	7.77
F	0.27	0.86	52.23	24.24
Cl	0.33	1.65	32.80	17.27
Br	0.36	2.34	24.53	13.94
I	0.39	3.11	24.36	12.35

Table S8: Final parameters in the **SH/SQE-M** scheme. The optimized parameters are the LJ collision radius σ (in nm), the LJ well depth ϵ (in kJ mol^{-1}), the hardness η (in $e^{-1}V$) and electronegativity χ (in V).

atom type	σ	ϵ	η	χ
CH0	0.62	0.01	19.88	6.07
CX4	0.62	0.01	17.05	8.68
CH1	0.46	0.10	20.64	7.56
CX3	0.46	0.10	27.08	5.93
CH2	0.40	0.43	51.86	7.79
CX2	0.40	0.43	27.88	5.46
CH3	0.38	0.92	34.87	7.97
F	0.26	0.78	61.35	33.87
Cl	0.34	1.63	14.54	18.14
Br	0.36	2.38	8.90	14.86
I	0.38	3.07	5.61	12.96

Table S9: Final bond hardness parameters η^{bond} (in $e^{-1}V$) for the **SH/SQE-M** scheme.

	bond type	η^{bond}
0	C-C	8.478339
1	C-F	9.777982
2	C-Cl	9.267636
3	C-Br	10.405338
4	C-I	10.115890

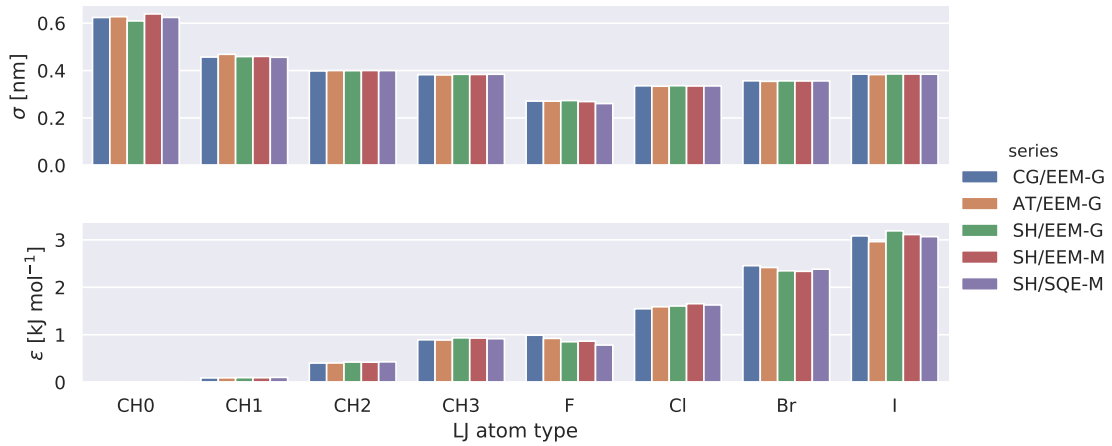


Figure S12: Final values for the LJ well depth ϵ and collision radius σ for each LJ atom type. Note that the CHn and CX$(4-n)$ atom types share the same LJ parameters. A comparison is shown for the different optimization schemes.

S6 Deviations to experiment

S6.1 Calibration set

Table S10: Comparison of experimental and simulated properties for the CG/EEM-G optimization.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	CCC	1.0	230	582.1	576.2	-5.9	18.8	19.0	0.2	Alk
2	CC(C)C	19.9	260	597.9	604.7	6.8	-	22.3	-	Alk
3	CC(C)C	1.0	265	-	597.7	-	22.4	22.0	-0.4	Alk
4	CCCC	1.0	273	601.0	598.2	-2.8	-	22.6	-	Alk
5	CCCC	9.9	300	572.5	571.5	-1.0	-	21.7	-	Alk
6	CCCC	1.0	264	-	607.5	-	23.1	23.0	-0.1	Alk
7	CC(C)(C)C	1.0	282	603.7	630.7	27.0	23.6	25.3	1.6	Alk
8	CC(C)(C)C	1.8	298	586.0	613.3	27.3	-	24.6	-	Alk
9	CCC(C)C	0.9	298	616.0	618.8	2.8	25.5	25.7	0.2	Alk
10	CCCCC	1.0	298	621.1	621.9	0.8	26.6	26.6	-0.0	Alk
11	CCC(C)(C)C	1.0	298	644.4	663.4	18.9	28.8	29.5	0.7	Alk
12	CC(C)C(C)C	1.0	298	658.6	661.7	3.1	30.0	29.8	-0.3	Alk
13	CCC(C)CC	1.0	298	659.9	659.5	-0.5	30.9	30.3	-0.5	Alk
14	CCCC(C)C	1.0	298	648.5	655.0	6.5	30.4	30.5	0.1	Alk
15	CCCCCC	1.0	298	656.1	657.4	1.3	31.8	31.4	-0.3	Alk
16	CCCCCCC	0.1	298	682.0	683.4	1.5	36.5	36.2	-0.3	Alk
17	CCCCCCCC	1.0	298	698.9	704.1	5.2	41.0	41.0	-0.0	Alk
18	CCBr	1.0	298	1451.2	1441.8	-9.5	-	27.2	-	Br
19	CCBr	1.0	305	-	1429.0	-	27.6	26.9	-0.7	Br
20	CC(Br)Br	1.0	298	2091.8	2088.7	-3.1	-	39.9	-	Br
21	BrCCBr	1.0	298	2169.5	2165.3	-4.2	41.7	43.1	1.4	Br
22	BrCC(Br)Br	1.0	298	2610.1	2598.4	-11.7	-	56.4	-	Br
23	CC(C)Br	1.0	298	1301.4	1302.1	0.8	30.2	30.1	-0.1	Br
24	CCCBr	1.0	298	1345.5	1337.1	-8.4	31.9	31.7	-0.2	Br
25	CC(Br)CBr	1.0	298	1925.0	1927.0	2.1	41.7	45.6	3.9	Br
26	BrCCCBr	1.0	298	1971.2	1958.8	-12.4	-	47.8	-	Br
27	CC(Br)(Br)CBr	1.0	293	2298.5	2361.2	62.7	-	58.0	-	Br
28	CC(Br)C(Br)Br	1.0	293	2354.8	2355.6	0.8	-	57.4	-	Br
29	BrCC(Br)CBr	1.0	298	2411.0	2390.1	-20.9	-	61.3	-	Br
30	CC(C)(C)Br	1.0	298	1212.5	1223.7	11.2	31.8	32.6	0.8	Br
31	CC(C)CBr	1.0	298	1257.1	1257.0	-0.1	34.9	35.3	0.4	Br
32	CCC(C)Br	1.0	298	1253.6	1248.1	-5.5	34.8	34.7	-0.1	Br
33	CCCCBr	1.0	298	1268.6	1265.5	-3.1	36.6	36.3	-0.3	Br
34	CC(CBr)CBr	1.0	298	1799.5	1804.0	4.5	-	50.0	-	Br
35	CCC(Br)CBr	1.0	298	1787.0	1787.2	0.2	45.6	49.2	3.6	Br
36	CC(Br)CCBr	1.0	293	1796.0	1794.4	-1.6	-	50.3	-	Br
37	CC(C)(Br)C(Br)Br	1.0	294	2175.3	2204.2	28.9	-	59.9	-	Br
38	CC(Br)(CBr)CBr	1.0	298	2180.3	2221.2	40.9	-	62.5	-	Br
39	CC(C)(C)CBr	0.0	298	1193.5	1220.4	26.9	-	38.4	-	Br
40	CCC(C)(C)Br	0.0	298	1209.5	1207.3	-2.3	-	37.5	-	Br
41	CCC(C)CBr	1.0	298	1214.4	1215.0	0.6	-	39.6	-	Br
42	CCC(Br)CC	1.0	298	1205.1	1203.0	-2.1	-	38.9	-	Br
43	CC(C)CCBr	1.0	298	1200.7	1209.7	9.0	-	40.0	-	Br
44	CCCC(C)Br	1.0	298	1200.5	1199.3	-1.2	38.5	39.3	0.8	Br
45	CCCCCBr	1.0	298	1211.4	1213.5	2.1	40.9	40.9	0.0	Br
46	CC(C)(C)C(Br)Br	1.0	293	1669.5	1702.9	33.4	-	51.0	-	Br
47	CCC(C)(Br)CC	1.0	293	1179.2	1190.6	11.4	-	42.3	-	Br
48	CCCC(Br)CC	1.0	298	1157.2	1164.3	7.1	-	43.4	-	Br
49	CCCCCCBr	1.0	298	1168.8	1173.0	4.2	45.6	45.5	-0.1	Br
50	CCCCCCCBr	1.0	298	1134.8	1141.2	6.4	50.4	50.2	-0.2	Br
51	CCCCCCCCBr	1.0	298	1107.7	1115.0	7.3	55.1	54.8	-0.3	Br
52	CCCl	1.0	285	906.2	894.2	-12.0	24.9	24.6	-0.3	Cl
53	CCCl	1.4	298	890.0	875.1	-14.9	-	24.0	-	Cl

Continued on next page (CG/EEM-G)

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
54	CC(Cl)Cl	1.0	298	1168.1	1155.5	-12.5	30.6	30.5	-0.1	Cl
55	ClCCCl	1.0	298	1245.6	1237.7	-7.8	34.4	34.6	0.2	Cl
56	CC(Cl)(Cl)Cl	1.0	298	1329.3	1319.7	-9.6	32.4	32.4	-0.0	Cl
57	ClCC(Cl)Cl	1.0	298	1432.8	1438.5	5.7	40.1	42.0	1.9	Cl
58	CC(C)Cl	1.0	298	855.6	845.3	-10.3	-	27.1	-	Cl
59	CC(Cl)CCl	1.0	298	1153.0	1145.2	-7.8	36.2	36.4	0.2	Cl
60	ClCCCCl	1.0	298	1180.0	1180.5	0.5	40.6	40.7	0.1	Cl
61	CC(C)(C)Cl	1.0	298	836.3	832.4	-3.9	28.6	28.7	0.1	Cl
62	CC(C)CCl	1.0	298	871.4	867.6	-3.8	31.7	31.8	0.1	Cl
63	CCC(C)Cl	1.0	298	867.5	858.7	-8.8	31.5	31.5	0.0	Cl
64	CCCCCl	1.0	298	880.4	874.4	-6.0	33.5	32.9	-0.6	Cl
65	CC(Cl)C(C)Cl	1.0	298	1106.3	1091.7	-14.6	-	40.3	-	Cl
66	CCC(Cl)CCl	1.0	298	1111.8	1107.6	-4.2	40.1	40.4	0.3	Cl
67	ClCCCCCl	1.0	298	-	1132.5	-	46.4	47.1	0.7	Cl
68	CCC(C)(C)Cl	1.0	298	859.6	858.2	-1.5	-	33.4	-	Cl
69	CCC(C)CCl	1.0	298	875.0	874.7	-0.3	-	36.1	-	Cl
70	CC(C)CCCl	1.0	298	870.0	871.2	1.2	36.2	36.4	0.2	Cl
71	CCCC(C)Cl	1.0	298	866.0	860.9	-5.1	36.0	36.0	-0.0	Cl
72	CCCCCCl	1.0	298	877.8	874.5	-3.3	38.2	37.4	-0.8	Cl
73	ClCCCCCCl	1.0	298	1095.6	1095.3	-0.3	51.3	51.2	-0.1	Cl
74	CCCCCCCl	1.0	298	873.5	873.0	-0.6	42.0	41.8	-0.2	Cl
75	CC(CCl)C(C)(C)Cl	1.0	298	1064.0	1075.8	11.8	-	49.0	-	Cl
76	CC(Cl)CCC(C)Cl	1.0	298	1044.1	1046.0	1.9	-	51.8	-	Cl
77	ClCCCCCCCl	1.0	298	1063.7	1067.6	3.9	-	55.6	-	Cl
78	CCCCCCCCl	1.0	298	871.5	872.4	0.9	47.0	46.4	-0.6	Cl
79	CCCCCCCCCl	1.0	298	869.4	872.0	2.6	51.4	51.0	-0.4	Cl
80	CCF	1.0	236	817.6	805.8	-11.8	20.7	20.7	-0.0	F
81	CCF	9.1	298	707.5	706.6	-0.9	-	18.3	-	F
82	CC(F)F	1.0	250	1009.0	994.2	-14.8	22.7	22.1	-0.6	F
83	CC(F)F	6.2	298	907.0	903.7	-3.3	-	20.1	-	F
84	CC(F)(F)F	1.0	220	1182.9	1121.4	-61.5	19.2	19.3	0.1	F
85	CC(C)F	1.0	264	769.2	749.7	-19.5	-	22.4	-	F
86	CCCF	1.0	271	781.8	784.3	2.5	-	24.0	-	F
87	CCC(F)F	0.6	276	-	946.7	-	25.1	25.7	0.5	F
88	FCCCF	1.0	298	1005.7	1003.6	-2.1	-	29.6	-	F
89	CC(C)(C)F	1.0	285	752.7	719.1	-33.6	-	23.4	-	F
90	CC(C)(C)F	1.4	298	735.3	704.4	-30.9	-	22.9	-	F
91	CCC(C)F	1.0	298	756.6	743.1	-13.4	-	25.7	-	F
92	CCCCF	1.0	298	770.8	772.8	2.0	-	27.5	-	F
93	FCCCCF	1.0	298	976.7	981.6	4.9	-	35.5	-	F
94	CCCC(F)(F)F	1.4	298	1010.0	961.7	-48.3	-	26.0	-	F
95	CCC(C)(C)F	1.0	298	773.7	748.0	-25.8	-	27.8	-	F
96	CCC(C)CF	0.3	298	791.5	785.9	-5.6	-	30.9	-	F
97	CCCCCF	1.0	298	784.9	788.2	3.3	30.9	32.1	1.1	F
98	CCCCC(C)F	1.0	293	791.4	784.3	-7.1	-	35.2	-	F
99	CCCCCCF	1.0	298	795.8	799.7	4.0	35.6	36.6	1.1	F
100	CC(C)CC(C)(F)F	1.0	293	888.2	868.3	-19.9	-	33.8	-	F
101	FCCCCCCF	1.0	298	940.7	949.9	9.2	-	44.4	-	F
102	CCCCCCCF	1.0	298	800.9	807.6	6.7	40.8	41.3	0.5	F
103	CCCCCCCCF	1.0	298	806.7	814.3	7.6	-	45.9	-	F
104	CCI	1.0	298	1924.0	1908.2	-15.8	31.7	30.8	-0.9	I
105	CC(C)I	1.0	298	1694.5	1694.3	-0.2	34.1	33.7	-0.4	I
106	CCCI	1.0	298	1737.2	1730.7	-6.5	36.0	35.3	-0.7	I
107	ICCCI	1.0	298	2565.1	2530.3	-34.8	-	54.6	-	I
108	ICCCI	0.0	369	-	2397.1	-	53.5	51.1	-2.4	I
109	CC(C)(C)I	0.1	298	1536.0	1569.3	33.3	35.7	36.6	0.9	I
110	CC(C)CI	0.0	298	1595.1	1599.0	3.9	38.8	39.1	0.3	I
111	CCC(C)I	1.0	298	1589.0	1591.0	2.0	38.5	38.3	-0.2	I
112	CCCCI	1.0	298	1606.7	1606.4	-0.4	40.3	39.9	-0.4	I
113	ICCCCI	1.0	298	2349.6	2323.6	-26.0	59.0	59.0	0.0	I
114	CC(C)(C)CI	1.0	293	1494.0	1533.6	39.6	-	42.1	-	I
115	CCC(C)(C)I	0.0	298	1486.6	1520.5	33.9	-	41.5	-	I
116	CC(C)C(C)I	1.0	293	1524.0	1518.2	-5.8	-	41.7	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
117	CCC(I)CC	1.0	298	1505.5	1507.9	2.5	-	42.4	-	I
118	CC(C)CCI	1.0	298	1495.2	1511.0	15.8	42.2	43.6	1.4	I
119	CCCC(C)I	1.0	293	1500.9	1507.8	6.9	-	43.0	-	I
120	CCCCCI	1.0	298	1507.3	1514.0	6.6	44.4	44.5	0.1	I
121	ICCCCCI	1.0	298	2173.4	2161.9	-11.5	-	63.3	-	I
122	CCCC(C)CI	1.0	293	1443.0	1451.2	8.2	-	47.8	-	I
123	CCCCC(C)I	1.0	293	1419.3	1438.2	18.9	-	47.6	-	I
124	CCCCCCI	1.0	298	1431.8	1441.1	9.3	-	49.1	-	I
125	CCCCCCI	1.0	346	-	1379.3	-	46.2	46.5	0.3	I
126	ICCCCCCI	1.0	298	2034.2	2034.1	-0.1	-	67.9	-	I
127	CCCCCCCI	1.0	298	1371.9	1383.9	12.0	-	53.8	-	I
128	CCCCCCCI	0.0	357	-	1313.1	-	48.4	50.3	1.9	I
129	CCCCCCCCI	1.0	298	1326.7	1337.0	10.3	-	58.4	-	I
130	CCCCCCCCI	0.0	374	-	1250.4	-	50.9	53.5	2.6	I
131	CC(Cl)Br	1.0	283	1667.0	1674.4	7.4	-	36.3	-	Mix
132	ClCCBr	1.0	298	1727.0	1722.3	-4.7	-	38.8	-	Mix
133	ClCCBr	1.0	308	-	1705.7	-	37.6	38.4	0.8	Mix
134	FCCBr	1.0	298	1704.4	1699.8	-4.6	-	33.5	-	Mix
135	FCCCl	0.3	298	1167.5	1150.2	-17.4	-	29.2	-	Mix
136	ClCCI	1.0	288	2133.6	2132.4	-1.2	-	43.2	-	Mix
137	CC(F)(F)Cl	1.1	265	1188.8	1168.8	-19.9	22.7	23.1	0.4	Mix
138	CC(F)(F)Cl	3.6	298	1107.7	1090.7	-17.0	19.7	21.5	1.8	Mix
139	CC(F)(Cl)Cl	1.0	298	1233.7	1223.0	-10.7	26.0	27.1	1.1	Mix
140	FC(Cl)CCl	1.0	298	1369.2	1379.0	9.8	-	37.0	-	Mix
141	FC(F)(Br)CBr	1.0	293	2223.8	2271.1	47.3	-	44.5	-	Mix
142	FC(F)(Cl)CCl	1.0	298	1406.6	1427.2	20.6	-	34.1	-	Mix
143	FC(F)C(F)Br	1.0	283	1874.0	1961.0	87.0	-	38.1	-	Mix
144	FC(F)(F)CCl	1.0	285	1353.9	1354.6	0.7	-	29.2	-	Mix
145	FC(Cl)(Cl)CCl	1.0	298	1482.6	1499.4	16.8	-	39.4	-	Mix
146	FC(Cl)C(Cl)Cl	1.0	298	1529.8	1550.5	20.7	-	41.9	-	Mix
147	FC(F)(F)CI	1.0	298	2130.0	2150.0	20.0	-	35.0	-	Mix
148	CC(C)(Cl)Br	1.0	293	1495.0	1489.3	-5.7	-	36.6	-	Mix
149	CC(Br)CCl	1.0	293	1537.0	1559.0	22.0	-	41.2	-	Mix
150	CC(Cl)CBr	1.0	293	1531.0	1556.7	25.7	-	41.5	-	Mix
151	ClCCCBr	1.0	293	1596.9	1591.9	-5.0	-	44.6	-	Mix
152	CC(C)(F)Cl	1.0	293	998.2	958.6	-39.6	-	25.9	-	Mix
153	CC(F)CCl	1.0	293	1086.0	1057.5	-28.5	-	30.9	-	Mix
154	ClCCCI	1.0	293	1904.0	1931.3	27.3	-	47.8	-	Mix
155	ClC(Cl)CCBr	1.0	293	1708.4	1718.1	9.7	-	50.1	-	Mix
156	ClCC(Br)CBr	1.0	287	2093.0	2099.4	6.4	-	57.7	-	Mix
157	CC(F)(Cl)CCl	0.1	298	1255.2	1243.6	-11.7	-	36.6	-	Mix
158	ClC(Cl)(Br)CCBr	1.0	293	2077.2	2110.8	33.6	-	59.4	-	Mix
159	ClCCCCBr	1.0	298	1485.1	1479.1	-6.1	-	49.5	-	Mix
160	CC(Cl)C(Cl)CBr	1.0	293	1598.5	1623.0	24.5	-	56.0	-	Mix
161	CCC(F)(F)C(C)Cl	1.0	293	1108.5	1087.1	-21.4	-	39.2	-	Mix
162	CC(C)(C)C(C)(Cl)Br	1.0	293	1250.0	1453.8	203.8	-	54.7	-	Mix

Table S11: Comparison of experimental and simulated properties for the AT/EEM-G optimization.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	CCC	1.0	230	582.1	577.2	-4.9	18.8	18.9	0.1	Alk
2	CC(C)C	19.9	260	597.9	602.7	4.8	-	22.2	-	Alk
3	CC(C)C	1.0	265	-	595.2	-	22.4	21.9	-0.5	Alk
4	CCCC	1.0	273	601.0	599.0	-2.0	-	22.6	-	Alk
5	CCCC	9.9	300	572.5	571.8	-0.7	-	21.6	-	Alk
6	CCCC	1.0	264	-	607.7	-	23.1	22.9	-0.2	Alk
7	CC(C)(C)C	1.0	282	603.7	628.5	24.8	23.6	24.8	1.2	Alk
8	CC(C)(C)C	1.8	298	586.0	615.1	29.2	-	24.3	-	Alk

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
9	CCC(C)C	0.9	298	616.0	619.0	2.9	25.5	25.7	0.3	Alk
10	CCCCC	1.0	298	621.1	622.3	1.1	26.6	26.6	0.0	Alk
11	CCC(C)(C)C	1.0	298	644.4	663.4	19.0	28.8	29.2	0.5	Alk
12	CC(C)C(C)C	1.0	298	658.6	660.9	2.3	30.0	30.0	-0.1	Alk
13	CCC(C)CC	1.0	298	659.9	659.9	-0.0	30.9	30.6	-0.3	Alk
14	CCCC(C)C	1.0	298	648.5	654.2	5.7	30.4	30.6	0.1	Alk
15	CCCCCC	1.0	298	656.1	657.3	1.2	31.8	31.5	-0.2	Alk
16	CCCCCCC	0.1	298	682.0	683.5	1.6	36.5	36.3	-0.2	Alk
17	CCCCCCCC	1.0	298	698.9	704.1	5.2	41.0	41.3	0.3	Alk
18	CCBr	1.0	298	1451.2	1445.8	-5.4	-	26.9	-	Br
19	CCBr	1.0	305	-	1432.3	-	27.6	26.6	-1.0	Br
20	CC(Br)Br	1.0	298	2091.8	2090.6	-1.1	-	39.3	-	Br
21	BrCCBr	1.0	298	2169.5	2170.4	0.9	41.7	42.6	0.9	Br
22	BrCC(Br)Br	1.0	298	2610.1	2596.7	-13.4	-	55.2	-	Br
23	CC(C)Br	1.0	298	1301.4	1301.5	0.1	30.2	30.1	-0.1	Br
24	CCCBr	1.0	298	1345.5	1339.3	-6.2	31.9	31.5	-0.4	Br
25	CC(Br)CBr	1.0	298	1925.0	1924.6	-0.3	41.7	45.1	3.4	Br
26	BrCCCBr	1.0	298	1971.2	1961.7	-9.4	-	47.4	-	Br
27	CC(Br)(Br)CBr	1.0	293	2298.5	2364.8	66.2	-	56.7	-	Br
28	CC(Br)C(Br)Br	1.0	293	2354.8	2347.5	-7.3	-	56.9	-	Br
29	BrCC(Br)CBr	1.0	298	2411.0	2388.4	-22.6	-	60.6	-	Br
30	CC(C)(C)Br	1.0	298	1212.5	1226.8	14.3	31.8	32.1	0.3	Br
31	CC(C)CBr	1.0	298	1257.1	1255.7	-1.4	34.9	35.1	0.2	Br
32	CCC(C)Br	1.0	298	1253.6	1248.5	-5.1	34.8	34.8	-0.0	Br
33	CCCCBr	1.0	298	1268.6	1266.4	-2.2	36.6	36.2	-0.4	Br
34	CC(CBr)CBr	1.0	298	1799.5	1804.3	4.8	-	49.6	-	Br
35	CCC(Br)CBr	1.0	298	1787.0	1786.8	-0.2	45.6	49.1	3.5	Br
36	CC(Br)CCBr	1.0	293	1796.0	1794.2	-1.8	-	50.2	-	Br
37	CC(C)(Br)C(Br)Br	1.0	294	2175.3	2204.6	29.3	-	58.9	-	Br
38	CC(Br)(CBr)CBr	1.0	298	2180.3	2225.3	45.0	-	61.6	-	Br
39	CC(C)(C)CBr	0.0	298	1193.5	1222.3	28.8	-	37.9	-	Br
40	CCC(C)(C)Br	0.0	298	1209.5	1208.4	-1.1	-	37.0	-	Br
41	CCC(C)CBr	1.0	298	1214.4	1214.9	0.5	-	39.5	-	Br
42	CCC(Br)CC	1.0	298	1205.1	1204.1	-1.0	-	39.1	-	Br
43	CC(C)CCBr	1.0	298	1200.7	1209.2	8.5	-	39.9	-	Br
44	CCCC(C)Br	1.0	298	1200.5	1198.7	-1.8	38.5	39.4	0.9	Br
45	CCCCCBr	1.0	298	1211.4	1212.7	1.3	40.9	40.8	-0.1	Br
46	CC(C)(C)C(Br)Br	1.0	293	1669.5	1704.1	34.6	-	50.4	-	Br
47	CCC(C)(Br)CC	1.0	293	1179.2	1191.8	12.6	-	41.9	-	Br
48	CCCC(Br)CC	1.0	298	1157.2	1165.6	8.4	-	43.7	-	Br
49	CCCCCCBr	1.0	298	1168.8	1171.8	3.0	45.6	45.5	-0.1	Br
50	CCCCCCCBr	1.0	298	1134.8	1139.7	4.9	50.4	50.2	-0.2	Br
51	CCCCCCCCBr	1.0	298	1107.7	1113.3	5.6	55.1	54.9	-0.2	Br
52	CCCl	1.0	285	906.2	900.2	-6.0	24.9	24.5	-0.4	Cl
53	CCCl	1.4	298	890.0	881.4	-8.6	-	24.0	-	Cl
54	CC(Cl)Cl	1.0	298	1168.1	1160.3	-7.7	30.6	30.5	-0.1	Cl
55	ClCCCl	1.0	298	1245.6	1245.1	-0.5	34.4	34.8	0.4	Cl
56	CC(Cl)(Cl)Cl	1.0	298	1329.3	1327.2	-2.1	32.4	32.2	-0.2	Cl
57	ClCC(Cl)Cl	1.0	298	1432.8	1434.9	2.1	40.1	41.7	1.6	Cl
58	CC(C)Cl	1.0	298	855.6	847.4	-8.3	-	27.0	-	Cl
59	CC(Cl)CCl	1.0	298	1153.0	1140.0	-13.0	36.2	36.3	0.1	Cl
60	ClCCCCl	1.0	298	1180.0	1178.4	-1.6	40.6	40.5	-0.1	Cl
61	CC(C)(C)Cl	1.0	298	836.3	835.3	-1.0	28.6	28.2	-0.4	Cl
62	CC(C)CCl	1.0	298	871.4	866.8	-4.5	31.7	31.7	0.0	Cl
63	CCC(C)Cl	1.0	298	867.5	857.8	-9.7	31.5	31.5	-0.0	Cl
64	CCCCCl	1.0	298	880.4	875.7	-4.7	33.5	32.9	-0.6	Cl
65	CC(Cl)C(C)Cl	1.0	298	1106.3	1083.1	-23.2	-	40.1	-	Cl
66	CCC(Cl)CCl	1.0	298	1111.8	1103.5	-8.3	40.1	40.5	0.4	Cl
67	ClCCCCCl	1.0	298	-	1131.7	-	46.4	47.0	0.6	Cl
68	CCC(C)(C)Cl	1.0	298	859.6	860.1	0.4	-	33.1	-	Cl
69	CCC(C)CCl	1.0	298	875.0	874.6	-0.4	-	36.2	-	Cl
70	CC(C)CCCl	1.0	298	870.0	870.7	0.7	36.2	36.5	0.3	Cl
71	CCCC(C)Cl	1.0	298	866.0	860.1	-5.9	36.0	36.0	0.0	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
72	CCCCCCl	1.0	298	877.8	875.0	-2.8	38.2	37.6	-0.6	Cl
73	ClCCCCCCl	1.0	298	1095.6	1094.7	-0.9	51.3	51.3	-0.0	Cl
74	CCCCCCCl	1.0	298	873.5	873.1	-0.5	42.0	42.1	0.1	Cl
75	CC(CCl)C(C)(C)Cl	1.0	298	1064.0	1076.7	12.7	-	49.0	-	Cl
76	CC(Cl)CCC(C)Cl	1.0	298	1044.1	1042.2	-1.9	-	51.8	-	Cl
77	ClCCCCCCCl	1.0	298	1063.7	1066.9	3.2	-	55.6	-	Cl
78	CCCCCCCCl	1.0	298	871.5	872.4	0.9	47.0	46.7	-0.3	Cl
79	CCCCCCCCCl	1.0	298	869.4	871.6	2.2	51.4	51.3	-0.1	Cl
80	CCF	1.0	236	817.6	805.2	-12.4	20.7	20.7	0.0	F
81	CCF	9.1	298	707.5	705.2	-2.3	-	18.3	-	F
82	CC(F)F	1.0	250	1009.0	1022.2	13.2	22.7	22.1	-0.6	F
83	CC(F)F	6.2	298	907.0	912.4	5.4	-	19.8	-	F
84	CC(F)(F)F	1.0	220	1182.9	1433.6	250.7	19.2	21.7	2.5	F
85	CC(C)F	1.0	264	769.2	748.8	-20.4	-	22.3	-	F
86	CCCF	1.0	271	781.8	782.9	1.1	-	24.0	-	F
87	CCC(F)F	0.6	276	-	929.5	-	25.1	25.0	-0.2	F
88	FCCCF	1.0	298	1005.7	1001.1	-4.6	-	29.8	-	F
89	CC(C)(C)F	1.0	285	752.7	723.9	-28.8	-	23.0	-	F
90	CC(C)(C)F	1.4	298	735.3	703.2	-32.1	-	22.4	-	F
91	CCC(C)F	1.0	298	756.6	737.1	-19.5	-	25.5	-	F
92	CCCCF	1.0	298	770.8	769.6	-1.2	-	27.5	-	F
93	FCCCCF	1.0	298	976.7	976.6	-0.1	-	35.8	-	F
94	CCCC(F)(F)F	1.4	298	1010.0	940.8	-69.2	-	24.7	-	F
95	CCC(C)(C)F	1.0	298	773.7	744.3	-29.4	-	27.3	-	F
96	CCC(C)CF	0.3	298	791.5	782.3	-9.2	-	31.0	-	F
97	CCCCCF	1.0	298	784.9	785.6	0.7	30.9	32.2	1.2	F
98	CCCCC(C)F	1.0	293	791.4	778.7	-12.7	-	35.1	-	F
99	CCCCCCF	1.0	298	795.8	796.7	0.9	35.6	36.7	1.2	F
100	CC(C)CC(C)(F)F	1.0	293	888.2	860.2	-28.0	-	33.0	-	F
101	FCCCCCCF	1.0	298	940.7	945.0	4.3	-	44.8	-	F
102	CCCCCCCF	1.0	298	800.9	805.0	4.1	40.8	41.4	0.6	F
103	CCCCCCCCF	1.0	298	806.7	811.2	4.6	-	46.1	-	F
104	CCI	1.0	298	1924.0	1913.6	-10.4	31.7	30.6	-1.1	I
105	CC(C)I	1.0	298	1694.5	1694.2	-0.3	34.1	33.9	-0.2	I
106	CCCI	1.0	298	1737.2	1732.5	-4.8	36.0	35.1	-0.9	I
107	ICCCI	1.0	298	2565.1	2540.4	-24.7	-	54.5	-	I
108	ICCCI	0.0	369	-	2405.3	-	53.5	50.9	-2.6	I
109	CC(C)(C)I	0.1	298	1536.0	1570.4	34.4	35.7	35.8	0.1	I
110	CC(C)CI	0.0	298	1595.1	1596.7	1.6	38.8	38.7	-0.1	I
111	CCC(C)I	1.0	298	1589.0	1591.0	2.0	38.5	38.5	0.0	I
112	CCCCI	1.0	298	1606.7	1607.1	0.3	40.3	39.7	-0.6	I
113	ICCCCI	1.0	298	2349.6	2329.8	-19.7	59.0	59.3	0.3	I
114	CC(C)(C)CI	1.0	293	1494.0	1535.6	41.6	-	41.6	-	I
115	CCC(C)(C)I	0.0	298	1486.6	1519.2	32.6	-	40.7	-	I
116	CC(C)C(C)I	1.0	293	1524.0	1516.7	-7.3	-	42.0	-	I
117	CCC(I)CC	1.0	298	1505.5	1509.1	3.6	-	42.7	-	I
118	CC(C)CCI	1.0	298	1495.2	1507.7	12.6	42.2	43.4	1.2	I
119	CCCC(C)I	1.0	293	1500.9	1507.9	7.0	-	43.2	-	I
120	CCCCCI	1.0	298	1507.3	1513.0	5.6	44.4	44.3	-0.1	I
121	ICCCCCI	1.0	298	2173.4	2165.6	-7.8	-	63.5	-	I
122	CCCC(C)CI	1.0	293	1443.0	1450.2	7.2	-	47.7	-	I
123	CCCCC(C)I	1.0	293	1419.3	1436.5	17.2	-	47.7	-	I
124	CCCCCCI	1.0	298	1431.8	1439.7	7.9	-	48.9	-	I
125	CCCCCCI	1.0	346	-	1377.0	-	46.2	46.3	0.1	I
126	ICCCCCCI	1.0	298	2034.2	2034.9	0.7	-	67.9	-	I
127	CCCCCCCI	1.0	298	1371.9	1381.5	9.6	-	53.6	-	I
128	CCCCCCCI	0.0	357	-	1310.2	-	48.4	50.1	1.7	I
129	CCCCCCCCI	1.0	298	1326.7	1334.0	7.4	-	58.3	-	I
130	CCCCCCCCI	0.0	374	-	1247.9	-	50.9	53.4	2.5	I
131	CC(Cl)Br	1.0	283	1667.0	1673.8	6.8	-	35.8	-	Mix
132	ClCCBr	1.0	298	1727.0	1728.6	1.6	-	38.6	-	Mix
133	ClCCBr	1.0	308	-	1710.4	-	37.6	38.2	0.6	Mix
134	FCCBr	1.0	298	1704.4	1700.9	-3.5	-	33.3	-	Mix

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
135	FCCCl	0.3	298	1167.5	1156.2	-11.3	-	29.4	-	Mix
136	ClCCI	1.0	288	2133.6	2140.2	6.7	-	42.9	-	Mix
137	CC(F)(F)Cl	1.1	265	1188.8	1193.5	4.7	22.7	22.6	-0.1	Mix
138	CC(F)(F)Cl	3.6	298	1107.7	1100.2	-7.5	19.7	20.8	1.1	Mix
139	CC(F)(Cl)Cl	1.0	298	1233.7	1227.3	-6.3	26.0	26.6	0.5	Mix
140	FC(Cl)CCl	1.0	298	1369.2	1375.9	6.7	-	36.8	-	Mix
141	FC(F)(Br)CBr	1.0	293	2223.8	2267.1	43.2	-	42.9	-	Mix
142	FC(F)(Cl)CCl	1.0	298	1406.6	1413.3	6.7	-	32.9	-	Mix
143	FC(F)C(F)Br	1.0	283	1874.0	1957.8	83.8	-	37.3	-	Mix
144	FC(F)(F)CCl	1.0	285	1353.9	1349.7	-4.2	-	28.1	-	Mix
145	FC(Cl)(Cl)CCl	1.0	298	1482.6	1488.6	6.0	-	38.3	-	Mix
146	FC(Cl)C(Cl)Cl	1.0	298	1529.8	1527.2	-2.6	-	41.1	-	Mix
147	FC(F)(F)CI	1.0	298	2130.0	2125.0	-5.0	-	33.5	-	Mix
148	CC(C)(Cl)Br	1.0	293	1495.0	1486.0	-9.0	-	35.7	-	Mix
149	CC(Br)CCl	1.0	293	1537.0	1555.1	18.1	-	40.9	-	Mix
150	CC(Cl)CBr	1.0	293	1531.0	1551.5	20.5	-	41.0	-	Mix
151	ClCCCBr	1.0	293	1596.9	1591.3	-5.6	-	44.2	-	Mix
152	CC(C)(F)Cl	1.0	293	998.2	959.5	-38.7	-	25.1	-	Mix
153	CC(F)CCl	1.0	293	1086.0	1051.0	-35.0	-	30.7	-	Mix
154	ClCCCI	1.0	293	1904.0	1937.1	33.1	-	47.8	-	Mix
155	ClC(Cl)CCBr	1.0	293	1708.4	1710.3	1.9	-	49.7	-	Mix
156	ClCC(Br)CBr	1.0	287	2093.0	2093.5	0.5	-	57.1	-	Mix
157	CC(F)(Cl)CCl	0.1	298	1255.2	1232.9	-22.4	-	35.6	-	Mix
158	ClC(Cl)(Br)CCBr	1.0	293	2077.2	2116.2	39.0	-	58.9	-	Mix
159	ClCCCCBr	1.0	298	1485.1	1480.0	-5.1	-	49.5	-	Mix
160	CC(Cl)C(Cl)CBr	1.0	293	1598.5	1611.3	12.8	-	55.3	-	Mix
161	CCC(F)(F)C(C)Cl	1.0	293	1108.5	1077.2	-31.3	-	38.2	-	Mix
162	CC(C)(C)C(C)(Cl)Br	1.0	293	1250.0	1451.9	201.9	-	53.7	-	Mix

Table S12: Comparison of experimental and simulated properties for the SH/EEM-G optimization.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	CCC	1.0	230	582.1	576.5	-5.7	18.8	19.1	0.3	Alk
2	CC(C)C	19.9	260	597.9	603.9	6.0	-	22.3	-	Alk
3	CC(C)C	1.0	265	-	598.6	-	22.4	22.1	-0.3	Alk
4	CCCC	1.0	273	601.0	599.5	-1.5	-	22.8	-	Alk
5	CCCC	9.9	300	572.5	574.1	1.7	-	21.8	-	Alk
6	CCCC	1.0	264	-	608.1	-	23.1	23.1	-0.0	Alk
7	CC(C)(C)C	1.0	282	603.7	635.6	31.9	23.6	25.4	1.8	Alk
8	CC(C)(C)C	1.8	298	586.0	620.0	34.0	-	24.8	-	Alk
9	CCC(C)C	0.9	298	616.0	619.6	3.6	25.5	25.7	0.3	Alk
10	CCCCC	1.0	298	621.1	623.5	2.4	26.6	26.7	0.1	Alk
11	CCC(C)(C)C	1.0	298	644.4	667.1	22.6	28.8	29.5	0.8	Alk
12	CC(C)C(C)C	1.0	298	658.6	662.2	3.6	30.0	29.8	-0.3	Alk
13	CCC(C)CC	1.0	298	659.9	660.2	0.3	30.9	30.3	-0.6	Alk
14	CCCC(C)C	1.0	298	648.5	655.4	7.0	30.4	30.5	0.1	Alk
15	CCCCCC	1.0	298	656.1	658.6	2.5	31.8	31.5	-0.2	Alk
16	CCCCCCC	0.1	298	682.0	684.5	2.5	36.5	36.2	-0.3	Alk
17	CCCCCCCC	1.0	298	698.9	704.9	6.0	41.0	41.1	0.0	Alk
18	CCBr	1.0	298	1451.2	1442.4	-8.8	-	27.5	-	Br
19	CCBr	1.0	305	-	1429.3	-	27.6	27.2	-0.4	Br
20	CC(Br)Br	1.0	298	2091.8	2079.4	-12.3	-	38.6	-	Br
21	BrCCBr	1.0	298	2169.5	2169.6	0.1	41.7	42.7	1.0	Br
22	BrCC(Br)Br	1.0	298	2610.1	2597.1	-13.0	-	54.8	-	Br
23	CC(C)Br	1.0	298	1301.4	1300.8	-0.6	30.2	30.2	-0.0	Br
24	CCCBr	1.0	298	1345.5	1337.5	-8.0	31.9	31.9	-0.0	Br
25	CC(Br)CBr	1.0	298	1925.0	1926.0	1.0	41.7	44.6	2.9	Br
26	BrCCCBr	1.0	298	1971.2	1967.2	-4.0	-	48.0	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
27	CC(Br)(Br)CBr	1.0	293	2298.5	2359.3	60.8	-	55.6	-	Br
28	CC(Br)C(Br)Br	1.0	293	2354.8	2351.3	-3.5	-	56.0	-	Br
29	BrCC(Br)CBr	1.0	298	2411.0	2403.1	-7.9	-	60.8	-	Br
30	CC(C)(C)Br	1.0	298	1212.5	1223.8	11.3	31.8	31.7	-0.1	Br
31	CC(C)CBr	1.0	298	1257.1	1256.4	-0.7	34.9	35.2	0.3	Br
32	CCC(C)Br	1.0	298	1253.6	1245.9	-7.7	34.8	34.6	-0.2	Br
33	CCCCBr	1.0	298	1268.6	1265.3	-3.3	36.6	36.3	-0.3	Br
34	CC(CBr)CBr	1.0	298	1799.5	1807.8	8.3	-	49.5	-	Br
35	CCC(Br)CBr	1.0	298	1787.0	1786.6	-0.4	45.6	48.2	2.6	Br
36	CC(Br)CCBr	1.0	293	1796.0	1795.6	-0.4	-	49.8	-	Br
37	CC(C)(Br)C(Br)Br	1.0	294	2175.3	2196.0	20.7	-	56.6	-	Br
38	CC(Br)(CBr)CBr	1.0	298	2180.3	2225.2	44.9	-	60.3	-	Br
39	CC(C)(C)CBr	0.0	298	1193.5	1225.3	31.9	-	38.3	-	Br
40	CCC(C)(C)Br	0.0	298	1209.5	1204.9	-4.6	-	36.4	-	Br
41	CCC(C)CBr	1.0	298	1214.4	1213.6	-0.8	-	39.4	-	Br
42	CCC(Br)CC	1.0	298	1205.1	1201.4	-3.7	-	38.8	-	Br
43	CC(C)CCBr	1.0	298	1200.7	1208.8	8.1	-	39.8	-	Br
44	CCCC(C)Br	1.0	298	1200.5	1196.5	-4.0	38.5	39.1	0.6	Br
45	CCCCCBr	1.0	298	1211.4	1212.6	1.2	40.9	40.8	-0.1	Br
46	CC(C)(C)C(Br)Br	1.0	293	1669.5	1700.2	30.7	-	49.3	-	Br
47	CCC(C)(Br)CC	1.0	293	1179.2	1186.2	7.0	-	40.9	-	Br
48	CCCC(Br)CC	1.0	298	1157.2	1162.3	5.1	-	43.1	-	Br
49	CCCCCCBr	1.0	298	1168.8	1171.7	2.9	45.6	45.3	-0.3	Br
50	CCCCCCCBr	1.0	298	1134.8	1140.0	5.2	50.4	49.9	-0.5	Br
51	CCCCCCCCBr	1.0	298	1107.7	1114.1	6.4	55.1	54.5	-0.6	Br
52	CCCl	1.0	285	906.2	896.5	-9.7	24.9	24.7	-0.2	Cl
53	CCCl	1.4	298	890.0	877.9	-12.1	-	24.2	-	Cl
54	CC(Cl)Cl	1.0	298	1168.1	1161.0	-7.0	30.6	30.6	0.0	Cl
55	ClCCCl	1.0	298	1245.6	1236.3	-9.3	34.4	34.7	0.3	Cl
56	CC(Cl)(Cl)Cl	1.0	298	1329.3	1334.4	5.1	32.4	32.3	-0.1	Cl
57	ClCC(Cl)Cl	1.0	298	1432.8	1435.7	3.0	40.1	41.9	1.8	Cl
58	CC(C)Cl	1.0	298	855.6	848.8	-6.9	-	27.0	-	Cl
59	CC(Cl)CCl	1.0	298	1153.0	1142.9	-10.1	36.2	36.4	0.2	Cl
60	ClCCCCl	1.0	298	1180.0	1180.1	0.1	40.6	40.8	0.2	Cl
61	CC(C)(C)Cl	1.0	298	836.3	837.2	0.9	28.6	28.0	-0.6	Cl
62	CC(C)CCl	1.0	298	871.4	868.3	-3.0	31.7	31.8	0.1	Cl
63	CCC(C)Cl	1.0	298	867.5	858.6	-8.9	31.5	31.3	-0.2	Cl
64	CCCCCl	1.0	298	880.4	875.9	-4.5	33.5	33.0	-0.5	Cl
65	CC(Cl)C(C)Cl	1.0	298	1106.3	1090.3	-16.0	-	39.9	-	Cl
66	CCC(Cl)CCl	1.0	298	1111.8	1106.4	-5.4	40.1	40.4	0.3	Cl
67	ClCCCCCl	1.0	298	-	1132.7	-	46.4	47.2	0.8	Cl
68	CCC(C)(C)Cl	1.0	298	859.6	859.9	0.2	-	32.6	-	Cl
69	CCC(C)CCl	1.0	298	875.0	874.8	-0.2	-	36.1	-	Cl
70	CC(C)CCCl	1.0	298	870.0	872.6	2.6	36.2	36.4	0.2	Cl
71	CCCC(C)Cl	1.0	298	866.0	860.6	-5.4	36.0	35.8	-0.2	Cl
72	CCCCCCl	1.0	298	877.8	875.4	-2.4	38.2	37.5	-0.7	Cl
73	ClCCCCCCl	1.0	298	1095.6	1096.1	0.5	51.3	51.3	-0.0	Cl
74	CCCCCCCl	1.0	298	873.5	874.1	0.5	42.0	41.9	-0.1	Cl
75	CC(CCl)C(C)(C)Cl	1.0	298	1064.0	1075.2	11.2	-	47.8	-	Cl
76	CC(Cl)CCC(C)Cl	1.0	298	1044.1	1043.7	-0.4	-	51.2	-	Cl
77	ClCCCCCCCl	1.0	298	1063.7	1068.0	4.3	-	55.6	-	Cl
78	CCCCCCCCl	1.0	298	871.5	873.4	1.9	47.0	46.5	-0.5	Cl
79	CCCCCCCCCl	1.0	298	869.4	873.0	3.7	51.4	51.0	-0.4	Cl
80	CCF	1.0	236	817.6	802.4	-15.2	20.7	21.1	0.4	F
81	CCF	9.1	298	707.5	705.9	-1.6	-	18.7	-	F
82	CC(F)F	1.0	250	1009.0	1009.8	0.8	22.7	22.2	-0.5	F
83	CC(F)F	6.2	298	907.0	904.4	-2.6	-	20.0	-	F
84	CC(F)(F)F	1.0	220	1182.9	1468.6	285.7	19.2	22.0	2.8	F
85	CC(C)F	1.0	264	769.2	752.0	-17.2	-	22.6	-	F
86	CCCF	1.0	271	781.8	782.2	0.4	-	24.3	-	F
87	CCC(F)F	0.6	276	-	932.3	-	25.1	25.2	0.1	F
88	FCCCF	1.0	298	1005.7	997.9	-7.8	-	29.8	-	F
89	CC(C)(C)F	1.0	285	752.7	728.5	-24.2	-	23.3	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
90	CC(C)(C)F	1.4	298	735.3	712.6	-22.7	-	22.8	-	F
91	CCC(C)F	1.0	298	756.6	739.7	-16.8	-	25.7	-	F
92	CCCCF	1.0	298	770.8	770.7	-0.1	-	27.6	-	F
93	FCCCCF	1.0	298	976.7	978.9	2.2	-	36.2	-	F
94	CCCC(F)(F)F	1.4	298	1010.0	953.1	-56.9	-	24.6	-	F
95	CCC(C)(C)F	1.0	298	773.7	749.3	-24.4	-	27.5	-	F
96	CCC(C)CF	0.3	298	791.5	783.3	-8.1	-	31.0	-	F
97	CCCCCF	1.0	298	784.9	786.7	1.8	30.9	32.2	1.3	F
98	CCCCC(C)F	1.0	293	791.4	781.1	-10.3	-	35.0	-	F
99	CCCCCCF	1.0	298	795.8	797.5	1.7	35.6	36.7	1.1	F
100	CC(C)CC(C)(F)F	1.0	293	888.2	866.3	-21.9	-	33.0	-	F
101	FCCCCCCF	1.0	298	940.7	947.0	6.3	-	44.9	-	F
102	CCCCCCCF	1.0	298	800.9	806.3	5.4	40.8	41.2	0.4	F
103	CCCCCCCCF	1.0	298	806.7	812.8	6.1	-	45.8	-	F
104	CCI	1.0	298	1924.0	1908.9	-15.1	31.7	30.9	-0.8	I
105	CC(C)I	1.0	298	1694.5	1690.3	-4.3	34.1	33.6	-0.5	I
106	CCCI	1.0	298	1737.2	1730.8	-6.4	36.0	35.4	-0.7	I
107	ICCCI	1.0	298	2565.1	2530.4	-34.7	-	54.6	-	I
108	ICCCI	0.0	369	-	2401.8	-	53.5	51.1	-2.4	I
109	CC(C)(C)I	0.1	298	1536.0	1577.8	41.7	35.7	36.5	0.8	I
110	CC(C)CI	0.0	298	1595.1	1597.8	2.7	38.8	39.0	0.2	I
111	CCC(C)I	1.0	298	1589.0	1588.4	-0.6	38.5	38.1	-0.4	I
112	CCCCI	1.0	298	1606.7	1606.2	-0.5	40.3	39.9	-0.4	I
113	ICCCCI	1.0	298	2349.6	2324.4	-25.1	59.0	59.1	0.1	I
114	CC(C)(C)CI	1.0	293	1494.0	1538.2	44.2	-	42.0	-	I
115	CCC(C)(C)I	0.0	298	1486.6	1521.8	35.2	-	41.2	-	I
116	CC(C)C(C)I	1.0	293	1524.0	1515.5	-8.5	-	41.3	-	I
117	CCC(I)CC	1.0	298	1505.5	1506.0	0.5	-	42.3	-	I
118	CC(C)CCI	1.0	298	1495.2	1509.4	14.2	42.2	43.5	1.3	I
119	CCCC(C)I	1.0	293	1500.9	1505.2	4.3	-	42.8	-	I
120	CCCCCI	1.0	298	1507.3	1513.6	6.2	44.4	44.5	0.1	I
121	ICCCCCI	1.0	298	2173.4	2162.7	-10.8	-	63.3	-	I
122	CCCC(C)CI	1.0	293	1443.0	1449.7	6.7	-	47.7	-	I
123	CCCCC(C)I	1.0	293	1419.3	1435.6	16.3	-	47.3	-	I
124	CCCCCCI	1.0	298	1431.8	1440.6	8.8	-	49.0	-	I
125	CCCCCCI	1.0	346	-	1380.6	-	46.2	46.5	0.3	I
126	ICCCCCCI	1.0	298	2034.2	2033.4	-0.8	-	67.8	-	I
127	CCCCCCCI	1.0	298	1371.9	1383.1	11.2	-	53.7	-	I
128	CCCCCCCI	0.0	357	-	1314.8	-	48.4	50.2	1.8	I
129	CCCCCCCCI	1.0	298	1326.7	1336.0	9.4	-	58.3	-	I
130	CCCCCCCCI	0.0	374	-	1253.4	-	50.9	53.5	2.6	I
131	CC(Cl)Br	1.0	283	1667.0	1667.2	0.2	-	35.4	-	Mix
132	ClCCBr	1.0	298	1727.0	1724.1	-2.9	-	38.7	-	Mix
133	ClCCBr	1.0	308	-	1707.2	-	37.6	38.2	0.6	Mix
134	FCCBr	1.0	298	1704.4	1694.6	-9.8	-	33.0	-	Mix
135	FCCCl	0.3	298	1167.5	1145.2	-22.3	-	29.0	-	Mix
136	ClCCI	1.0	288	2133.6	2133.4	-0.2	-	43.2	-	Mix
137	CC(F)(F)Cl	1.1	265	1188.8	1173.0	-15.8	22.7	22.2	-0.5	Mix
138	CC(F)(F)Cl	3.6	298	1107.7	1099.8	-7.9	19.7	20.8	1.0	Mix
139	CC(F)(Cl)Cl	1.0	298	1233.7	1231.3	-2.4	26.0	26.6	0.6	Mix
140	FC(Cl)CCl	1.0	298	1369.2	1369.0	-0.2	-	36.5	-	Mix
141	FC(F)(Br)CBr	1.0	293	2223.8	2269.0	45.2	-	42.0	-	Mix
142	FC(F)(Cl)CCl	1.0	298	1406.6	1422.4	15.8	-	33.0	-	Mix
143	FC(F)C(F)Br	1.0	283	1874.0	1929.3	55.3	-	35.4	-	Mix
144	FC(F)(F)CCl	1.0	285	1353.9	1343.7	-10.2	-	27.7	-	Mix
145	FC(Cl)(Cl)CCl	1.0	298	1482.6	1501.8	19.2	-	38.6	-	Mix
146	FC(Cl)C(Cl)Cl	1.0	298	1529.8	1541.6	11.8	-	41.3	-	Mix
147	FC(F)(F)CI	1.0	298	2130.0	2137.7	7.7	-	33.4	-	Mix
148	CC(C)(Cl)Br	1.0	293	1495.0	1487.0	-8.0	-	34.9	-	Mix
149	CC(Br)CCl	1.0	293	1537.0	1556.5	19.5	-	40.7	-	Mix
150	CC(Cl)CBr	1.0	293	1531.0	1553.6	22.6	-	40.7	-	Mix
151	ClCCCBr	1.0	293	1596.9	1595.9	-1.0	-	44.7	-	Mix
152	CC(C)(F)Cl	1.0	293	998.2	965.5	-32.7	-	25.2	-	Mix

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
153	CC(F)CCl	1.0	293	1086.0	1051.4	-34.6	-	30.6	-	Mix
154	ClCCCI	1.0	293	1904.0	1933.1	29.1	-	48.0	-	Mix
155	ClC(Cl)CCBr	1.0	293	1708.4	1722.5	14.1	-	49.8	-	Mix
156	ClCC(Br)CBr	1.0	287	2093.0	2107.2	14.2	-	57.7	-	Mix
157	CC(F)(Cl)CCl	0.1	298	1255.2	1245.4	-9.8	-	35.9	-	Mix
158	ClC(Cl)(Br)CCBr	1.0	293	2077.2	2116.4	39.2	-	57.4	-	Mix
159	ClCCCCBr	1.0	298	1485.1	1483.0	-2.1	-	50.2	-	Mix
160	CC(Cl)C(Cl)CBr	1.0	293	1598.5	1622.9	24.4	-	55.4	-	Mix
161	CCC(F)(F)C(C)Cl	1.0	293	1108.5	1084.4	-24.1	-	38.1	-	Mix
162	CC(C)(C)C(C)(Cl)Br	1.0	293	1250.0	1450.4	200.4	-	52.4	-	Mix

Table S13: Comparison of experimental and simulated properties for the SH/EEM-M optimization.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	CCC	1.0	230	582.1	577.2	-4.9	18.8	19.0	0.2	Alk
2	CC(C)C	19.9	260	597.9	605.5	7.5	-	22.1	-	Alk
3	CC(C)C	1.0	265	-	597.7	-	22.4	21.9	-0.5	Alk
4	CCCC	1.0	273	601.0	598.3	-2.7	-	22.6	-	Alk
5	CCCC	9.9	300	572.5	573.6	1.2	-	21.7	-	Alk
6	CCCC	1.0	264	-	607.9	-	23.1	22.9	-0.2	Alk
7	CC(C)(C)C	1.0	282	603.7	622.9	19.2	23.6	24.7	1.0	Alk
8	CC(C)(C)C	1.8	298	586.0	609.7	23.8	-	24.1	-	Alk
9	CCC(C)C	0.9	298	616.0	619.8	3.7	25.5	25.5	0.1	Alk
10	CCCCC	1.0	298	621.1	622.4	1.3	26.6	26.5	-0.1	Alk
11	CCC(C)(C)C	1.0	298	644.4	658.8	14.4	28.8	29.0	0.2	Alk
12	CC(C)C(C)C	1.0	298	658.6	661.8	3.3	30.0	29.4	-0.6	Alk
13	CCC(C)CC	1.0	298	659.9	659.8	-0.1	30.9	30.1	-0.7	Alk
14	CCCC(C)C	1.0	298	648.5	655.0	6.6	30.4	30.3	-0.1	Alk
15	CCCCCC	1.0	298	656.1	657.2	1.1	31.8	31.3	-0.4	Alk
16	CCCCCCC	0.1	298	682.0	683.1	1.1	36.5	36.0	-0.5	Alk
17	CCCCCCCC	1.0	298	698.9	703.4	4.6	41.0	40.8	-0.2	Alk
18	CCBr	1.0	298	1451.2	1440.6	-10.6	-	27.2	-	Br
19	CCBr	1.0	305	-	1428.4	-	27.6	27.0	-0.6	Br
20	CC(Br)Br	1.0	298	2091.8	2072.0	-19.8	-	37.8	-	Br
21	BrCCBr	1.0	298	2169.5	2166.6	-2.9	41.7	42.4	0.7	Br
22	BrCC(Br)Br	1.0	298	2610.1	2593.5	-16.6	-	53.9	-	Br
23	CC(C)Br	1.0	298	1301.4	1301.1	-0.3	30.2	30.1	-0.1	Br
24	CCCBr	1.0	298	1345.5	1335.1	-10.4	31.9	31.5	-0.4	Br
25	CC(Br)CBr	1.0	298	1925.0	1926.0	1.1	41.7	44.2	2.5	Br
26	BrCCCBr	1.0	298	1971.2	1947.5	-23.7	-	45.8	-	Br
27	CC(Br)(Br)CBr	1.0	293	2298.5	2346.5	47.9	-	56.4	-	Br
28	CC(Br)C(Br)Br	1.0	293	2354.8	2353.5	-1.3	-	55.5	-	Br
29	BrCC(Br)CBr	1.0	298	2411.0	2393.6	-17.4	-	59.6	-	Br
30	CC(C)(C)Br	1.0	298	1212.5	1207.2	-5.3	31.8	31.9	0.1	Br
31	CC(C)CBr	1.0	298	1257.1	1258.2	1.1	34.9	35.4	0.5	Br
32	CCC(C)Br	1.0	298	1253.6	1246.1	-7.5	34.8	34.5	-0.3	Br
33	CCCCBr	1.0	298	1268.6	1264.6	-4.0	36.6	36.3	-0.3	Br
34	CC(CBr)CBr	1.0	298	1799.5	1800.0	0.5	-	48.7	-	Br
35	CCC(Br)CBr	1.0	298	1787.0	1786.7	-0.3	45.6	47.9	2.3	Br
36	CC(Br)CCBr	1.0	293	1796.0	1784.9	-11.1	-	48.5	-	Br
37	CC(C)(Br)C(Br)Br	1.0	294	2175.3	2190.3	15.0	-	56.8	-	Br
38	CC(Br)(CBr)CBr	1.0	298	2180.3	2208.6	28.3	-	58.5	-	Br
39	CC(C)(C)CBr	0.0	298	1193.5	1219.9	26.4	-	39.0	-	Br
40	CCC(C)(C)Br	0.0	298	1209.5	1198.3	-11.2	-	36.8	-	Br
41	CCC(C)CBr	1.0	298	1214.4	1215.9	1.5	-	39.6	-	Br
42	CCC(Br)CC	1.0	298	1205.1	1200.8	-4.3	-	38.4	-	Br
43	CC(C)CCBr	1.0	298	1200.7	1210.9	10.2	-	40.1	-	Br
44	CCCC(C)Br	1.0	298	1200.5	1197.1	-3.4	38.5	39.0	0.5	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
45	CCCCCBr	1.0	298	1211.4	1211.8	0.4	40.9	40.9	0.0	Br
46	CC(C)(C)C(Br)Br	1.0	293	1669.5	1700.0	30.5	-	51.1	-	Br
47	CCC(C)(Br)CC	1.0	293	1179.2	1183.4	4.2	-	41.5	-	Br
48	CCCC(Br)CC	1.0	298	1157.2	1162.5	5.4	-	43.0	-	Br
49	CCCCCCBr	1.0	298	1168.8	1171.3	2.5	45.6	45.5	-0.1	Br
50	CCCCCCCBr	1.0	298	1134.8	1139.1	4.3	50.4	50.1	-0.3	Br
51	CCCCCCCCBr	1.0	298	1107.7	1113.5	5.8	55.1	54.8	-0.3	Br
52	CCCl	1.0	285	906.2	896.4	-9.8	24.9	24.3	-0.6	Cl
53	CCCl	1.4	298	890.0	878.7	-11.3	-	23.9	-	Cl
54	CC(Cl)Cl	1.0	298	1168.1	1162.8	-5.3	30.6	30.4	-0.2	Cl
55	ClCCCl	1.0	298	1245.6	1238.1	-7.5	34.4	34.4	-0.0	Cl
56	CC(Cl)(Cl)Cl	1.0	298	1329.3	1330.8	1.5	32.4	33.7	1.3	Cl
57	ClCC(Cl)Cl	1.0	298	1432.8	1440.7	7.9	40.1	42.1	2.0	Cl
58	CC(C)Cl	1.0	298	855.6	852.5	-3.1	-	27.0	-	Cl
59	CC(Cl)CCl	1.0	298	1153.0	1146.0	-7.0	36.2	36.2	0.0	Cl
60	ClCCCCl	1.0	298	1180.0	1165.6	-14.4	40.6	38.5	-2.1	Cl
61	CC(C)(C)Cl	1.0	298	836.3	834.9	-1.4	28.6	29.1	0.5	Cl
62	CC(C)CCl	1.0	298	871.4	872.3	0.9	31.7	32.1	0.4	Cl
63	CCC(C)Cl	1.0	298	867.5	860.5	-7.0	31.5	31.2	-0.3	Cl
64	CCCCCl	1.0	298	880.4	877.8	-2.6	33.5	33.2	-0.3	Cl
65	CC(Cl)C(C)Cl	1.0	298	1106.3	1095.0	-11.3	-	40.1	-	Cl
66	CCC(Cl)CCl	1.0	298	1111.8	1108.7	-3.1	40.1	40.3	0.2	Cl
67	ClCCCCCl	1.0	298	-	1126.5	-	46.4	45.1	-1.3	Cl
68	CCC(C)(C)Cl	1.0	298	859.6	859.3	-0.4	-	33.7	-	Cl
69	CCC(C)CCl	1.0	298	875.0	879.3	4.3	-	36.7	-	Cl
70	CC(C)CCCl	1.0	298	870.0	876.7	6.7	36.2	37.1	0.9	Cl
71	CCCC(C)Cl	1.0	298	866.0	862.6	-3.4	36.0	36.0	-0.0	Cl
72	CCCCCCl	1.0	298	877.8	876.9	-0.9	38.2	37.8	-0.4	Cl
73	ClCCCCCCl	1.0	298	1095.6	1092.1	-3.5	51.3	49.9	-1.4	Cl
74	CCCCCCCl	1.0	298	873.5	875.3	1.8	42.0	42.4	0.4	Cl
75	CC(CCl)C(C)(C)Cl	1.0	298	1064.0	1073.0	9.0	-	48.2	-	Cl
76	CC(Cl)CCC(C)Cl	1.0	298	1044.1	1043.3	-0.8	-	50.2	-	Cl
77	ClCCCCCCCl	1.0	298	1063.7	1065.2	1.5	-	54.5	-	Cl
78	CCCCCCCCl	1.0	298	871.5	874.1	2.6	47.0	47.1	0.1	Cl
79	CCCCCCCCCl	1.0	298	869.4	873.6	4.3	51.4	51.7	0.3	Cl
80	CCF	1.0	236	817.6	806.4	-11.2	20.7	21.1	0.4	F
81	CCF	9.1	298	707.5	709.6	2.1	-	18.7	-	F
82	CC(F)F	1.0	250	1009.0	1002.9	-6.1	22.7	22.5	-0.2	F
83	CC(F)F	6.2	298	907.0	905.5	-1.5	-	20.4	-	F
84	CC(F)(F)F	1.0	220	1182.9	1401.9	219.0	19.2	22.1	2.9	F
85	CC(C)F	1.0	264	769.2	755.5	-13.7	-	22.9	-	F
86	CCCF	1.0	271	781.8	783.1	1.3	-	24.2	-	F
87	CCC(F)F	0.6	276	-	941.5	-	25.1	25.9	0.8	F
88	FCCCF	1.0	298	1005.7	984.4	-21.3	-	28.2	-	F
89	CC(C)(C)F	1.0	285	752.7	714.6	-38.1	-	23.7	-	F
90	CC(C)(C)F	1.4	298	735.3	697.4	-37.9	-	23.1	-	F
91	CCC(C)F	1.0	298	756.6	743.2	-13.3	-	25.9	-	F
92	CCCCF	1.0	298	770.8	773.5	2.6	-	28.0	-	F
93	FCCCCF	1.0	298	976.7	972.5	-4.2	-	34.4	-	F
94	CCCC(F)(F)F	1.4	298	1010.0	945.5	-64.5	-	28.2	-	F
95	CCC(C)(C)F	1.0	298	773.7	741.2	-32.5	-	27.9	-	F
96	CCC(C)CF	0.3	298	791.5	788.4	-3.1	-	31.6	-	F
97	CCCCCF	1.0	298	784.9	789.7	4.8	30.9	32.7	1.8	F
98	CCCCC(C)F	1.0	293	791.4	784.7	-6.7	-	35.6	-	F
99	CCCCCCF	1.0	298	795.8	800.4	4.6	35.6	37.3	1.7	F
100	CC(C)CC(C)(F)F	1.0	293	888.2	868.4	-19.8	-	35.9	-	F
101	FCCCCCCF	1.0	298	940.7	946.6	5.9	-	44.4	-	F
102	CCCCCCCF	1.0	298	800.9	808.1	7.2	40.8	42.0	1.2	F
103	CCCCCCCCF	1.0	298	806.7	813.9	7.2	-	46.6	-	F
104	CCI	1.0	298	1924.0	1911.7	-12.4	31.7	31.1	-0.6	I
105	CC(C)I	1.0	298	1694.5	1694.9	0.4	34.1	33.7	-0.4	I
106	CCCI	1.0	298	1737.2	1730.8	-6.4	36.0	35.4	-0.7	I
107	ICCCI	1.0	298	2565.1	2529.1	-36.0	-	54.2	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
108	ICCCI	0.0	369	-	2398.7	-	53.5	50.6	-2.9	I
109	CC(C)(C)I	0.1	298	1536.0	1552.3	16.3	35.7	35.7	-0.0	I
110	CC(C)CI	0.0	298	1595.1	1598.5	3.4	38.8	38.9	0.1	I
111	CCC(C)I	1.0	298	1589.0	1589.7	0.7	38.5	38.1	-0.4	I
112	CCCCI	1.0	298	1606.7	1605.5	-1.3	40.3	40.0	-0.3	I
113	ICCCCI	1.0	298	2349.6	2323.9	-25.6	59.0	59.3	0.3	I
114	CC(C)(C)CI	1.0	293	1494.0	1527.0	33.0	-	42.2	-	I
115	CCC(C)(C)I	0.0	298	1486.6	1509.0	22.4	-	40.6	-	I
116	CC(C)C(C)I	1.0	293	1524.0	1517.2	-6.8	-	41.4	-	I
117	CCC(I)CC	1.0	298	1505.5	1505.9	0.4	-	42.1	-	I
118	CC(C)CCI	1.0	298	1495.2	1510.4	15.2	42.2	43.6	1.4	I
119	CCCC(C)I	1.0	293	1500.9	1506.6	5.7	-	42.8	-	I
120	CCCCCI	1.0	298	1507.3	1512.2	4.8	44.4	44.5	0.1	I
121	ICCCCCI	1.0	298	2173.4	2160.7	-12.7	-	63.6	-	I
122	CCCC(C)CI	1.0	293	1443.0	1449.9	6.9	-	47.7	-	I
123	CCCCC(C)I	1.0	293	1419.3	1436.1	16.8	-	47.3	-	I
124	CCCCCCI	1.0	298	1431.8	1439.4	7.6	-	49.0	-	I
125	CCCCCCI	1.0	346	-	1378.7	-	46.2	46.4	0.2	I
126	ICCCCCCI	1.0	298	2034.2	2032.1	-2.1	-	68.0	-	I
127	CCCCCCCI	1.0	298	1371.9	1381.4	9.5	-	53.6	-	I
128	CCCCCCCI	0.0	357	-	1312.2	-	48.4	50.1	1.6	I
129	CCCCCCCCI	1.0	298	1326.7	1334.1	7.4	-	58.2	-	I
130	CCCCCCCCI	0.0	374	-	1250.5	-	50.9	53.3	2.4	I
131	CC(Cl)Br	1.0	283	1667.0	1664.5	-2.5	-	34.8	-	Mix
132	ClCCBr	1.0	298	1727.0	1724.2	-2.8	-	38.5	-	Mix
133	ClCCBr	1.0	308	-	1707.2	-	37.6	38.0	0.4	Mix
134	FCCBr	1.0	298	1704.4	1700.0	-4.4	-	33.0	-	Mix
135	FCCCl	0.3	298	1167.5	1149.4	-18.1	-	28.9	-	Mix
136	ClCCI	1.0	288	2133.6	2141.3	7.8	-	43.5	-	Mix
137	CC(F)(F)Cl	1.1	265	1188.8	1138.8	-49.9	22.7	22.7	0.0	Mix
138	CC(F)(F)Cl	3.6	298	1107.7	1066.6	-41.1	19.7	21.3	1.5	Mix
139	CC(F)(Cl)Cl	1.0	298	1233.7	1213.8	-19.9	26.0	27.5	1.4	Mix
140	FC(Cl)CCl	1.0	298	1369.2	1380.2	11.0	-	36.9	-	Mix
141	FC(F)(Br)CBr	1.0	293	2223.8	2238.5	14.7	-	43.4	-	Mix
142	FC(F)(Cl)CCl	1.0	298	1406.6	1409.0	2.4	-	34.4	-	Mix
143	FC(F)C(F)Br	1.0	283	1874.0	1933.8	59.8	-	34.6	-	Mix
144	FC(F)(F)CCl	1.0	285	1353.9	1319.0	-34.9	-	29.0	-	Mix
145	FC(Cl)(Cl)CCl	1.0	298	1482.6	1498.5	15.9	-	40.2	-	Mix
146	FC(Cl)C(Cl)Cl	1.0	298	1529.8	1545.2	15.4	-	40.9	-	Mix
147	FC(F)(F)CI	1.0	298	2130.0	2135.4	5.4	-	38.2	-	Mix
148	CC(C)(Cl)Br	1.0	293	1495.0	1478.5	-16.5	-	36.2	-	Mix
149	CC(Br)CCl	1.0	293	1537.0	1558.9	21.9	-	40.5	-	Mix
150	CC(Cl)CBr	1.0	293	1531.0	1557.6	26.6	-	40.5	-	Mix
151	ClCCCBr	1.0	293	1596.9	1578.7	-18.2	-	42.4	-	Mix
152	CC(C)(F)Cl	1.0	293	998.2	958.9	-39.3	-	27.1	-	Mix
153	CC(F)CCl	1.0	293	1086.0	1057.2	-28.8	-	30.5	-	Mix
154	ClCCCI	1.0	293	1904.0	1927.2	23.2	-	46.9	-	Mix
155	ClC(Cl)CCBr	1.0	293	1708.4	1707.8	-0.6	-	48.6	-	Mix
156	ClCC(Br)CBr	1.0	287	2093.0	2098.8	5.8	-	56.4	-	Mix
157	CC(F)(Cl)CCl	0.1	298	1255.2	1239.0	-16.3	-	37.2	-	Mix
158	ClC(Cl)(Br)CCBr	1.0	293	2077.2	2096.7	19.5	-	56.9	-	Mix
159	ClCCCCBr	1.0	298	1485.1	1474.6	-10.5	-	48.4	-	Mix
160	CC(Cl)C(Cl)CBr	1.0	293	1598.5	1622.6	24.1	-	54.5	-	Mix
161	CCC(F)(F)C(C)Cl	1.0	293	1108.5	1083.8	-24.7	-	39.5	-	Mix
162	CC(C)(C)C(C)(Cl)Br	1.0	293	1250.0	1456.3	206.3	-	57.2	-	Mix

Table S14: Comparison of experimental and simulated properties for the AT+SH/SQE-M optimization.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	CCC	1.0	230	582.1	572.9	-9.2	18.8	18.8	0.0	Alk
2	CC(C)C	19.9	260	597.9	601.7	3.7	-	22.0	-	Alk
3	CC(C)C	1.0	265	-	595.4	-	22.4	21.8	-0.6	Alk
4	CCCC	1.0	273	601.0	596.9	-4.1	-	22.6	-	Alk
5	CCCC	9.9	300	572.5	571.3	-1.1	-	21.6	-	Alk
6	CCCC	1.0	264	-	605.4	-	23.1	22.9	-0.2	Alk
7	CC(C)(C)C	1.0	282	603.7	625.2	21.5	23.6	24.6	1.0	Alk
8	CC(C)(C)C	1.8	298	586.0	608.4	22.4	-	24.0	-	Alk
9	CCC(C)C	0.9	298	616.0	617.9	1.8	25.5	25.4	-0.0	Alk
10	CCCCC	1.0	298	621.1	621.8	0.6	26.6	26.6	-0.0	Alk
11	CCC(C)(C)C	1.0	298	644.4	659.4	15.0	28.8	28.9	0.1	Alk
12	CC(C)C(C)C	1.0	298	658.6	660.2	1.7	30.0	29.4	-0.6	Alk
13	CCC(C)CC	1.0	298	659.9	658.8	-1.1	30.9	30.2	-0.7	Alk
14	CCCC(C)C	1.0	298	648.5	654.3	5.9	30.4	30.3	-0.1	Alk
15	CCCCCC	1.0	298	656.1	657.2	1.1	31.8	31.5	-0.3	Alk
16	CCCCCCC	0.1	298	682.0	683.5	1.5	36.5	36.3	-0.2	Alk
17	CCCCCCCC	1.0	298	698.9	704.4	5.6	41.0	41.2	0.1	Alk
18	CCBr	1.0	298	1451.2	1437.2	-14.0	-	27.1	-	Br
19	CCBr	1.0	305	-	1424.4	-	27.6	26.9	-0.7	Br
20	CC(Br)Br	1.0	298	2091.8	2075.7	-16.1	-	38.1	-	Br
21	BrCCBr	1.0	298	2169.5	2166.7	-2.8	41.7	42.6	0.9	Br
22	BrCC(Br)Br	1.0	298	2610.1	2594.2	-15.9	-	53.8	-	Br
23	CC(C)Br	1.0	298	1301.4	1297.7	-3.7	30.2	29.8	-0.4	Br
24	CCCBr	1.0	298	1345.5	1334.0	-11.5	31.9	31.6	-0.3	Br
25	CC(Br)CBr	1.0	298	1925.0	1925.7	0.8	41.7	44.6	2.9	Br
26	BrCCCBr	1.0	298	1971.2	1954.8	-16.4	-	46.8	-	Br
27	CC(Br)(Br)CBr	1.0	293	2298.5	2356.4	57.9	-	57.1	-	Br
28	CC(Br)C(Br)Br	1.0	293	2354.8	2349.4	-5.4	-	55.0	-	Br
29	BrCC(Br)CBr	1.0	298	2411.0	2393.5	-17.5	-	59.7	-	Br
30	CC(C)(C)Br	1.0	298	1212.5	1215.4	2.9	31.8	32.0	0.2	Br
31	CC(C)CBr	1.0	298	1257.1	1257.0	-0.1	34.9	35.3	0.4	Br
32	CCC(C)Br	1.0	298	1253.6	1244.9	-8.7	34.8	34.4	-0.4	Br
33	CCCCBr	1.0	298	1268.6	1263.5	-5.1	36.6	36.2	-0.4	Br
34	CC(CBr)CBr	1.0	298	1799.5	1804.2	4.7	-	49.4	-	Br
35	CCC(Br)CBr	1.0	298	1787.0	1786.3	-0.7	45.6	48.2	2.6	Br
36	CC(Br)CCBr	1.0	293	1796.0	1790.1	-5.9	-	49.2	-	Br
37	CC(C)(Br)C(Br)Br	1.0	294	2175.3	2194.9	19.6	-	57.1	-	Br
38	CC(Br)(CBr)CBr	1.0	298	2180.3	2216.5	36.2	-	59.7	-	Br
39	CC(C)(C)CBr	0.0	298	1193.5	1216.7	23.3	-	38.1	-	Br
40	CCC(C)(C)Br	0.0	298	1209.5	1201.5	-8.0	-	36.9	-	Br
41	CCC(C)CBr	1.0	298	1214.4	1214.4	-0.0	-	39.4	-	Br
42	CCC(Br)CC	1.0	298	1205.1	1201.1	-4.0	-	38.5	-	Br
43	CC(C)CCBr	1.0	298	1200.7	1209.4	8.7	-	39.8	-	Br
44	CCCC(C)Br	1.0	298	1200.5	1196.4	-4.1	38.5	38.9	0.4	Br
45	CCCCCBr	1.0	298	1211.4	1211.6	0.2	40.9	40.9	-0.0	Br
46	CC(C)(C)C(Br)Br	1.0	293	1669.5	1695.0	25.5	-	49.3	-	Br
47	CCC(C)(Br)CC	1.0	293	1179.2	1184.4	5.2	-	41.5	-	Br
48	CCCC(Br)CC	1.0	298	1157.2	1162.5	5.3	-	43.1	-	Br
49	CCCCCCBr	1.0	298	1168.8	1171.4	2.6	45.6	45.4	-0.2	Br
50	CCCCCCCBr	1.0	298	1134.8	1139.8	5.0	50.4	50.1	-0.3	Br
51	CCCCCCCCBr	1.0	298	1107.7	1114.3	6.6	55.1	54.8	-0.3	Br
52	CCCl	1.0	285	906.2	895.5	-10.7	24.9	24.6	-0.3	Cl
53	CCCl	1.4	298	890.0	877.7	-12.2	-	24.1	-	Cl
54	CC(Cl)Cl	1.0	298	1168.1	1160.1	-8.0	30.6	30.1	-0.5	Cl
55	ClCCCl	1.0	298	1245.6	1237.6	-8.0	34.4	34.5	0.1	Cl
56	CC(Cl)(Cl)Cl	1.0	298	1329.3	1340.7	11.4	32.4	33.9	1.5	Cl
57	ClCC(Cl)Cl	1.0	298	1432.8	1432.3	-0.5	40.1	40.7	0.6	Cl
58	CC(C)Cl	1.0	298	855.6	850.3	-5.4	-	27.1	-	Cl
59	CC(Cl)CCl	1.0	298	1153.0	1146.3	-6.7	36.2	36.2	0.0	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
60	ClCCCCCl	1.0	298	1180.0	1170.7	-9.3	40.6	39.4	-1.2	Cl
61	CC(C)(C)Cl	1.0	298	836.3	840.1	3.8	28.6	29.6	1.0	Cl
62	CC(C)CCl	1.0	298	871.4	871.7	0.4	31.7	32.1	0.4	Cl
63	CCC(C)Cl	1.0	298	867.5	860.4	-7.1	31.5	31.5	0.0	Cl
64	CCCCCl	1.0	298	880.4	876.7	-3.7	33.5	33.1	-0.4	Cl
65	CC(Cl)C(C)Cl	1.0	298	1106.3	1094.2	-12.1	-	40.0	-	Cl
66	CCC(Cl)CCl	1.0	298	1111.8	1108.5	-3.3	40.1	40.2	0.1	Cl
67	ClCCCCCl	1.0	298	-	1131.1	-	46.4	46.1	-0.3	Cl
68	CCC(C)(C)Cl	1.0	298	859.6	861.9	2.3	-	34.1	-	Cl
69	CCC(C)CCl	1.0	298	875.0	877.6	2.6	-	36.5	-	Cl
70	CC(C)CCCl	1.0	298	870.0	873.9	3.9	36.2	36.6	0.4	Cl
71	CCCC(C)Cl	1.0	298	866.0	862.8	-3.2	36.0	36.1	0.1	Cl
72	CCCCCCl	1.0	298	877.8	875.7	-2.1	38.2	37.6	-0.6	Cl
73	ClCCCCCCl	1.0	298	1095.6	1096.8	1.2	51.3	51.3	-0.0	Cl
74	CCCCCCCl	1.0	298	873.5	874.6	1.0	42.0	42.1	0.1	Cl
75	CC(CCl)C(C)(C)Cl	1.0	298	1064.0	1079.1	15.1	-	49.4	-	Cl
76	CC(Cl)CCC(C)Cl	1.0	298	1044.1	1046.4	2.3	-	50.8	-	Cl
77	ClCCCCCCCl	1.0	298	1063.7	1069.6	5.9	-	55.9	-	Cl
78	CCCCCCCCl	1.0	298	871.5	874.2	2.7	47.0	46.8	-0.2	Cl
79	CCCCCCCCCl	1.0	298	869.4	873.7	4.3	51.4	51.4	0.0	Cl
80	CCF	1.0	236	817.6	804.2	-13.4	20.7	20.7	0.0	F
81	CCF	9.1	298	707.5	702.7	-4.8	-	18.3	-	F
82	CC(F)F	1.0	250	1009.0	1007.1	-1.9	22.7	22.4	-0.3	F
83	CC(F)F	6.2	298	907.0	906.2	-0.8	-	20.3	-	F
84	CC(F)(F)F	1.0	220	1182.9	1452.0	269.2	19.2	22.5	3.3	F
85	CC(C)F	1.0	264	769.2	752.6	-16.6	-	22.6	-	F
86	CCCF	1.0	271	781.8	781.2	-0.6	-	23.7	-	F
87	CCC(F)F	0.6	276	-	941.8	-	25.1	25.2	0.1	F
88	FCCCF	1.0	298	1005.7	997.0	-8.7	-	28.4	-	F
89	CC(C)(C)F	1.0	285	752.7	718.1	-34.6	-	23.4	-	F
90	CC(C)(C)F	1.4	298	735.3	699.9	-35.4	-	22.8	-	F
91	CCC(C)F	1.0	298	756.6	740.5	-16.1	-	25.5	-	F
92	CCCCF	1.0	298	770.8	770.6	-0.2	-	27.2	-	F
93	FCCCCF	1.0	298	976.7	981.3	4.6	-	34.1	-	F
94	CCCC(F)(F)F	1.4	298	1010.0	934.4	-75.6	-	24.8	-	F
95	CCC(C)(C)F	1.0	298	773.7	742.2	-31.5	-	27.6	-	F
96	CCC(C)CF	0.3	298	791.5	786.3	-5.2	-	30.8	-	F
97	CCCCCF	1.0	298	784.9	787.7	2.8	30.9	31.8	0.8	F
98	CCCCC(C)F	1.0	293	791.4	783.4	-8.0	-	35.0	-	F
99	CCCCCCF	1.0	298	795.8	798.8	3.0	35.6	36.3	0.7	F
100	CC(C)CC(C)(F)F	1.0	293	888.2	867.1	-21.1	-	34.2	-	F
101	FCCCCCCF	1.0	298	940.7	953.6	12.9	-	44.3	-	F
102	CCCCCCCF	1.0	298	800.9	807.3	6.4	40.8	40.9	0.1	F
103	CCCCCCCCF	1.0	298	806.7	813.2	6.5	-	45.4	-	F
104	CCI	1.0	298	1924.0	1907.2	-16.9	31.7	30.9	-0.8	I
105	CC(C)I	1.0	298	1694.5	1691.8	-2.7	34.1	33.4	-0.7	I
106	CCCI	1.0	298	1737.2	1730.8	-6.4	36.0	35.3	-0.7	I
107	ICCCI	1.0	298	2565.1	2536.4	-28.7	-	54.3	-	I
108	ICCCI	0.0	369	-	2404.4	-	53.5	50.7	-2.8	I
109	CC(C)(C)I	0.1	298	1536.0	1558.8	22.8	35.7	35.7	-0.0	I
110	CC(C)CI	0.0	298	1595.1	1599.6	4.5	38.8	38.9	0.1	I
111	CCC(C)I	1.0	298	1589.0	1589.3	0.3	38.5	38.0	-0.5	I
112	CCCCI	1.0	298	1606.7	1605.7	-1.0	40.3	39.9	-0.4	I
113	ICCCCI	1.0	298	2349.6	2330.8	-18.8	59.0	59.6	0.6	I
114	CC(C)(C)CI	1.0	293	1494.0	1530.1	36.1	-	41.8	-	I
115	CCC(C)(C)I	0.0	298	1486.6	1510.0	23.4	-	40.4	-	I
116	CC(C)C(C)I	1.0	293	1524.0	1516.7	-7.3	-	41.3	-	I
117	CCC(I)CC	1.0	298	1505.5	1505.5	0.1	-	42.1	-	I
118	CC(C)CCI	1.0	298	1495.2	1510.2	15.0	42.2	43.3	1.1	I
119	CCCC(C)I	1.0	293	1500.9	1506.1	5.2	-	42.7	-	I
120	CCCCCI	1.0	298	1507.3	1513.4	6.0	44.4	44.5	0.1	I
121	ICCCCCI	1.0	298	2173.4	2167.4	-6.0	-	64.1	-	I
122	CCCC(C)CI	1.0	293	1443.0	1450.3	7.3	-	47.7	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
123	CCCCC(C)I	1.0	293	1419.3	1435.6	16.3	-	47.2	-	I
124	CCCCCCI	1.0	298	1431.8	1440.9	9.1	-	49.1	-	I
125	CCCCCCI	1.0	346	-	1379.9	-	46.2	46.5	0.3	I
126	ICCCCCCI	1.0	298	2034.2	2038.9	4.7	-	68.6	-	I
127	CCCCCCCI	1.0	298	1371.9	1383.0	11.1	-	53.8	-	I
128	CCCCCCCI	0.0	357	-	1313.9	-	48.4	50.2	1.8	I
129	CCCCCCCCI	1.0	298	1326.7	1336.4	9.7	-	58.4	-	I
130	CCCCCCCCI	0.0	374	-	1253.0	-	50.9	53.6	2.7	I
131	CC(Cl)Br	1.0	283	1667.0	1666.7	-0.3	-	34.9	-	Mix
132	ClCCBr	1.0	298	1727.0	1724.5	-2.5	-	38.6	-	Mix
133	ClCCBr	1.0	308	-	1708.0	-	37.6	38.2	0.6	Mix
134	FCCBr	1.0	298	1704.4	1704.0	-0.4	-	32.6	-	Mix
135	FCCCl	0.3	298	1167.5	1151.5	-16.0	-	28.3	-	Mix
136	ClCCI	1.0	288	2133.6	2143.6	10.1	-	43.4	-	Mix
137	CC(F)(F)Cl	1.1	265	1188.8	1160.2	-28.6	22.7	22.8	0.1	Mix
138	CC(F)(F)Cl	3.6	298	1107.7	1089.1	-18.6	19.7	21.3	1.6	Mix
139	CC(F)(Cl)Cl	1.0	298	1233.7	1227.4	-6.2	26.0	27.5	1.4	Mix
140	FC(Cl)CCl	1.0	298	1369.2	1373.6	4.4	-	35.1	-	Mix
141	FC(F)(Br)CBr	1.0	293	2223.8	2266.1	42.3	-	42.2	-	Mix
142	FC(F)(Cl)CCl	1.0	298	1406.6	1413.3	6.7	-	32.2	-	Mix
143	FC(F)C(F)Br	1.0	283	1874.0	1941.0	67.0	-	32.7	-	Mix
144	FC(F)(F)CCl	1.0	285	1353.9	1321.0	-32.9	-	26.4	-	Mix
145	FC(Cl)(Cl)CCl	1.0	298	1482.6	1502.7	20.1	-	38.7	-	Mix
146	FC(Cl)C(Cl)Cl	1.0	298	1529.8	1536.7	6.9	-	39.0	-	Mix
147	FC(F)(F)CI	1.0	298	2130.0	2133.9	3.9	-	33.6	-	Mix
148	CC(C)(Cl)Br	1.0	293	1495.0	1490.2	-4.8	-	36.8	-	Mix
149	CC(Br)CCl	1.0	293	1537.0	1559.5	22.5	-	40.6	-	Mix
150	CC(Cl)CBr	1.0	293	1531.0	1558.3	27.3	-	40.9	-	Mix
151	ClCCCBr	1.0	293	1596.9	1584.9	-12.0	-	43.4	-	Mix
152	CC(C)(F)Cl	1.0	293	998.2	970.6	-27.6	-	27.3	-	Mix
153	CC(F)CCl	1.0	293	1086.0	1058.5	-27.5	-	30.0	-	Mix
154	ClCCCI	1.0	293	1904.0	1932.0	28.0	-	47.2	-	Mix
155	ClC(Cl)CCBr	1.0	293	1708.4	1709.8	1.4	-	48.6	-	Mix
156	ClCC(Br)CBr	1.0	287	2093.0	2099.9	6.9	-	56.4	-	Mix
157	CC(F)(Cl)CCl	0.1	298	1255.2	1249.0	-6.3	-	36.9	-	Mix
158	ClC(Cl)(Br)CCBr	1.0	293	2077.2	2106.8	29.6	-	57.3	-	Mix
159	ClCCCCBr	1.0	298	1485.1	1480.2	-5.0	-	49.3	-	Mix
160	CC(Cl)C(Cl)CBr	1.0	293	1598.5	1623.0	24.5	-	54.8	-	Mix
161	CCC(F)(F)C(C)Cl	1.0	293	1108.5	1082.9	-25.6	-	37.9	-	Mix
162	CC(C)(C)C(C)(Cl)Br	1.0	293	1250.0	1452.3	202.3	-	54.7	-	Mix

S6.2 Validation set

Table S15: Comparison of experimental and simulated properties validation using the CG/EEM-G scheme.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	BrCBr	0.1	298	2482.0	2470.3	-11.7	-	38.6	-	Br
2	BrCBr	1.0	298	-	2471.0	-	37.0	38.6	1.6	Br
3	BrC(Br)Br	1.0	298	2877.2	2895.5	18.4	46.1	50.3	4.2	Br
4	BrC(Br)(Br)Br	1.0	374	2953.3	3025.7	72.4	-	56.9	-	Br
5	BrC(Br)(Br)Br	1.0	384	-	3005.5	-	48.2	56.4	8.2	Br
6	CC(Br)Br	1.0	316	-	2055.4	-	39.6	39.1	-0.5	Br
7	BrCC(Br)Br	1.0	321	-	2556.6	-	52.9	54.4	1.5	Br
8	CC(C)(Br)Br	0.0	298	1820.0	1871.3	51.3	37.3	41.3	4.0	Br
9	CCC(Br)Br	0.0	302	1968.8	1901.4	-67.4	43.1	43.9	0.9	Br
10	CC(Br)(Br)CBr	0.0	349	-	2267.4	-	47.5	54.6	7.1	Br
11	BrCC(Br)CBr	0.0	374	-	2261.1	-	52.1	56.7	4.6	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
12	BrCCC(Br)Br	1.0	290	2350.0	2384.0	34.0	-	60.5	-	Br
13	CC(C)(Br)CBr	1.0	293	1760.4	1795.9	35.5	-	47.4	-	Br
14	CC(C)(Br)CBr	0.0	322	-	1752.1	-	41.8	46.2	4.4	Br
15	CCC(C)(Br)Br	0.0	318	1718.7	1735.7	17.1	41.0	44.8	3.8	Br
16	CC(C)C(Br)Br	0.0	321	1733.3	1737.2	3.9	-	45.7	-	Br
17	CC(Br)C(C)Br	1.0	295	1789.3	1779.0	-10.3	-	47.3	-	Br
18	CC(Br)C(C)Br	0.0	325	-	1734.5	-	43.0	45.9	2.8	Br
19	CC(Br)CCBr	0.0	343	-	1719.4	-	45.1	47.7	2.6	Br
20	CCCC(Br)Br	1.0	298	1784.0	1765.5	-18.5	-	48.4	-	Br
21	CCCC(Br)Br	1.0	357	-	1676.0	-	45.8	45.4	-0.4	Br
22	BrCCCCBr	1.0	298	1818.8	1806.4	-12.5	52.6	52.6	0.0	Br
23	CC(Br)C(C)(Br)Br	1.0	293	2172.4	2195.2	22.8	-	59.4	-	Br
24	CC(Br)C(C)(Br)Br	1.0	326	-	2146.6	-	51.7	57.6	5.9	Br
25	CCC(Br)(Br)CBr	1.0	293	2168.5	2203.3	34.8	-	60.4	-	Br
26	CCC(Br)(Br)CBr	1.0	329	-	2148.8	-	50.7	58.5	7.8	Br
27	CC(Br)C(Br)CBr	1.0	293	2183.5	2204.8	21.3	-	64.0	-	Br
28	CC(Br)C(Br)CBr	1.0	333	-	2142.3	-	51.3	61.9	10.6	Br
29	CCC(Br)C(Br)Br	1.0	293	2183.5	2182.2	-1.3	-	61.1	-	Br
30	CCC(Br)C(Br)Br	0.0	369	-	2062.2	-	51.1	56.7	5.6	Br
31	BrCC(CBr)CBr	1.0	490	-	1925.4	-	66.1	54.1	-12.0	Br
32	BrCCC(Br)CBr	1.0	298	2210.0	2206.4	-3.6	-	65.0	-	Br
33	BrCCC(Br)CBr	1.0	405	-	2041.1	-	53.5	58.7	5.2	Br
34	CC(C)(C)CBr	1.0	308	-	1207.6	-	35.6	37.9	2.3	Br
35	CC(C)C(C)Br	0.0	298	1215.6	1205.9	-9.7	-	38.2	-	Br
36	CC(C)C(C)Br	1.0	316	-	1183.3	-	37.2	37.3	0.1	Br
37	CCC(Br)CC	0.0	298	-	1203.2	-	39.3	39.0	-0.3	Br
38	CC(Br)C(C)(C)C	0.0	298	1169.8	1194.7	24.9	-	42.4	-	Br
39	CC(Br)C(C)(C)C	1.0	330	-	1159.0	-	39.5	40.8	1.3	Br
40	CC(C)C(C)(C)Br	1.0	292	1187.4	1194.3	6.9	-	41.9	-	Br
41	CCCC(C)(C)Br	1.0	293	1180.4	1174.7	-5.7	-	42.4	-	Br
42	ClCCl	1.0	298	1316.4	1315.8	-0.6	28.8	29.5	0.7	Cl
43	ClC(Cl)Cl	1.0	298	1479.5	1496.4	16.9	31.1	32.5	1.4	Cl
44	ClC(Cl)(Cl)Cl	1.0	298	1584.3	1596.0	11.7	-	33.9	-	Cl
45	ClC(Cl)(Cl)Cl	0.1	298	-	1594.3	-	32.4	33.9	1.4	Cl
46	CC(C)Cl	0.7	298	-	844.3	-	26.4	27.0	0.6	Cl
47	CCCCl	1.0	298	884.1	875.7	-8.4	28.5	28.4	-0.1	Cl
48	CC(C)(Cl)Cl	0.2	298	1107.3	1068.9	-38.4	-	31.1	-	Cl
49	CC(C)(Cl)Cl	1.0	298	-	1070.0	-	32.1	31.2	-0.9	Cl
50	CCC(Cl)Cl	0.1	298	1126.0	1113.3	-12.6	-	34.7	-	Cl
51	CCC(Cl)Cl	1.0	298	-	1113.6	-	35.2	34.7	-0.5	Cl
52	CC(Cl)(Cl)CCl	0.0	298	1317.9	1325.1	7.3	40.5	42.6	2.1	Cl
53	CCC(Cl)(Cl)Cl	1.0	298	1283.6	1274.0	-9.6	-	36.8	-	Cl
54	CCC(Cl)(Cl)Cl	1.0	259	-	1327.4	-	38.8	38.7	-0.1	Cl
55	CC(Cl)C(Cl)Cl	1.0	289	1353.0	1343.7	-9.3	-	44.3	-	Cl
56	CC(Cl)C(Cl)Cl	0.0	302	-	1328.4	-	42.3	43.4	1.1	Cl
57	ClCC(Cl)CCl	1.0	298	1388.8	1392.3	3.5	46.8	50.4	3.6	Cl
58	ClCCC(Cl)Cl	1.0	293	1355.5	1366.1	10.6	-	45.9	-	Cl
59	ClCCC(Cl)Cl	0.0	313	-	1342.0	-	44.2	44.8	0.6	Cl
60	CC(C)(Cl)CCl	0.0	298	1089.0	1094.4	5.5	36.8	37.7	0.9	Cl
61	CCC(C)(Cl)Cl	0.1	298	1065.1	1062.2	-2.9	-	35.7	-	Cl
62	CCC(C)(Cl)Cl	1.0	298	-	1062.1	-	36.7	35.7	-1.0	Cl
63	CC(C)C(Cl)Cl	0.0	298	1100.1	1078.8	-21.3	36.5	37.7	1.2	Cl
64	CC(Cl)C(C)Cl	0.0	298	-	1096.0	-	38.5	42.1	3.6	Cl
65	CC(CCl)CCl	0.0	307	1090.0	1116.1	26.0	-	42.5	-	Cl
66	CC(CCl)CCl	1.0	285	-	1140.1	-	45.1	43.9	-1.2	Cl
67	CC(Cl)CCCl	1.0	298	1108.3	1111.9	3.6	42.1	42.6	0.5	Cl
68	CCCC(Cl)Cl	0.0	298	1080.1	1077.6	-2.5	-	39.0	-	Cl
69	CCCC(Cl)Cl	1.0	298	-	1079.0	-	39.4	39.0	-0.4	Cl
70	CC(C)(Cl)C(Cl)Cl	1.0	298	1267.7	1273.3	5.6	-	45.3	-	Cl
71	CC(Cl)C(C)(Cl)Cl	1.0	291	1263.0	1275.1	12.1	-	45.4	-	Cl
72	CC(Cl)C(C)(Cl)Cl	0.0	310	-	1250.0	-	42.7	44.2	1.5	Cl
73	CC(Cl)(CCl)CCl	1.0	298	1301.2	1313.8	12.6	-	50.0	-	Cl
74	CC(Cl)(CCl)CCl	0.0	327	-	1281.0	-	45.9	48.2	2.2	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
75	CCCC(Cl)(Cl)Cl	0.0	298	1231.0	1224.0	-7.0	-	41.5	-	Cl
76	CC(CCl)C(Cl)Cl	0.0	312	1251.1	1276.1	25.0	-	46.6	-	Cl
77	CC(Cl)C(Cl)CCl	1.0	293	1316.4	1311.6	-4.8	-	51.8	-	Cl
78	CC(Cl)C(Cl)CCl	1.0	288	-	1316.5	-	41.3	52.1	10.8	Cl
79	CC(Cl)CC(Cl)Cl	1.0	288	1317.0	1284.1	-32.9	-	48.2	-	Cl
80	CC(Cl)CC(Cl)Cl	0.0	318	-	1248.2	-	43.9	46.1	2.2	Cl
81	ClCCC(Cl)CCl	1.0	293	1317.5	1325.5	8.0	-	53.2	-	Cl
82	CC(C)(C)CCl	0.1	298	860.9	876.6	15.7	-	35.0	-	Cl
83	CC(C)(C)CCl	1.0	294	-	881.9	-	34.9	35.3	0.4	Cl
84	CC(C)C(C)Cl	0.1	298	857.0	865.0	7.9	-	34.9	-	Cl
85	CC(C)C(C)Cl	1.0	300	-	863.2	-	35.9	34.9	-1.0	Cl
86	CCC(Cl)CC	1.0	298	884.0	863.8	-20.2	-	35.7	-	Cl
87	CCC(Cl)CC	1.0	304	-	858.3	-	36.5	35.4	-1.1	Cl
88	CC(C)(C)C(Cl)Cl	0.0	312	1074.8	1059.0	-15.8	-	40.8	-	Cl
89	CC(C)C(C)(C)Cl	1.0	298	874.9	877.1	2.2	-	37.7	-	Cl
90	CC(C)C(C)(C)Cl	1.0	316	-	861.4	-	38.0	36.8	-1.2	Cl
91	CCC(C)(Cl)CC	1.0	293	883.9	878.2	-5.7	-	38.2	-	Cl
92	CCCC(C)(C)Cl	0.0	298	858.3	861.8	3.4	37.7	38.1	0.3	Cl
93	FCF	1.0	221	1213.8	1259.8	46.0	20.9	22.6	1.7	F
94	FCF	17.6	298	891.6	1086.9	195.3	-	19.6	-	F
95	FCF	1.0	298	961.0	1084.4	123.4	-	19.6	-	F
96	FC(F)F	1.0	191	1442.9	1546.5	103.6	16.7	22.5	5.8	F
97	FC(F)F	47.1	298	636.7	1218.0	581.4	-	17.7	-	F
98	FC(F)F	1.0	298	666.7	1202.9	536.2	-	17.5	-	F
99	FC(F)(F)F	1.0	145	1605.2	1879.9	274.7	12.3	18.8	6.5	F
100	FCCF	1.0	283	1024.0	1055.9	31.9	-	24.2	-	F
101	FCCF	1.8	298	-	1030.6	-	22.5	23.6	1.1	F
102	CC(F)(F)F	12.9	298	-	912.6	-	13.1	15.9	2.8	F
103	FCC(F)F	1.0	314	1175.5	1178.9	3.4	-	25.6	-	F
104	FCC(F)F	1.0	278	-	1251.0	-	23.2	27.4	4.2	F
105	FCC(F)F	2.0	296	-	1214.6	-	20.6	26.5	5.9	F
106	CC(C)F	1.0	293	723.8	709.2	-14.6	-	21.2	-	F
107	CC(C)F	1.0	249	-	768.6	-	23.7	23.0	-0.7	F
108	CC(C)(F)F	1.0	271	943.8	846.5	-97.3	22.6	21.2	-1.5	F
109	CC(C)(F)F	2.1	291	911.4	814.6	-96.8	21.6	20.4	-1.2	F
110	CC(F)CF	1.4	298	960.0	941.7	-18.3	-	25.2	-	F
111	CCC(F)F	1.3	298	920.1	913.8	-6.3	23.7	24.7	1.0	F
112	CCC(F)(F)F	0.9	259	1148.2	1032.5	-115.7	21.8	22.8	1.0	F
113	CC(C)(C)F	1.0	237	-	776.6	-	27.6	25.4	-2.2	F
114	CC(C)CF	0.9	286	764.5	776.1	11.6	-	26.9	-	F
115	CC(C)CF	1.4	298	750.0	761.9	11.9	-	26.4	-	F
116	CCC(C)F	1.0	248	-	800.5	-	29.2	27.9	-1.3	F
117	CCCCF	1.0	237	-	840.0	-	30.1	30.2	0.1	F
118	CCC(C)(F)F	1.0	293	915.9	855.9	-60.0	-	25.3	-	F
119	CCC(C)(F)F	0.8	298	-	848.3	-	25.9	25.1	-0.8	F
120	CCCC(F)F	0.4	298	910.1	910.9	0.8	-	29.3	-	F
121	CCCC(F)F	1.0	261	-	958.0	-	31.0	31.1	0.1	F
122	FCCCCF	0.1	298	-	981.7	-	34.6	35.5	0.9	F
123	CCC(C)(C)F	0.4	298	-	747.3	-	29.4	27.7	-1.7	F
124	CC(C)(C)C(F)(F)F	1.0	293	990.5	1002.5	12.0	-	30.7	-	F
125	ICI	1.0	298	3307.8	3176.2	-131.6	49.0	45.8	-3.2	I
126	IC(I)I	0.0	396	3685.6	3428.7	-257.0	47.9	57.1	9.2	I
127	IC(I)(I)I	0.0	447	3819.2	3670.3	-148.9	-	69.0	-	I
128	CCI	0.2	298	-	1907.9	-	31.7	30.8	-0.9	I
129	CC(I)I	0.0	336	2682.9	2649.6	-33.3	-	45.8	-	I
130	ICCI	0.0	356	2551.8	2673.8	121.9	48.1	47.9	-0.2	I
131	CCCI	0.1	298	-	1730.5	-	36.0	35.3	-0.7	I
132	CC(C)(I)I	0.0	352	2379.7	2319.2	-60.5	-	46.4	-	I
133	CC(I)CI	0.0	330	2506.9	2442.6	-64.4	-	50.9	-	I
134	CCC(I)I	0.0	357	2370.2	2378.5	8.2	-	48.7	-	I
135	CC(C)CI	1.0	298	-	1599.4	-	38.8	38.7	-0.1	I
136	CC(C)(I)CI	0.0	370	2163.1	2205.4	42.3	-	51.6	-	I
137	CCC(C)(I)I	0.0	370	2163.1	2191.3	28.2	-	50.5	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
138	CC(C)C(I)I	0.0	365	2171.2	2191.0	19.8	-	51.0	-	I
139	CC(I)C(C)I	0.0	374	2155.0	2167.6	12.6	-	50.7	-	I
140	CC(CI)CI	0.0	374	2155.0	2194.7	39.8	-	52.9	-	I
141	CCC(I)CI	0.0	371	2160.5	2185.0	24.5	-	52.3	-	I
142	CC(I)CCI	0.0	382	2141.4	2162.9	21.5	-	52.6	-	I
143	CCCC(I)I	0.0	373	2144.3	2163.8	19.5	-	52.0	-	I
144	CCC(C)(C)I	1.0	323	-	1484.4	-	40.4	40.4	0.0	I
145	CC(I)C(C)(C)C	0.0	320	1392.3	1446.5	54.1	-	44.9	-	I
146	CC(C)C(C)(C)I	1.0	293	1448.0	1477.8	29.8	-	45.8	-	I
147	CCC(C)(I)CC	0.0	319	1393.3	1440.0	46.6	-	44.9	-	I
148	CCCC(C)(C)I	0.0	332	1376.8	1404.4	27.6	-	44.5	-	I
149	ClCBr	1.0	298	1924.9	1929.8	4.9	-	34.4	-	Mix
150	ClCBr	1.0	304	-	1917.7	-	33.5	34.2	0.7	Mix
151	FCCl	1.0	260	1282.1	1297.9	15.7	21.9	26.1	4.2	Mix
152	BrCI	1.0	290	2926.0	2877.4	-48.6	-	42.7	-	Mix
153	ClCI	1.0	293	2422.0	2407.5	-14.5	-	38.9	-	Mix
154	FC(F)Br	1.0	298	1775.5	2027.3	251.8	-	29.5	-	Mix
155	FC(F)Br	1.0	244	-	2166.2	-	24.0	31.8	7.8	Mix
156	FC(F)Cl	1.0	233	1408.0	1500.6	92.6	20.2	25.5	5.3	Mix
157	FC(F)Cl	10.8	298	1193.0	1348.1	155.1	-	22.7	-	Mix
158	FC(Cl)Cl	1.8	298	1367.0	1434.4	67.4	-	27.8	-	Mix
159	FC(Cl)Cl	1.0	267	-	1498.7	-	26.1	29.3	3.2	Mix
160	FC(I)I	1.0	295	3196.9	3221.8	24.9	-	49.0	-	Mix
161	FC(I)I	1.0	314	-	3174.8	-	32.9	48.1	15.2	Mix
162	FC(F)I	1.0	272	-	2599.3	-	26.0	36.0	10.0	Mix
163	FC(Br)Br	1.0	293	2421.0	2551.1	130.1	-	40.5	-	Mix
164	ClC(Cl)Br	1.0	298	1983.5	2010.6	27.1	-	39.1	-	Mix
165	ClC(Br)Br	1.0	293	2451.0	2486.9	35.9	-	45.3	-	Mix
166	ClC(Cl)(Cl)Br	1.0	298	2002.1	2036.7	34.5	-	40.8	-	Mix
167	ClC(Cl)(Cl)Br	0.1	298	-	2036.2	-	36.1	40.7	4.6	Mix
168	ClC(Cl)(Br)Br	1.0	298	2420.0	2447.3	27.3	-	47.6	-	Mix
169	ClC(Br)(Br)Br	1.0	288	2710.0	2850.6	140.6	-	54.7	-	Mix
170	FC(F)(F)Br	1.0	215	1989.9	2177.4	187.5	17.5	28.0	10.5	Mix
171	FC(F)(F)Br	16.6	298	1536.1	1908.6	372.5	-	24.4	-	Mix
172	FC(Br)(Br)Br	1.0	330	-	2808.3	-	34.4	47.6	13.2	Mix
173	FC(F)(Br)Br	1.0	298	2251.2	2484.6	233.4	25.0	37.0	12.1	Mix
174	FC(F)(F)Cl	1.0	190	1527.8	1766.7	238.9	15.4	23.3	7.9	Mix
175	FC(F)(F)Cl	36.7	298	840.9	1319.0	478.1	-	17.8	-	Mix
176	FC(F)(Cl)Cl	1.0	243	1488.0	1553.4	65.4	20.1	25.3	5.2	Mix
177	FC(F)(Cl)Cl	6.7	298	1307.0	1421.1	114.1	-	23.1	-	Mix
178	FC(Cl)(Cl)Cl	1.1	298	1477.0	1522.0	44.9	24.9	28.6	3.7	Mix
179	FC(F)(F)I	20.0	298	2046.8	2380.6	333.8	-	30.0	-	Mix
180	FC(F)(F)I	1.0	281	-	2422.2	-	22.5	30.6	8.1	Mix
181	FC(Cl)Br	1.0	273	1977.1	2073.7	96.6	-	35.5	-	Mix
182	FC(F)(Cl)Br	1.0	269	1899.6	2046.6	147.0	23.1	31.3	8.2	Mix
183	FC(F)(Cl)Br	2.6	298	1810.0	1975.3	165.3	-	30.1	-	Mix
184	FC(Cl)(Cl)Br	1.0	295	1950.0	2015.1	65.1	-	35.6	-	Mix
185	FC(Cl)(Cl)Br	0.4	298	-	2006.6	-	29.1	35.5	6.4	Mix
186	FC(Cl)(Br)Br	1.0	295	2317.3	2467.0	149.7	-	42.5	-	Mix
187	CC(Cl)Br	1.0	305	-	1635.7	-	33.1	35.4	2.3	Mix
188	CC(F)Cl	1.4	298	-	1045.6	-	23.7	25.4	1.7	Mix
189	FCCCl	1.0	303	-	1141.9	-	32.1	28.9	-3.2	Mix
190	CC(F)(F)Cl	1.0	263	-	1172.0	-	22.7	23.1	0.4	Mix
191	FCC(F)Cl	0.8	298	-	1308.1	-	26.6	31.5	5.0	Mix
192	FC(F)CCl	1.0	288	1312.0	1323.3	11.3	-	32.6	-	Mix
193	FC(F)CCl	0.7	298	-	1305.3	-	26.6	32.0	5.5	Mix
194	CC(F)(Cl)Cl	0.8	298	-	1222.1	-	26.0	27.1	1.0	Mix
195	FC(Cl)CCl	0.1	298	-	1378.4	-	32.8	37.0	4.3	Mix
196	ClC(Cl)(Br)CBr	1.0	273	2298.0	2316.7	18.7	-	56.2	-	Mix
197	ClC(Cl)(Br)CBr	1.0	369	-	2145.3	-	45.9	50.3	4.4	Mix
198	ClC(Br)C(Cl)Br	1.0	293	2135.0	2331.6	196.6	-	59.6	-	Mix
199	ClC(Br)C(Cl)Br	1.0	335	-	2254.2	-	45.9	56.7	10.8	Mix
200	FC(F)(Cl)CCl	0.4	298	-	1425.4	-	28.3	34.1	5.8	Mix

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
201	FC(Cl)C(F)Cl	0.4	298	1405.4	1498.9	93.4	-	36.9	-	Mix
202	FC(F)(F)CBr	1.0	293	1788.1	1789.6	1.5	-	31.8	-	Mix
203	FC(F)(F)CCl	1.9	298	-	1325.1	-	22.3	28.5	6.2	Mix
204	FC(Cl)(Cl)CCl	0.1	298	-	1497.6	-	34.7	39.2	4.6	Mix
205	FCC(Cl)(Cl)Cl	0.1	298	1575.0	1516.2	-58.8	-	38.8	-	Mix
206	FC(Cl)C(Cl)Cl	0.0	298	-	1550.4	-	36.9	41.8	4.9	Mix
207	ClCCCBr	1.0	341	-	1520.7	-	42.0	42.1	0.1	Mix
208	CC(C)(F)Cl	0.1	298	-	951.8	-	31.5	25.7	-5.8	Mix
209	CC(F)(F)CCl	0.4	298	1191.6	1146.1	-45.5	-	31.2	-	Mix
210	FC(F)(F)CCCl	0.5	298	1290.1	1277.1	-13.0	-	33.1	-	Mix
211	FC(F)(F)CCCl	1.0	306	-	1263.2	-	29.9	32.7	2.8	Mix
212	FCCCCCl	0.0	298	1062.7	1063.6	0.9	-	41.3	-	Mix
213	CC(CI)C(F)(F)F	1.0	313	-	1828.7	-	30.4	43.0	12.6	Mix
214	CC(I)CC(F)(F)F	1.0	312	-	1798.3	-	32.4	42.1	9.7	Mix
215	CCC(C)CBr	1.0	321	-	1186.6	-	37.9	38.4	0.5	Br
216	CC(C)CCBr	0.0	298	-	1210.4	-	39.7	40.0	0.3	Br
217	CC(Br)C(C)(C)Br	1.0	298	1663.0	1690.9	27.9	-	51.2	-	Br
218	CC(Br)C(C)(C)Br	0.0	335	-	1640.7	-	-	49.2	-	Br
219	CC(C)C(C)(Br)Br	0.0	337	1622.0	1631.5	9.5	-	47.7	-	Br
220	CC(C)(CBr)CBr	1.0	293	1693.4	1720.5	27.1	-	52.7	-	Br
221	CC(C)(CBr)CBr	0.0	345	-	1651.1	-	-	49.8	-	Br
222	CCC(C)(Br)CBr	1.0	294	1663.8	1701.1	37.3	-	51.1	-	Br
223	CCC(C)(Br)CBr	0.0	337	-	1644.1	-	-	49.0	-	Br
224	CCC(Br)(Br)CC	0.0	332	1610.0	1630.3	20.3	-	48.1	-	Br
225	CC(C)(Br)CCBr	1.0	273	1696.0	1720.1	24.1	-	54.3	-	Br
226	CC(C)(Br)CCBr	0.0	337	-	1633.5	-	-	50.8	-	Br
227	CCCC(C)(Br)Br	1.0	289	1645.2	1672.1	26.9	-	50.9	-	Br
228	CCCC(C)(Br)Br	0.0	335	-	1610.2	-	-	48.5	-	Br
229	CC(Br)C(C)CBr	0.0	337	1751.0	1636.4	-114.6	-	50.8	-	Br
230	CCC(C)C(Br)Br	0.0	337	1602.8	1619.0	16.3	-	49.1	-	Br
231	CC(C)C(Br)CBr	1.0	293	1677.0	1688.7	11.7	-	52.3	-	Br
232	CC(C)C(Br)CBr	0.0	337	-	1628.9	-	-	50.2	-	Br
233	CCC(Br)C(C)Br	1.0	293	1673.0	1677.2	4.2	-	52.4	-	Br
234	CCC(Br)C(C)Br	0.0	341	-	1610.7	-	-	49.7	-	Br
235	CC(C)CC(Br)Br	0.0	337	1602.8	1603.8	1.0	-	49.6	-	Br
236	CC(Br)CC(C)Br	1.0	293	1665.9	1664.5	-1.4	-	51.9	-	Br
237	CC(Br)CC(C)Br	0.0	344	-	1594.9	-	-	49.2	-	Br
238	CC(CBr)CCBr	1.0	293	1711.5	1701.0	-10.5	-	55.7	-	Br
239	CC(CBr)CCBr	0.0	337	-	1641.3	-	-	53.1	-	Br
240	CCC(Br)CCBr	1.0	293	1665.3	1687.2	21.9	-	54.2	-	Br
241	CCC(Br)CCBr	0.0	351	-	1608.2	-	-	50.9	-	Br
242	CCCC(Br)CBr	1.0	293	1670.8	1681.1	10.3	49.0	53.5	4.5	Br
243	CC(Br)CCCBr	1.0	293	1683.0	1683.5	0.5	-	55.4	-	Br
244	CC(Br)CCCBr	1.0	392	-	1547.3	-	51.8	49.6	-2.2	Br
245	CCCCC(Br)Br	0.0	343	1588.3	1596.4	8.0	-	50.3	-	Br
246	CCCCC(Br)Br	1.0	375	-	1550.8	-	48.8	48.5	-0.3	Br
247	BrCCCCCBr	1.0	298	1694.0	1690.1	-3.9	-	56.8	-	Br
248	BrCCCCCBr	1.0	411	-	1535.8	-	54.4	50.2	-4.2	Br
249	CC(Br)C(C)(Br)CBr	1.0	293	2082.1	2100.3	18.2	-	66.1	-	Br
250	CC(CBr)(CBr)CBr	1.0	293	2091.7	2122.8	31.1	-	68.0	-	Br
251	CCCCC(Br)(Br)Br	1.0	293	1988.2	2024.0	35.8	-	63.6	-	Br
252	CCCCC(Br)(Br)Br	0.1	427	-	1826.6	-	-	55.6	-	Br
253	BrCCC(Br)CCBr	1.0	292	2065.0	2073.2	8.2	-	70.0	-	Br
254	BrCCCC(Br)CBr	1.0	295	2073.0	2062.5	-10.5	-	69.9	-	Br
255	CCC(C)(C)CBr	0.0	311	1150.8	1183.8	33.0	-	42.2	-	Br
256	CC(C)(C)CCBr	1.0	293	1155.6	1192.2	36.6	-	44.2	-	Br
257	CC(C)(C)CCBr	0.0	308	-	1175.0	-	-	43.4	-	Br
258	CC(C)C(C)CBr	1.0	298	1190.0	1183.6	-6.4	-	43.3	-	Br
259	CC(C)C(C)CBr	0.0	311	-	1169.9	-	-	42.7	-	Br
260	CCC(C)C(C)Br	0.0	303	1163.1	1169.5	6.4	-	42.5	-	Br
261	CCC(Br)C(C)C	0.0	303	1163.1	1163.9	0.8	-	42.0	-	Br
262	CC(C)CC(C)Br	0.0	303	1144.3	1154.2	9.9	40.9	42.4	1.6	Br
263	CCC(CC)CBr	0.0	313	1159.9	1162.7	2.9	42.7	42.9	0.2	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
264	CCC(C)CCBr	1.0	296	1171.0	1180.2	9.2	-	44.6	-	Br
265	CCC(C)CCBr	0.0	317	-	1156.3	-	-	43.5	-	Br
266	CCCC(C)CBr	1.0	293	1177.9	1180.0	2.1	-	44.3	-	Br
267	CCCC(C)CBr	0.0	314	-	1156.5	-	-	43.2	-	Br
268	CCCC(Br)CC	0.0	312	-	1149.0	-	42.5	42.7	0.2	Br
269	CC(C)CCCBr	1.0	293	1168.3	1176.6	8.3	-	44.9	-	Br
270	CC(C)CCCBr	0.0	316	-	1150.4	-	-	43.6	-	Br
271	CCCCC(C)Br	1.0	298	1159.7	1161.5	1.8	-	43.8	-	Br
272	CCCCC(C)Br	1.0	318	-	1138.9	-	43.8	42.7	-1.1	Br
273	CC(C)(Br)C(C)(C)Br	0.3	435	-	1473.3	-	-	47.8	-	Br
274	CC(C)C(C)(Br)CBr	0.1	400	1450.3	1503.9	53.5	-	49.7	-	Br
275	CC(C)(C)C(Br)CBr	0.1	400	1462.2	1495.0	32.8	-	51.5	-	Br
276	CCCCC(C)(Br)Br	1.0	295	1546.3	1580.2	33.9	-	55.0	-	Br
277	CCCCC(C)(Br)Br	0.1	400	-	1443.5	-	-	49.0	-	Br
278	CC(C)C(CBr)CBr	1.0	293	1605.0	1623.7	18.7	-	58.2	-	Br
279	CC(CBr)C(C)CBr	0.1	400	1465.9	1488.3	22.4	-	52.2	-	Br
280	CCC(Br)C(Br)CC	1.0	293	1602.7	1594.5	-8.2	-	55.5	-	Br
281	CCC(Br)C(Br)CC	0.1	400	-	1455.0	-	-	49.5	-	Br
282	CCCC(Br)C(C)Br	1.0	293	1581.2	1591.8	10.6	-	56.2	-	Br
283	CCCC(Br)C(C)Br	0.1	400	-	1451.9	-	-	49.6	-	Br
284	CC(Br)CCC(C)Br	1.0	293	1578.8	1582.9	4.1	-	57.8	-	Br
285	CC(Br)CCC(C)Br	0.0	365	-	1490.2	-	49.5	53.3	3.8	Br
286	CCCC(CBr)CBr	1.0	293	1577.1	1613.5	36.4	-	58.9	-	Br
287	CC(CCBr)CCBr	0.1	426	1395.4	1443.0	47.6	50.8	52.2	1.4	Br
288	CCC(Br)CCCBr	0.1	400	1443.8	1461.0	17.2	-	52.6	-	Br
289	CCCCC(Br)CBr	1.0	293	1560.4	1593.1	32.7	56.5	57.8	1.3	Br
290	CC(Br)CCCCBr	0.1	400	1415.4	1456.7	41.3	-	53.0	-	Br
291	CCCCCC(Br)Br	0.1	400	1416.2	1440.1	23.9	-	51.1	-	Br
292	CCCCCC(Br)Br	1.0	393	-	1448.8	-	51.6	51.5	-0.1	Br
293	BrCCCCCCBr	1.0	298	1602.5	1600.0	-2.5	-	61.2	-	Br
294	BrCCCCCCBr	0.0	364	-	1517.1	-	57.1	57.0	-0.1	Br
295	CCC(CBr)(CBr)CBr	1.0	293	1912.2	2016.6	104.4	-	71.8	-	Br
296	CCCC(Br)CCC	1.0	296	1133.0	1136.7	3.7	-	48.1	-	Br
297	CCCC(Br)CCC	0.0	327	-	1101.9	-	-	46.3	-	Br
298	CCCCC(Br)CC	1.0	295	1134.1	1137.0	2.9	-	48.1	-	Br
299	CCCCCC(C)Br	0.0	320	1095.5	1107.5	11.9	46.2	47.1	0.9	Br
300	CCC(Br)(CBr)C(C)C	1.0	293	1526.1	1577.8	51.7	-	59.8	-	Br
301	CC(C)(C)CC(Br)CBr	1.0	293	1502.0	1540.5	38.5	-	59.6	-	Br
302	CCCC(Br)(CC)CBr	1.0	293	1492.9	1555.7	62.8	-	60.5	-	Br
303	CC(C)(CCBr)CCBr	1.0	293	1532.0	1568.1	36.1	-	64.8	-	Br
304	CCCC(Br)C(Br)CC	1.0	293	1516.2	1524.5	8.3	-	60.3	-	Br
305	CCCC(Br)C(Br)CC	0.1	418	-	1370.6	-	-	52.0	-	Br
306	CCCCC(Br)C(C)Br	1.0	293	1513.2	1521.0	7.8	-	60.2	-	Br
307	CCCCC(Br)C(C)Br	0.1	418	-	1366.4	-	-	52.3	-	Br
308	CCC(Br)CCCCBr	0.1	418	-	1376.0	-	-	55.3	-	Br
309	CCCCCC(Br)CBr	1.0	293	1518.0	1522.3	4.3	-	62.3	-	Br
310	CCCCCC(Br)CBr	1.0	300	-	1514.2	-	54.4	61.8	7.4	Br
311	CCCCCCC(Br)Br	1.0	294	1500.0	1509.5	9.5	-	62.1	-	Br
312	CCCCCCC(Br)Br	1.0	410	-	1367.8	-	54.4	54.5	0.1	Br
313	BrCCCCCCCBr	0.0	385	1469.2	1425.9	-43.3	57.8	59.8	2.0	Br
314	CC(C)CCCC(C)Br	1.0	293	1091.0	1108.4	17.4	-	52.1	-	Br
315	CCCCCCC(C)Br	1.0	298	1096.8	1106.4	9.6	-	53.0	-	Br
316	CCCCCCC(C)Br	1.0	358	-	1045.1	-	48.4	49.3	0.9	Br
317	CCC(C)(C)CC(Br)CBr	1.0	293	1468.9	1496.3	27.4	-	64.0	-	Br
318	CCCC(Br)C(Br)CCC	0.1	435	-	1298.3	-	-	54.6	-	Br
319	CCCCC(Br)CCCBr	0.1	435	-	1304.4	-	-	57.8	-	Br
320	CCCC(Br)CCCCBr	0.1	435	-	1305.0	-	-	57.9	-	Br
321	CCCCCCC(Br)CBr	1.0	293	1458.0	1463.9	5.9	-	66.7	-	Br
322	CCCCCCC(Br)CBr	0.1	435	-	1298.6	-	-	57.0	-	Br
323	CCCCCCCC(Br)Br	0.1	435	-	1289.3	-	-	56.9	-	Br
324	CCCCCCCC(Br)Br	1.0	427	-	1299.0	-	57.1	57.4	0.3	Br
325	BrCCCCCCCCBr	0.0	399	1413.1	1355.1	-58.0	59.6	62.7	3.1	Br
326	CCCCCCCC(C)Br	1.0	298	1076.0	1086.1	10.1	-	57.6	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
327	CCCCCCCCCBr	1.0	298	1084.9	1093.8	8.9	-	59.4	-	Br
328	CCCCCCCCCBr	1.0	391	-	1004.1	-	53.1	53.1	-0.0	Br
329	CCCCCCCC(Br)CBr	1.0	293	1398.0	1415.9	17.9	-	71.4	-	Br
330	CCCCCCCC(Br)CBr	0.1	451	-	1239.4	-	-	59.6	-	Br
331	CCCCCCCCC(Br)Br	0.1	451	-	1231.1	-	-	59.5	-	Br
332	CCCCCCCCC(Br)Br	1.0	442	-	1242.1	-	59.5	60.1	0.6	Br
333	BrCCCCCCCCCBr	1.0	298	1428.0	1420.1	-7.9	-	74.6	-	Br
334	BrCCCCCCCCCBr	0.0	415	-	1294.6	-	61.8	65.5	3.7	Br
335	CCCCCCCCC(C)Br	1.0	298	1047.0	1069.0	22.0	-	62.2	-	Br
336	CCCCCCCCC(C)Br	0.0	383	-	989.1	-	-	56.0	-	Br
337	CCCCCCCCCCBr	1.0	298	1062.5	1075.8	13.3	-	64.1	-	Br
338	CCCCCCCCCCBr	1.0	398	-	983.1	-	56.6	56.8	0.2	Br
339	CCCCCCCCC(Br)CBr	1.0	383	-	1280.3	-	67.0	68.7	1.7	Br
340	CCCCCCCCCC(Br)Br	1.0	457	-	1191.7	-	62.2	62.9	0.7	Br
341	CCC(C)CCl	0.0	298	-	874.2	-	36.3	36.1	-0.2	Cl
342	CC(Cl)C(C)(C)Cl	0.0	307	1080.9	1059.8	-21.1	-	40.6	-	Cl
343	CC(C)C(C)(Cl)Cl	0.0	333	1051.1	1016.6	-34.4	-	38.0	-	Cl
344	CC(C)(CCl)CCl	0.0	314	1066.8	1088.4	21.6	-	44.8	-	Cl
345	CCC(C)(Cl)CCl	0.0	306	1061.9	1070.0	8.1	35.9	41.4	5.5	Cl
346	CCC(Cl)(Cl)CC	0.0	303	1043.7	1045.2	1.5	40.3	39.8	-0.5	Cl
347	CC(C)(Cl)CCCl	1.0	293	1075.8	1083.8	8.0	-	45.3	-	Cl
348	CC(C)(Cl)CCCl	0.0	314	-	1063.6	-	-	44.2	-	Cl
349	CCCC(C)(Cl)Cl	0.0	299	1034.6	1038.2	3.6	40.0	40.3	0.3	Cl
350	CC(Cl)C(C)CCl	1.0	293	1093.8	1092.7	-1.1	-	46.5	-	Cl
351	CC(Cl)C(C)CCl	0.0	313	-	1072.4	-	-	45.3	-	Cl
352	CCC(C)C(Cl)Cl	0.0	302	1045.7	1055.1	9.4	-	41.8	-	Cl
353	CC(C)C(Cl)CCl	1.0	293	1080.5	1084.2	3.7	-	43.7	-	Cl
354	CC(C)C(Cl)CCl	0.0	312	-	1064.1	-	42.1	42.5	0.4	Cl
355	CCC(Cl)C(C)Cl	1.0	298	1075.0	1074.9	-0.1	-	47.3	-	Cl
356	CCC(Cl)C(C)Cl	0.0	309	-	1062.6	-	41.6	46.2	4.6	Cl
357	CC(C)CC(Cl)Cl	1.0	293	1047.3	1056.4	9.1	-	42.6	-	Cl
358	CC(C)CC(Cl)Cl	0.0	302	-	1046.5	-	40.1	42.1	2.0	Cl
359	CC(Cl)CC(C)Cl	1.0	291	1063.0	1067.0	4.0	-	44.7	-	Cl
360	CC(Cl)CC(C)Cl	0.0	317	-	1039.7	-	41.5	43.1	1.6	Cl
361	CC(CCl)CCCl	1.0	294	1103.0	1102.8	-0.2	-	50.4	-	Cl
362	CC(CCl)CCCl	0.0	324	-	1071.6	-	-	48.5	-	Cl
363	CCC(Cl)CCCl	1.0	293	1083.4	1087.0	3.6	-	46.4	-	Cl
364	CCC(Cl)CCCl	0.0	322	-	1056.8	-	-	44.8	-	Cl
365	CCCC(Cl)CCl	1.0	298	1074.1	1074.6	0.5	43.9	44.4	0.5	Cl
366	CC(Cl)CCCCl	1.0	293	1073.4	1088.3	14.9	48.1	49.7	1.6	Cl
367	CCCCC(Cl)Cl	0.0	304	1041.7	1045.1	3.4	-	43.0	-	Cl
368	CCCCC(Cl)Cl	1.0	298	-	1052.6	-	44.3	43.5	-0.8	Cl
369	CC(C)(Cl)C(C)(Cl)Cl	0.0	342	1144.6	1209.1	64.5	-	49.1	-	Cl
370	CC(Cl)C(C)(Cl)CCl	0.0	343	1184.5	1220.4	35.8	-	50.7	-	Cl
371	CC(C)(Cl)C(Cl)CCl	1.0	293	1264.1	1265.3	1.2	-	54.1	-	Cl
372	CC(CCl)(CCl)CCl	0.0	338	1215.5	1261.0	45.5	-	54.6	-	Cl
373	CCCCC(Cl)(Cl)Cl	0.0	298	1183.9	1185.0	1.1	-	46.0	-	Cl
374	CCC(C)(C)CCl	0.0	298	874.6	890.7	16.1	-	39.4	-	Cl
375	CC(C)(C)CCCl	0.0	298	863.1	883.3	20.2	38.5	40.1	1.7	Cl
376	CC(C)C(C)CCl	1.0	298	881.6	880.8	-0.8	-	39.7	-	Cl
377	CC(C)C(C)CCl	0.0	298	-	880.9	-	-	39.8	-	Cl
378	CCC(C)C(C)Cl	0.0	298	869.9	873.1	3.2	-	39.5	-	Cl
379	CCC(Cl)C(C)C	0.0	298	869.9	867.9	-2.0	-	39.2	-	Cl
380	CC(C)CC(C)Cl	0.0	298	855.9	861.4	5.4	-	39.4	-	Cl
381	CCC(CC)CCl	0.0	300	884.2	876.3	-7.8	-	40.1	-	Cl
382	CCC(C)CCCl	1.0	300	892.0	875.2	-16.8	-	40.7	-	Cl
383	CCC(C)CCCl	0.0	303	-	872.7	-	-	40.6	-	Cl
384	CCCC(C)CCl	0.0	298	869.9	873.6	3.8	-	40.5	-	Cl
385	CCCC(Cl)CC	1.0	297	871.0	865.6	-5.4	-	40.2	-	Cl
386	CCCC(Cl)CC	0.0	298	-	864.5	-	39.9	40.1	0.2	Cl
387	CC(C)CCCCl	0.0	300	868.5	870.6	2.1	-	40.9	-	Cl
388	CCCCC(C)Cl	0.0	299	864.8	861.9	-2.9	41.2	40.4	-0.8	Cl
389	CC(C)(C)C(C)(Cl)Cl	0.0	317	-	1051.0	-	-	43.5	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
390	CC(C)(C)CC(Cl)Cl	1.0	293	1027.1	1050.6	23.5	-	45.8	-	Cl
391	CC(C)(C)CC(Cl)Cl	0.0	322	-	1021.8	-	41.8	44.2	2.4	Cl
392	CC(Cl)CC(C)(C)Cl	1.0	293	1036.0	1049.9	13.9	-	46.8	-	Cl
393	CCCCC(C)(Cl)Cl	1.0	298	1015.0	1022.1	7.1	-	44.8	-	Cl
394	CCCCC(C)(Cl)Cl	0.0	338	-	981.2	-	-	42.6	-	Cl
395	CCC(Cl)C(Cl)CC	1.0	293	1061.7	1061.0	-0.7	-	52.5	-	Cl
396	CCCC(Cl)C(C)Cl	0.0	334	1015.7	1011.0	-4.7	-	46.7	-	Cl
397	CCCC(Cl)CCCl	0.0	343	-	1011.3	-	-	47.7	-	Cl
398	CCC(Cl)CCCCl	0.0	350	-	1009.1	-	-	49.8	-	Cl
399	CCCCC(Cl)CCl	1.0	293	1080.0	1054.6	-25.4	48.2	49.1	0.9	Cl
400	CC(Cl)CCCCCl	1.0	293	1108.6	1061.8	-46.8	-	54.1	-	Cl
401	CCCCCC(Cl)Cl	0.0	335	987.4	993.3	5.9	-	45.6	-	Cl
402	CCCCCC(Cl)Cl	1.0	298	-	1030.8	-	48.7	47.8	-0.9	Cl
403	CCCCCC(Cl)(Cl)Cl	0.1	390	1033.3	1050.1	16.8	-	44.9	-	Cl
404	CC(C)(C)C(C)(C)Cl	0.0	298	864.3	908.8	44.5	-	42.6	-	Cl
405	CCC(C)(Cl)C(C)C	0.0	301	861.7	887.0	25.3	-	42.2	-	Cl
406	CCC(C)C(C)(C)Cl	0.0	301	-	881.6	-	-	42.2	-	Cl
407	CC(Cl)CC(C)(C)C	0.0	302	852.3	871.1	18.8	-	42.6	-	Cl
408	CC(C)CC(C)(C)Cl	1.0	293	862.8	868.1	5.3	-	41.6	-	Cl
409	CC(C)CC(C)(C)Cl	0.0	302	-	860.2	-	-	41.1	-	Cl
410	CCC(Cl)(CC)CC	0.0	314	865.9	869.5	3.6	-	41.5	-	Cl
411	CCCC(C)(Cl)CC	0.0	308	865.5	864.8	-0.7	-	42.0	-	Cl
412	CCCCC(C)(C)Cl	1.0	293	863.5	868.3	4.8	-	42.9	-	Cl
413	CCCCC(C)(C)Cl	0.0	309	-	854.2	-	-	42.0	-	Cl
414	CC(C)CCC(C)Cl	0.0	309	848.9	851.8	3.0	-	43.3	-	Cl
415	CCCC(C)CCCl	0.0	320	851.3	855.6	4.3	-	44.0	-	Cl
416	CCCC(Cl)CCC	1.0	295	869.4	867.4	-2.0	-	44.8	-	Cl
417	CCCC(Cl)CCC	0.0	315	-	850.0	-	-	43.6	-	Cl
418	CCCCC(Cl)CC	1.0	298	857.9	865.1	7.2	-	44.6	-	Cl
419	CCCCC(Cl)CC	0.0	315	-	850.1	-	-	43.6	-	Cl
420	CCCCCC(C)Cl	1.0	295	865.1	865.5	0.4	-	45.1	-	Cl
421	CCCCCC(C)Cl	1.0	328	-	835.9	-	44.8	43.1	-1.7	Cl
422	CC(C)(Cl)CC(C)(C)Cl	0.0	339	986.3	998.3	12.1	-	47.9	-	Cl
423	CCC(C)(C)CC(Cl)Cl	1.0	293	1032.1	1045.9	13.8	-	50.4	-	Cl
424	CC(C)(C)CC(Cl)CCl	1.0	293	1025.9	1047.6	21.7	-	50.9	-	Cl
425	CC(C)(C)CC(Cl)CCl	0.0	344	-	1000.5	-	45.1	47.9	2.8	Cl
426	CC(C)(CCCl)CCCl	1.0	293	1056.3	1077.5	21.2	-	58.9	-	Cl
427	CC(C)(CCCl)CCCl	0.0	339	-	1036.7	-	-	55.8	-	Cl
428	CCCC(Cl)(Cl)CCC	0.0	349	1021.9	966.0	-56.0	-	46.2	-	Cl
429	CCCCCC(C)(Cl)Cl	0.0	340	968.2	965.0	-3.2	-	46.7	-	Cl
430	CCCCCC(Cl)CCl	1.0	293	1062.5	1034.5	-28.0	53.2	53.3	0.1	Cl
431	CCCCCCC(Cl)Cl	0.0	353	995.8	961.1	-34.8	-	48.7	-	Cl
432	CCCCCCC(Cl)Cl	1.0	298	-	1014.7	-	53.5	52.4	-1.1	Cl
433	ClCCCCCCCCCl	1.0	298	1040.8	1045.6	4.8	61.2	59.8	-1.5	Cl
434	CCCCCCC(Cl)(Cl)Cl	1.0	298	1121.2	1126.7	5.5	-	55.2	-	Cl
435	CCCCCCC(Cl)(Cl)Cl	0.1	410	-	1008.4	-	-	47.8	-	Cl
436	ClCCCCCCC(Cl)Cl	1.0	293	1174.4	1172.0	-2.4	-	66.4	-	Cl
437	CCC(C)(C)C(C)(C)Cl	1.0	298	906.5	919.2	12.7	-	47.3	-	Cl
438	CCC(C)(Cl)C(C)(C)C	1.0	293	906.6	921.3	14.7	-	47.4	-	Cl
439	CC(C)(C)CC(C)(C)Cl	1.0	293	874.1	883.0	8.9	-	45.2	-	Cl
440	CC(C)(C)CC(C)(C)Cl	0.0	332	-	850.1	-	-	43.1	-	Cl
441	CC(C)C(C)C(C)(C)Cl	1.0	293	888.0	893.8	5.8	-	45.9	-	Cl
442	CCCC(C)(Cl)C(C)C	0.0	332	834.5	857.5	22.9	-	44.7	-	Cl
443	CC(C)CCC(C)(C)Cl	0.0	332	-	832.5	-	-	43.8	-	Cl
444	CCCC(C)(Cl)CCC	0.0	332	834.8	844.7	9.9	-	45.2	-	Cl
445	CCCCC(C)(Cl)CC	0.0	328	845.6	847.6	2.0	-	45.1	-	Cl
446	CCCCCC(C)(C)Cl	1.0	298	856.8	863.9	7.1	-	47.1	-	Cl
447	CCCCCC(C)(C)Cl	0.0	328	-	837.9	-	-	45.2	-	Cl
448	CC(C)CCCC(C)Cl	0.0	328	-	834.9	-	-	46.4	-	Cl
449	CCCCC(CC)CCl	1.0	293	876.9	880.2	3.3	-	49.3	-	Cl
450	CCCCC(CC)CCl	0.0	337	-	841.2	-	47.4	46.5	-0.9	Cl
451	CCC(C)CCCCCl	0.0	336	-	841.8	-	-	47.3	-	Cl
452	CCCCCCC(C)Cl	1.0	298	861.5	863.5	2.1	-	49.5	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
453	CCCCCCC(C)Cl	1.0	345	-	822.8	-	47.8	46.4	-1.4	Cl
454	CC(C)(Cl)CCC(C)(C)Cl	0.0	363	-	952.0	-	-	49.7	-	Cl
455	CCC(C)(C)CC(Cl)CCl	1.0	293	1029.0	1042.1	13.1	-	55.1	-	Cl
456	CCCCCC(Cl)C(C)Cl	0.0	368	-	945.1	-	-	51.3	-	Cl
457	CCCCCCC(Cl)CCl	1.0	298	-	1014.1	-	57.6	57.4	-0.2	Cl
458	CCCCCCCC(Cl)Cl	0.0	370	-	934.3	-	-	51.8	-	Cl
459	CCCCCCCC(Cl)Cl	1.0	298	-	1000.9	-	57.7	56.9	-0.8	Cl
460	ClCCCCCCCCCl	1.0	298	1024.8	1028.0	3.2	65.6	63.9	-1.7	Cl
461	CCCCCCCC(Cl)(Cl)Cl	0.1	430	948.0	971.9	23.9	-	50.4	-	Cl
462	CCC(Cl)(CC)C(C)(C)C	0.0	344	-	884.3	-	-	48.3	-	Cl
463	CCCC(C)(Cl)C(C)(C)C	0.0	340	858.2	878.8	20.6	-	49.0	-	Cl
464	CCCCC(Cl)(CC)CC	0.0	351	836.3	837.3	1.0	-	47.7	-	Cl
465	CCCCC(C)(Cl)CCC	0.0	347	827.0	832.6	5.6	-	48.4	-	Cl
466	CCCCCC(C)(Cl)CC	0.0	347	826.8	831.9	5.1	-	48.3	-	Cl
467	CCCCCC(Cl)C(C)C	1.0	293	856.6	872.1	15.5	-	52.9	-	Cl
468	CCCCC(Cl)CCCC	0.0	351	815.6	821.8	6.2	-	49.9	-	Cl
469	CCCCCCC(Cl)CC	0.0	352	807.5	820.3	12.7	-	49.9	-	Cl
470	CCCCCCCC(C)Cl	1.0	293	879.0	868.1	-10.9	-	54.4	-	Cl
471	CCCCCCCCCCl	1.0	298	867.4	871.8	4.4	55.9	55.6	-0.3	Cl
472	CC(C)(Cl)CCCC(C)(C)Cl	0.0	374	-	929.4	-	-	53.4	-	Cl
473	CCCCCCCC(Cl)CCl	1.0	298	-	1000.7	-	62.1	61.8	-0.3	Cl
474	CCCCCCCCC(Cl)Cl	0.1	436	-	862.2	-	-	51.0	-	Cl
475	CCCCCCCCC(Cl)Cl	1.0	298	-	990.1	-	62.3	61.4	-0.9	Cl
476	ClCCCCCCCCCCl	1.0	298	1017.3	1013.4	-3.9	-	68.2	-	Cl
477	ClCCCCCCCCCCl	0.1	453	-	876.3	-	54.6	55.8	1.2	Cl
478	CCCCCCCCC(Cl)(Cl)Cl	0.1	449	914.4	939.0	24.6	-	53.0	-	Cl
479	CCCCCCCCC(C)Cl	1.0	293	870.6	868.3	-2.3	-	59.0	-	Cl
480	CCCCCCCCCCCl	1.0	298	865.8	871.5	5.7	64.0	60.1	-3.9	Cl
481	CCCCCCCCCC(Cl)Cl	0.1	456	-	838.1	-	-	53.4	-	Cl
482	CCCCCCCCCC(Cl)Cl	1.0	430	-	863.4	-	56.9	55.4	-1.5	Cl
483	ClCCCCCCCCCCCl	1.0	298	992.9	1001.7	8.7	73.1	72.6	-0.5	Cl
484	CCCCCCCCCC(Cl)(Cl)Cl	0.1	439	917.0	939.2	22.1	52.5	57.5	5.0	Cl
485	CCC(C)CF	1.0	302	-	781.9	-	30.7	30.7	0.0	F
486	CC(C)CCF	1.0	293	694.1	791.1	97.0	-	31.5	-	F
487	CC(C)CCF	0.4	298	-	785.8	-	-	31.2	-	F
488	CCCCCF	0.2	298	-	788.6	-	30.9	32.1	1.2	F
489	CC(F)C(C)(C)F	0.1	298	-	884.1	-	-	30.1	-	F
490	CC(C)C(C)(F)F	0.1	298	-	871.9	-	-	29.5	-	F
491	CC(C)(CF)CF	0.1	298	-	960.5	-	-	35.9	-	F
492	CCC(C)(F)CF	0.1	298	-	908.2	-	-	31.2	-	F
493	CCC(F)(F)CC	1.0	293	910.6	872.5	-38.1	-	30.2	-	F
494	CCC(F)(F)CC	1.0	277	-	891.8	-	33.8	30.9	-2.9	F
495	CC(C)(F)CCF	0.1	298	-	915.7	-	-	33.8	-	F
496	CCCC(C)(F)F	1.0	293	898.7	863.5	-35.2	-	30.1	-	F
497	CCCC(C)(F)F	1.0	277	-	883.2	-	33.7	30.9	-2.8	F
498	CC(F)C(C)CF	0.1	298	-	935.0	-	-	35.1	-	F
499	CCC(C)C(F)F	0.1	298	-	910.6	-	-	32.8	-	F
500	CC(C)C(F)CF	0.1	298	-	924.6	-	-	33.0	-	F
501	CCC(F)C(C)F	0.1	298	-	905.0	-	-	32.1	-	F
502	CC(C)CC(F)F	0.1	298	-	906.0	-	-	33.0	-	F
503	CC(F)CC(C)F	0.1	298	-	901.6	-	-	33.8	-	F
504	CC(CF)CCF	0.1	298	-	961.4	-	-	38.4	-	F
505	CCC(F)CCF	0.1	298	-	934.0	-	-	35.9	-	F
506	CCCC(F)CF	0.1	298	-	924.4	-	-	34.1	-	F
507	CC(F)CCCF	0.1	298	-	936.8	-	-	37.6	-	F
508	CCCCC(F)F	0.1	298	-	907.0	-	-	33.9	-	F
509	CCCCC(F)F	1.0	283	-	924.4	-	34.4	34.7	0.3	F
510	FCCCCCF	1.0	298	957.2	963.8	6.6	-	40.0	-	F
511	FCCCCCF	0.0	298	-	963.7	-	-	40.0	-	F
512	CC(C)CC(F)(F)F	1.0	298	978.8	959.3	-19.5	-	29.8	-	F
513	CCCCC(F)(F)F	1.0	293	970.1	964.5	-5.6	-	30.9	-	F
514	CCCCC(F)(F)F	0.3	298	-	957.2	-	-	30.7	-	F
515	CCC(C)(C)CF	0.1	298	-	811.4	-	-	34.6	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
516	CC(C)(C)CCF	1.0	293	780.9	814.6	33.7	-	35.3	-	F
517	CC(C)(C)CCF	0.1	298	-	810.2	-	-	35.1	-	F
518	CC(C)C(C)CF	0.1	298	-	804.4	-	-	34.8	-	F
519	CCC(C)C(C)F	0.1	298	-	786.9	-	-	34.0	-	F
520	CCC(F)C(C)C	0.1	298	-	780.8	-	-	33.9	-	F
521	CC(C)CC(C)F	0.1	298	-	777.8	-	-	34.1	-	F
522	CCC(C)CCF	0.1	298	-	803.6	-	-	35.7	-	F
523	CCCC(C)CF	0.1	298	-	797.5	-	-	35.5	-	F
524	CCCC(F)CC	0.1	298	-	780.4	-	-	34.8	-	F
525	CCCC(F)CC	1.0	296	-	782.4	-	36.8	34.9	-1.9	F
526	CC(C)CCCF	0.1	298	-	797.5	-	-	35.8	-	F
527	CCCCC(C)F	0.1	298	-	779.4	-	-	34.9	-	F
528	CCCCCCF	0.1	298	-	799.6	-	35.6	36.6	1.0	F
529	CCCCCC(F)F	0.1	310	-	890.4	-	-	37.8	-	F
530	CCCCCC(F)F	1.0	305	-	896.5	-	37.7	38.1	0.4	F
531	CCCCCC(F)(F)F	1.0	293	960.8	958.4	-2.4	-	35.7	-	F
532	CCCCCC(F)(F)F	0.1	298	-	951.8	-	-	35.4	-	F
533	CCCCCCC(F)F	1.0	293	-	904.7	-	-	43.3	-	F
534	CCCCCCC(F)F	1.0	326	-	872.7	-	41.1	41.4	0.3	F
535	CCCCCCC(F)(F)F	0.1	317	-	925.3	-	-	38.9	-	F
536	CCCCCCCCF	1.0	322	-	794.3	-	44.1	44.4	0.3	F
537	CCCCCCCC(F)F	0.1	365	-	834.3	-	-	43.4	-	F
538	CCCCCCCC(F)F	1.0	344	-	854.9	-	44.2	44.7	0.5	F
539	CCCCCCCC(F)(F)F	0.1	341	-	895.2	-	-	41.9	-	F
540	CCCCCCCCCF	1.0	293	-	823.5	-	-	50.8	-	F
541	CCCCCCCCCF	1.0	348	-	778.3	-	46.8	47.1	0.3	F
542	CCCCCCCCC(F)F	0.1	389	-	812.2	-	-	45.9	-	F
543	CCCCCCCCC(F)F	1.0	362	-	837.4	-	47.2	47.8	0.6	F
544	CCCCCCCCC(F)(F)F	1.0	293	935.7	940.1	4.4	-	49.7	-	F
545	CCCCCCCCC(F)(F)F	0.1	363	-	870.2	-	-	45.0	-	F
546	CCCCCCCCCCF	1.0	293	819.4	827.6	8.2	-	55.4	-	F
547	CCCCCCCCCCF	1.0	357	-	776.6	-	50.4	50.9	0.5	F
548	CCCCCCCCCC(F)F	0.1	412	-	791.7	-	-	48.5	-	F
549	CCCCCCCCCC(F)F	1.0	379	-	822.8	-	50.2	50.9	0.7	F
550	CCCCCCCCCC(F)(F)F	0.1	385	-	847.9	-	-	47.7	-	F
551	CCC(C)CI	0.0	310	1496.8	1499.5	2.8	43.1	42.3	-0.8	I
552	CC(I)C(C)(C)I	0.0	378	-	2063.2	-	-	53.9	-	I
553	CC(C)(CI)CI	0.0	385	-	2069.9	-	-	54.8	-	I
554	CCC(C)(I)CI	0.0	392	-	2046.2	-	-	53.9	-	I
555	CCC(I)(I)CC	0.0	386	-	2042.1	-	-	53.3	-	I
556	CC(C)(I)CCI	0.0	381	-	2044.7	-	-	56.0	-	I
557	CCCC(C)(I)I	0.0	386	-	2017.9	-	-	53.7	-	I
558	CCC(C)C(I)I	0.0	386	-	2023.1	-	-	53.8	-	I
559	CC(C)C(I)CI	0.0	378	-	2039.3	-	-	55.1	-	I
560	CCC(I)C(C)I	0.0	389	-	2011.5	-	-	53.7	-	I
561	CC(C)CC(I)I	0.0	389	-	1991.5	-	-	54.1	-	I
562	CC(I)CC(C)I	0.0	392	-	1985.0	-	-	53.6	-	I
563	CC(CI)CCI	0.0	398	-	2008.6	-	-	55.9	-	I
564	CCC(I)CCI	0.0	400	1966.0	1996.1	30.1	-	55.1	-	I
565	CCCC(I)CI	0.0	397	1961.6	1994.1	32.4	-	54.7	-	I
566	CC(I)CCCI	0.0	403	1970.4	1982.4	12.0	-	55.3	-	I
567	CCCCC(I)I	0.0	394	1962.8	1984.6	21.8	-	54.7	-	I
568	ICCCCCI	0.0	406	-	1992.1	-	59.7	57.0	-2.7	I
569	CCCCC(I)(I)I	0.0	469	-	2335.2	-	-	64.3	-	I
570	CCC(C)(C)CI	0.0	319	1393.3	1447.9	54.6	-	45.4	-	I
571	CC(C)(C)CCI	0.0	324	1387.2	1424.1	36.9	-	46.3	-	I
572	CC(C)C(C)CI	0.0	326	1385.2	1420.9	35.7	-	45.6	-	I
573	CCC(C)C(C)I	0.0	332	1376.8	1405.0	28.2	-	44.6	-	I
574	CCC(I)C(C)C	0.0	319	1393.3	1417.3	24.0	-	44.8	-	I
575	CC(C)CC(C)I	0.0	319	1393.3	1401.6	8.3	-	45.0	-	I
576	CCC(CC)CI	1.0	296	1440.0	1454.7	14.7	-	47.4	-	I
577	CCC(C)CCI	0.0	333	1349.7	1402.6	52.9	-	46.2	-	I
578	CCCC(C)CI	0.0	328	-	1405.5	-	-	45.9	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
579	CCCC(I)CC	0.0	328	1382.1	1397.9	15.9	-	45.3	-	I
580	CC(C)CCCI	1.0	293	1428.3	1445.5	17.2	-	48.4	-	I
581	CC(C)CCCI	0.0	332	-	1394.9	-	-	46.2	-	I
582	CCCCC(C)I	0.0	329	-	1391.4	-	-	45.6	-	I
583	CCCCCC(I)I	0.0	410	-	1844.6	-	-	57.7	-	I
584	ICCCCCCI	0.0	402	-	1882.8	-	-	61.3	-	I
585	CCCC(I)CCC	0.1	387	-	1269.5	-	-	46.3	-	I
586	CCCCC(I)CC	1.0	295	1365.6	1383.2	17.6	-	51.5	-	I
587	CCCCC(I)CC	0.0	349	-	1317.5	-	-	48.4	-	I
588	CCCCCC(C)I	0.0	349	1285.9	1312.2	26.3	-	48.9	-	I
589	CCCCCCC(I)I	0.1	491	-	1630.8	-	-	56.4	-	I
590	CCCCCCC(C)I	1.0	299	1316.4	1327.4	11.0	-	56.4	-	I
591	CCCCCCC(C)I	0.1	406	-	1203.6	-	-	49.8	-	I
592	CCCCCCCC(I)I	0.0	442	-	1632.5	-	-	63.5	-	I
593	ICCCCCCCCI	0.0	453	-	1637.7	-	-	65.6	-	I
594	CCCCCCCCCI	1.0	298	1283.6	1297.8	14.2	64.5	63.1	-1.4	I
595	CCCCCCCCC(C)I	1.0	298	1241.2	1257.9	16.7	-	65.6	-	I
596	CCCCCCCCCCI	1.0	293	1256.7	1269.6	12.9	69.8	68.0	-1.8	I
597	FCCCCCCl	0.0	325	1006.0	1006.2	0.2	-	44.0	-	Mix
598	FCCCCCCCl	0.0	353	962.2	958.8	-3.4	-	46.5	-	Mix
599	FCCCCCCCCl	0.1	379	923.4	919.8	-3.7	-	48.7	-	Mix
600	FCCCCCCCCCCl	0.1	426	870.8	858.2	-12.6	-	53.0	-	Mix
601	FCCCCCCCCCCCl	0.1	447	851.5	833.5	-17.9	-	55.2	-	Mix

Table S16: Comparison of experimental and simulated properties validation using the AT/EEM-G scheme.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	BrCBr	0.1	298	2482.0	2485.7	3.7	-	38.2	-	Br
2	BrCBr	1.0	298	-	2487.1	-	37.0	38.2	1.2	Br
3	BrC(Br)Br	1.0	298	2877.2	2896.2	19.0	46.1	49.1	3.0	Br
4	BrC(Br)(Br)Br	1.0	374	2953.3	3028.2	74.9	-	54.9	-	Br
5	BrC(Br)(Br)Br	1.0	384	-	3007.0	-	48.2	54.4	6.2	Br
6	CC(Br)Br	1.0	316	-	2055.2	-	39.6	38.6	-1.0	Br
7	BrCC(Br)Br	1.0	321	-	2554.4	-	52.9	53.4	0.5	Br
8	CC(C)(Br)Br	0.0	298	1820.0	1872.9	52.9	37.3	40.3	2.9	Br
9	CCC(Br)Br	0.0	302	1968.8	1898.7	-70.2	43.1	43.4	0.3	Br
10	CC(Br)(Br)CBr	0.0	349	-	2267.6	-	47.5	53.0	5.4	Br
11	BrCC(Br)CBr	0.0	374	-	2259.4	-	52.1	56.3	4.1	Br
12	BrCCC(Br)Br	1.0	290	2350.0	2382.7	32.7	-	59.7	-	Br
13	CC(C)(Br)CBr	1.0	293	1760.4	1794.2	33.8	-	46.5	-	Br
14	CC(C)(Br)CBr	0.0	322	-	1751.4	-	41.8	45.1	3.3	Br
15	CCC(C)(Br)Br	0.0	318	1718.7	1738.3	19.6	41.0	44.0	3.0	Br
16	CC(C)C(Br)Br	0.0	321	1733.3	1733.1	-0.2	-	45.4	-	Br
17	CC(Br)C(C)Br	1.0	295	1789.3	1773.8	-15.5	-	47.1	-	Br
18	CC(Br)C(C)Br	0.0	325	-	1730.8	-	43.0	45.7	2.7	Br
19	CC(Br)CCBr	0.0	343	-	1719.7	-	45.1	47.5	2.5	Br
20	CCCC(Br)Br	1.0	298	1784.0	1764.2	-19.8	-	48.1	-	Br
21	CCCC(Br)Br	1.0	357	-	1674.1	-	45.8	45.0	-0.8	Br
22	BrCCCCBr	1.0	298	1818.8	1807.6	-11.2	52.6	52.4	-0.2	Br
23	CC(Br)C(C)(Br)Br	1.0	293	2172.4	2197.3	24.9	-	58.5	-	Br
24	CC(Br)C(C)(Br)Br	1.0	326	-	2147.8	-	51.7	56.8	5.1	Br
25	CCC(Br)(Br)CBr	1.0	293	2168.5	2207.8	39.3	-	59.4	-	Br
26	CCC(Br)(Br)CBr	1.0	329	-	2152.4	-	50.7	57.4	6.7	Br
27	CC(Br)C(Br)CBr	1.0	293	2183.5	2202.8	19.3	-	64.1	-	Br
28	CC(Br)C(Br)CBr	1.0	333	-	2141.9	-	51.3	61.3	10.0	Br
29	CCC(Br)C(Br)Br	1.0	293	2183.5	2181.5	-2.0	-	60.7	-	Br
30	CCC(Br)C(Br)Br	0.0	369	-	2063.2	-	51.1	56.6	5.5	Br
31	BrCC(CBr)CBr	1.0	490	-	1933.2	-	66.1	54.0	-12.1	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
32	BrCCC(Br)CBr	1.0	298	2210.0	2208.7	-1.3	-	64.6	-	Br
33	BrCCC(Br)CBr	1.0	405	-	2042.7	-	53.5	58.4	4.9	Br
34	CC(C)(C)CBr	1.0	308	-	1210.8	-	35.6	37.5	1.9	Br
35	CC(C)C(C)Br	0.0	298	1215.6	1204.2	-11.4	-	38.3	-	Br
36	CC(C)C(C)Br	1.0	316	-	1182.7	-	37.2	37.5	0.3	Br
37	CCC(Br)CC	0.0	298	-	1203.9	-	39.3	39.0	-0.3	Br
38	CC(Br)C(C)(C)C	0.0	298	1169.8	1195.2	25.5	-	42.2	-	Br
39	CC(Br)C(C)(C)C	1.0	330	-	1161.3	-	39.5	40.7	1.2	Br
40	CC(C)C(C)(C)Br	1.0	292	1187.4	1195.5	8.1	-	41.6	-	Br
41	CCCC(C)(C)Br	1.0	293	1180.4	1176.3	-4.1	-	42.1	-	Br
42	ClCCl	1.0	298	1316.4	1338.6	22.2	28.8	30.5	1.7	Cl
43	ClC(Cl)Cl	1.0	298	1479.5	1526.6	47.1	31.1	33.5	2.4	Cl
44	ClC(Cl)(Cl)Cl	1.0	298	1584.3	1638.7	54.4	-	35.3	-	Cl
45	ClC(Cl)(Cl)Cl	0.1	298	-	1639.0	-	32.4	35.3	2.9	Cl
46	CC(C)Cl	0.7	298	-	846.2	-	26.4	26.9	0.5	Cl
47	CCCCl	1.0	298	884.1	876.6	-7.5	28.5	28.3	-0.2	Cl
48	CC(C)(Cl)Cl	0.2	298	1107.3	1068.6	-38.7	-	30.5	-	Cl
49	CC(C)(Cl)Cl	1.0	298	-	1069.1	-	32.1	30.5	-1.6	Cl
50	CCC(Cl)Cl	0.1	298	1126.0	1110.2	-15.8	-	34.5	-	Cl
51	CCC(Cl)Cl	1.0	298	-	1110.2	-	35.2	34.5	-0.7	Cl
52	CC(Cl)(Cl)CCl	0.0	298	1317.9	1314.1	-3.8	40.5	41.7	1.2	Cl
53	CCC(Cl)(Cl)Cl	1.0	298	1283.6	1274.1	-9.5	-	36.7	-	Cl
54	CCC(Cl)(Cl)Cl	1.0	259	-	1328.3	-	38.8	38.5	-0.3	Cl
55	CC(Cl)C(Cl)Cl	1.0	289	1353.0	1328.4	-24.6	-	43.7	-	Cl
56	CC(Cl)C(Cl)Cl	0.0	302	-	1311.7	-	42.3	42.9	0.6	Cl
57	ClCC(Cl)CCl	1.0	298	1388.8	1379.3	-9.5	46.8	49.7	2.9	Cl
58	ClCCC(Cl)Cl	1.0	293	1355.5	1356.0	0.5	-	45.5	-	Cl
59	ClCCC(Cl)Cl	0.0	313	-	1331.8	-	44.2	44.5	0.3	Cl
60	CC(C)(Cl)CCl	0.0	298	1089.0	1089.8	0.9	36.8	37.1	0.3	Cl
61	CCC(C)(Cl)Cl	0.1	298	1065.1	1062.1	-3.0	-	35.2	-	Cl
62	CCC(C)(Cl)Cl	1.0	298	-	1061.8	-	36.7	35.2	-1.5	Cl
63	CC(C)C(Cl)Cl	0.0	298	1100.1	1074.2	-25.9	36.5	37.7	1.2	Cl
64	CC(Cl)C(C)Cl	0.0	298	-	1087.7	-	38.5	41.6	3.1	Cl
65	CC(CCl)CCl	0.0	307	1090.0	1111.6	21.6	-	42.4	-	Cl
66	CC(CCl)CCl	1.0	285	-	1136.3	-	45.1	43.7	-1.4	Cl
67	CC(Cl)CCCl	1.0	298	1108.3	1107.2	-1.1	42.1	42.4	0.3	Cl
68	CCCC(Cl)Cl	0.0	298	1080.1	1075.8	-4.3	-	39.0	-	Cl
69	CCCC(Cl)Cl	1.0	298	-	1076.6	-	39.4	39.0	-0.4	Cl
70	CC(C)(Cl)C(Cl)Cl	1.0	298	1267.7	1263.1	-4.6	-	44.7	-	Cl
71	CC(Cl)C(C)(Cl)Cl	1.0	291	1263.0	1264.1	1.1	-	44.6	-	Cl
72	CC(Cl)C(C)(Cl)Cl	0.0	310	-	1240.7	-	42.7	43.5	0.8	Cl
73	CC(Cl)(CCl)CCl	1.0	298	1301.2	1302.0	0.8	-	49.0	-	Cl
74	CC(Cl)(CCl)CCl	0.0	327	-	1270.2	-	45.9	47.1	1.2	Cl
75	CCCC(Cl)(Cl)Cl	0.0	298	1231.0	1229.6	-1.4	-	41.7	-	Cl
76	CC(CCl)C(Cl)Cl	0.0	312	1251.1	1266.8	15.7	-	46.8	-	Cl
77	CC(Cl)C(Cl)CCl	1.0	293	1316.4	1298.0	-18.4	-	51.3	-	Cl
78	CC(Cl)C(Cl)CCl	1.0	288	-	1303.5	-	41.3	51.6	10.3	Cl
79	CC(Cl)CC(Cl)Cl	1.0	288	1317.0	1274.1	-42.9	-	48.0	-	Cl
80	CC(Cl)CC(Cl)Cl	0.0	318	-	1239.9	-	43.9	46.3	2.5	Cl
81	ClCCC(Cl)CCl	1.0	293	1317.5	1318.9	1.4	-	53.2	-	Cl
82	CC(C)(C)CCl	0.1	298	860.9	878.7	17.8	-	34.7	-	Cl
83	CC(C)(C)CCl	1.0	294	-	883.1	-	34.9	34.9	0.0	Cl
84	CC(C)C(C)Cl	0.1	298	857.0	863.0	6.0	-	34.9	-	Cl
85	CC(C)C(C)Cl	1.0	300	-	861.5	-	35.9	34.9	-1.0	Cl
86	CCC(Cl)CC	1.0	298	884.0	863.5	-20.5	-	35.8	-	Cl
87	CCC(Cl)CC	1.0	304	-	857.9	-	36.5	35.5	-1.0	Cl
88	CC(C)(C)C(Cl)Cl	0.0	312	1074.8	1058.7	-16.1	-	40.6	-	Cl
89	CC(C)C(C)(C)Cl	1.0	298	874.9	878.5	3.6	-	37.5	-	Cl
90	CC(C)C(C)(C)Cl	1.0	316	-	861.7	-	38.0	36.6	-1.4	Cl
91	CCC(C)(Cl)CC	1.0	293	883.9	879.3	-4.6	-	38.0	-	Cl
92	CCCC(C)(C)Cl	0.0	298	858.3	862.8	4.4	37.7	37.8	0.1	Cl
93	FCF	1.0	221	1213.8	1246.5	32.7	20.9	22.7	1.8	F
94	FCF	17.6	298	891.6	1076.4	184.8	-	19.7	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
95	FCF	1.0	298	961.0	1071.9	110.9	-	19.7	-	F
96	FC(F)F	1.0	191	1442.9	1734.7	291.8	16.7	23.1	6.4	F
97	FC(F)F	47.1	298	636.7	1325.2	688.5	-	17.4	-	F
98	FC(F)(F)F	1.0	145	1605.2	1507.4	-97.8	12.3	19.7	7.4	F
99	FCCF	1.0	283	1024.0	1048.6	24.6	-	24.1	-	F
100	FCCF	1.8	298	-	1024.2	-	22.5	23.5	1.0	F
101	CC(F)(F)F	12.9	298	-	902.4	-	13.1	14.7	1.6	F
102	CC(C)F	1.0	293	723.8	706.4	-17.4	-	21.1	-	F
103	CC(C)F	1.0	249	-	769.2	-	23.7	23.0	-0.7	F
104	CC(C)(F)F	1.0	271	943.8	855.3	-88.4	22.6	20.5	-2.1	F
105	CC(C)(F)F	2.1	291	911.4	817.6	-93.8	21.6	19.6	-1.9	F
106	CC(F)CF	1.4	298	960.0	932.3	-27.7	-	24.9	-	F
107	CCC(F)F	1.3	298	920.1	892.5	-27.6	23.7	23.9	0.2	F
108	CCC(F)(F)F	0.9	259	1148.2	1014.0	-134.1	21.8	21.5	-0.3	F
109	CC(C)(C)F	1.0	237	-	778.1	-	27.6	24.9	-2.7	F
110	CC(C)CF	0.9	286	764.5	770.8	6.3	-	26.8	-	F
111	CC(C)CF	1.4	298	750.0	757.4	7.4	-	26.3	-	F
112	CCC(C)F	1.0	248	-	795.0	-	29.2	27.7	-1.5	F
113	CCCCF	1.0	237	-	837.3	-	30.1	30.3	0.2	F
114	CCC(C)(F)F	1.0	293	915.9	842.5	-73.4	-	24.3	-	F
115	CCC(C)(F)F	0.8	298	-	836.8	-	25.9	24.2	-1.8	F
116	CCCC(F)F	0.4	298	910.1	892.1	-18.0	-	28.5	-	F
117	CCCC(F)F	1.0	261	-	941.4	-	31.0	30.4	-0.6	F
118	FCCCCF	0.1	298	-	976.0	-	34.6	35.7	1.2	F
119	CCC(C)(C)F	0.4	298	-	743.6	-	29.4	27.2	-2.1	F
120	CC(C)(C)C(F)(F)F	1.0	293	990.5	979.6	-10.9	-	28.8	-	F
121	ICI	1.0	298	3307.8	3194.6	-113.3	49.0	45.1	-3.9	I
122	IC(I)I	0.0	396	3685.6	3415.7	-269.9	47.9	54.8	7.0	I
123	IC(I)(I)I	0.0	447	3819.2	3667.0	-152.3	-	65.6	-	I
124	CCI	0.2	298	-	1913.3	-	31.7	30.6	-1.1	I
125	CC(I)I	0.0	336	2682.9	2644.6	-38.3	-	44.8	-	I
126	ICCI	0.0	356	2551.8	2681.3	129.5	48.1	47.3	-0.8	I
127	CCCI	0.1	298	-	1732.4	-	36.0	35.1	-0.9	I
128	CC(C)(I)I	0.0	352	2379.7	2324.5	-55.1	-	44.9	-	I
129	CC(I)CI	0.0	330	2506.9	2445.7	-61.3	-	50.8	-	I
130	CCC(I)I	0.0	357	2370.2	2375.3	5.1	-	47.9	-	I
131	CC(C)CI	1.0	298	-	1598.2	-	38.8	38.4	-0.4	I
132	CC(C)(I)CI	0.0	370	2163.1	2205.7	42.6	-	50.4	-	I
133	CCC(C)(I)I	0.0	370	2163.1	2187.5	24.4	-	48.9	-	I
134	CC(C)C(I)I	0.0	365	2171.2	2188.4	17.2	-	50.3	-	I
135	CC(I)C(C)I	0.0	374	2155.0	2174.1	19.1	-	51.6	-	I
136	CC(CI)CI	0.0	374	2155.0	2200.2	45.3	-	52.7	-	I
137	CCC(I)CI	0.0	371	2160.5	2189.3	28.8	-	52.4	-	I
138	CC(I)CCI	0.0	382	2141.4	2168.2	26.8	-	52.6	-	I
139	CCCC(I)I	0.0	373	2144.3	2160.1	15.8	-	51.2	-	I
140	CCC(C)(C)I	1.0	323	-	1483.5	-	40.4	39.6	-0.8	I
141	CC(I)C(C)(C)C	0.0	320	1392.3	1448.1	55.7	-	44.8	-	I
142	CC(C)C(C)(C)I	1.0	293	1448.0	1476.7	28.7	-	45.2	-	I
143	CCC(C)(I)CC	0.0	319	1393.3	1440.7	47.4	-	44.3	-	I
144	CCCC(C)(C)I	0.0	332	1376.8	1403.8	27.0	-	43.8	-	I
145	ClCBr	1.0	298	1924.9	1946.6	21.8	-	34.5	-	Mix
146	ClCBr	1.0	304	-	1934.0	-	33.5	34.3	0.8	Mix
147	FCCl	1.0	260	1282.1	1302.6	20.4	21.9	26.6	4.7	Mix
148	BrCI	1.0	290	2926.0	2894.1	-31.9	-	42.0	-	Mix
149	ClCI	1.0	293	2422.0	2419.9	-2.1	-	38.3	-	Mix
150	FC(F)Br	1.0	298	1775.5	2051.2	275.7	-	28.8	-	Mix
151	FC(F)Br	1.0	244	-	2287.0	-	24.0	32.4	8.4	Mix
152	FC(F)Cl	1.0	233	1408.0	1732.6	324.6	20.2	28.2	8.0	Mix
153	FC(F)Cl	10.8	298	1193.0	1390.2	197.2	-	22.6	-	Mix
154	FC(Cl)Cl	1.8	298	1367.0	1461.6	94.6	-	28.2	-	Mix
155	FC(Cl)Cl	1.0	267	-	1535.7	-	26.1	29.9	3.8	Mix
156	FC(I)I	1.0	295	3196.9	3258.9	62.0	-	47.3	-	Mix
157	FC(I)I	1.0	314	-	3199.4	-	32.9	46.3	13.4	Mix

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
158	FC(F)I	1.0	272	-	2642.2	-	26.0	34.5	8.5	Mix
159	FC(Br)Br	1.0	293	2421.0	2579.1	158.1	-	39.8	-	Mix
160	ClC(Cl)Br	1.0	298	1983.5	2026.5	43.0	-	39.2	-	Mix
161	ClC(Br)Br	1.0	293	2451.0	2494.7	43.7	-	44.6	-	Mix
162	ClC(Cl)(Cl)Br	1.0	298	2002.1	2063.7	61.6	-	41.1	-	Mix
163	ClC(Cl)(Cl)Br	0.1	298	-	2062.5	-	36.1	41.0	4.9	Mix
164	ClC(Cl)(Br)Br	1.0	298	2420.0	2465.3	45.3	-	47.0	-	Mix
165	ClC(Br)(Br)Br	1.0	288	2710.0	2863.6	153.6	-	53.3	-	Mix
166	FC(F)(F)Br	1.0	215	1989.9	2511.7	521.8	17.5	30.5	13.0	Mix
167	FC(F)(F)Br	16.6	298	1536.1	2503.8	967.7	-	29.2	-	Mix
168	FC(Br)(Br)Br	1.0	330	-	2819.3	-	34.4	46.0	11.6	Mix
169	FC(F)(Br)Br	1.0	298	2251.2	2741.5	490.3	25.0	39.2	14.2	Mix
170	FC(F)(F)Cl	1.0	190	1527.8	1792.4	264.6	15.4	24.3	8.9	Mix
171	FC(F)(Cl)Cl	1.0	243	1488.0	1846.3	358.3	20.1	30.1	10.0	Mix
172	FC(F)(Cl)Cl	6.7	298	1307.0	1547.3	240.3	-	24.7	-	Mix
173	FC(Cl)(Cl)Cl	1.1	298	1477.0	1589.0	112.0	24.9	30.0	5.2	Mix
174	FC(F)(F)I	20.0	298	2046.8	2957.0	910.2	-	34.2	-	Mix
175	FC(F)(F)I	1.0	281	-	2964.9	-	22.5	34.5	12.0	Mix
176	FC(Cl)Br	1.0	273	1977.1	2108.7	131.6	-	35.5	-	Mix
177	FC(F)(Cl)Br	1.0	269	1899.6	2151.9	252.2	23.1	32.1	9.0	Mix
178	FC(F)(Cl)Br	2.6	298	1810.0	2046.8	236.8	-	30.4	-	Mix
179	FC(Cl)(Cl)Br	1.0	295	1950.0	2090.8	140.8	-	36.7	-	Mix
180	FC(Cl)(Cl)Br	0.4	298	-	2084.3	-	29.1	36.6	7.5	Mix
181	FC(Cl)(Br)Br	1.0	295	2317.3	2513.7	196.4	-	42.3	-	Mix
182	CC(Cl)Br	1.0	305	-	1633.1	-	33.1	34.8	1.7	Mix
183	CC(F)Cl	1.4	298	-	1050.5	-	23.7	25.1	1.4	Mix
184	FCCCl	1.0	303	-	1148.8	-	32.1	29.2	-2.9	Mix
185	CC(F)(F)Cl	1.0	263	-	1192.7	-	22.7	22.6	-0.1	Mix
186	FCC(F)Cl	0.8	298	-	1306.5	-	26.6	31.5	4.9	Mix
187	FC(F)CCl	1.0	288	1312.0	1318.4	6.4	-	32.3	-	Mix
188	FC(F)CCl	0.7	298	-	1299.9	-	26.6	31.7	5.2	Mix
189	CC(F)(Cl)Cl	0.8	298	-	1222.8	-	26.0	26.5	0.5	Mix
190	FC(Cl)CCl	0.1	298	-	1376.4	-	32.8	36.8	4.0	Mix
191	ClC(Cl)(Br)CBr	1.0	273	2298.0	2315.8	17.8	-	55.1	-	Mix
192	ClC(Cl)(Br)CBr	1.0	369	-	2143.3	-	45.9	49.4	3.5	Mix
193	ClC(Br)C(Cl)Br	1.0	293	2135.0	2306.7	171.7	-	58.0	-	Mix
194	ClC(Br)C(Cl)Br	1.0	335	-	2230.1	-	45.9	55.2	9.3	Mix
195	FC(F)(Cl)CCl	0.4	298	-	1413.4	-	28.3	32.9	4.6	Mix
196	FC(Cl)C(F)Cl	0.4	298	1405.4	1493.6	88.2	-	36.4	-	Mix
197	FC(F)(F)CBr	1.0	293	1788.1	1770.1	-18.0	-	30.2	-	Mix
198	FC(F)(F)CCl	1.9	298	-	1314.3	-	22.3	27.3	5.0	Mix
199	FC(Cl)(Cl)CCl	0.1	298	-	1488.0	-	34.7	38.3	3.6	Mix
200	FCC(Cl)(Cl)Cl	0.1	298	1575.0	1511.1	-63.9	-	38.4	-	Mix
201	FC(Cl)C(Cl)Cl	0.0	298	-	1527.5	-	36.9	40.9	4.0	Mix
202	ClCCCBr	1.0	341	-	1520.2	-	42.0	41.8	-0.2	Mix
203	CC(C)(F)Cl	0.1	298	-	950.0	-	31.5	24.9	-6.6	Mix
204	CC(F)(F)CCl	0.4	298	1191.6	1135.4	-56.2	-	30.2	-	Mix
205	FC(F)(F)CCCl	0.5	298	1290.1	1244.5	-45.6	-	31.2	-	Mix
206	FC(F)(F)CCCl	1.0	306	-	1230.7	-	29.9	30.8	0.9	Mix
207	FCCCCCl	0.0	298	1062.7	1060.6	-2.1	-	41.3	-	Mix
208	CC(CI)C(F)(F)F	1.0	313	-	1805.9	-	30.4	41.5	11.1	Mix
209	CC(I)CC(F)(F)F	1.0	312	-	1778.6	-	32.4	41.3	8.9	Mix
210	CCC(C)CBr	1.0	321	-	1187.0	-	37.9	38.4	0.5	Br
211	CC(C)CCBr	0.0	298	-	1209.2	-	39.7	39.9	0.2	Br
212	CC(Br)C(C)(C)Br	1.0	298	1663.0	1692.6	29.6	-	51.0	-	Br
213	CC(Br)C(C)(C)Br	0.0	335	-	1643.6	-	-	49.1	-	Br
214	CC(C)C(C)(Br)Br	0.0	337	1622.0	1633.1	11.1	-	47.1	-	Br
215	CC(C)(CBr)CBr	1.0	293	1693.4	1724.5	31.1	-	52.2	-	Br
216	CC(C)(CBr)CBr	0.0	345	-	1656.1	-	-	49.4	-	Br
217	CCC(C)(Br)CBr	1.0	294	1663.8	1705.0	41.2	-	50.4	-	Br
218	CCC(C)(Br)CBr	0.0	337	-	1647.4	-	-	48.1	-	Br
219	CCC(Br)(Br)CC	0.0	332	1610.0	1632.9	22.9	-	47.5	-	Br
220	CC(C)(Br)CCBr	1.0	273	1696.0	1722.5	26.5	-	53.6	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
221	CC(C)(Br)CCBr	0.0	337	-	1637.5	-	-	50.2	-	Br
222	CCCC(C)(Br)Br	1.0	289	1645.2	1675.4	30.2	-	50.2	-	Br
223	CCCC(C)(Br)Br	0.0	335	-	1612.5	-	-	47.8	-	Br
224	CC(Br)C(C)CBr	0.0	337	1751.0	1638.6	-112.5	-	51.0	-	Br
225	CCC(C)C(Br)Br	0.0	337	1602.8	1619.5	16.7	-	49.1	-	Br
226	CC(C)C(Br)CBr	1.0	293	1677.0	1689.7	12.7	-	52.3	-	Br
227	CC(C)C(Br)CBr	0.0	337	-	1630.6	-	-	50.2	-	Br
228	CCC(Br)C(C)Br	1.0	293	1673.0	1679.7	6.7	-	52.9	-	Br
229	CCC(Br)C(C)Br	0.0	341	-	1613.5	-	-	50.1	-	Br
230	CC(C)CC(Br)Br	0.0	337	1602.8	1602.1	-0.6	-	49.5	-	Br
231	CC(Br)CC(C)Br	1.0	293	1665.9	1664.0	-1.9	-	52.0	-	Br
232	CC(Br)CC(C)Br	0.0	344	-	1594.8	-	-	49.3	-	Br
233	CC(CBr)CCBr	1.0	293	1711.5	1701.8	-9.7	-	55.7	-	Br
234	CC(CBr)CCBr	0.0	337	-	1642.0	-	-	53.0	-	Br
235	CCC(Br)CCBr	1.0	293	1665.3	1689.0	23.8	-	54.1	-	Br
236	CCC(Br)CCBr	0.0	351	-	1610.4	-	-	50.9	-	Br
237	CCCC(Br)CBr	1.0	293	1670.8	1681.8	11.0	49.0	53.3	4.3	Br
238	CC(Br)CCCBr	1.0	293	1683.0	1682.5	-0.5	-	55.4	-	Br
239	CC(Br)CCCBr	1.0	392	-	1547.8	-	51.8	49.7	-2.1	Br
240	CCCCC(Br)Br	0.0	343	1588.3	1594.0	5.6	-	50.0	-	Br
241	CCCCC(Br)Br	1.0	375	-	1548.7	-	48.8	48.3	-0.5	Br
242	BrCCCCCBr	1.0	298	1694.0	1690.2	-3.8	-	56.6	-	Br
243	BrCCCCCBr	1.0	411	-	1535.5	-	54.4	50.0	-4.4	Br
244	CC(Br)C(C)(Br)CBr	1.0	293	2082.1	2105.9	23.8	-	65.8	-	Br
245	CC(CBr)(CBr)CBr	1.0	293	2091.7	2129.8	38.1	-	67.4	-	Br
246	CCCCC(Br)(Br)Br	1.0	293	1988.2	2028.4	40.2	-	62.7	-	Br
247	CCCCC(Br)(Br)Br	0.1	427	-	1829.7	-	-	54.8	-	Br
248	BrCCC(Br)CCBr	1.0	292	2065.0	2074.2	9.2	-	69.7	-	Br
249	BrCCCC(Br)CBr	1.0	295	2073.0	2064.0	-9.0	-	69.8	-	Br
250	CCC(C)(C)CBr	0.0	311	1150.8	1186.1	35.3	-	41.9	-	Br
251	CC(C)(C)CCBr	1.0	293	1155.6	1194.0	38.4	-	43.8	-	Br
252	CC(C)(C)CCBr	0.0	308	-	1177.0	-	-	43.1	-	Br
253	CC(C)C(C)CBr	1.0	298	1190.0	1184.1	-5.9	-	43.5	-	Br
254	CC(C)C(C)CBr	0.0	311	-	1170.1	-	-	42.9	-	Br
255	CCC(C)C(C)Br	0.0	303	1163.1	1170.3	7.2	-	42.8	-	Br
256	CCC(Br)C(C)C	0.0	303	1163.1	1165.0	1.9	-	42.4	-	Br
257	CC(C)CC(C)Br	0.0	303	1144.3	1154.5	10.1	40.9	42.8	2.0	Br
258	CCC(CC)CBr	0.0	313	1159.9	1165.1	5.3	42.7	43.1	0.4	Br
259	CCC(C)CCBr	1.0	296	1171.0	1180.5	9.5	-	44.7	-	Br
260	CCC(C)CCBr	0.0	317	-	1156.5	-	-	43.6	-	Br
261	CCCC(C)CBr	1.0	293	1177.9	1179.8	1.9	-	44.4	-	Br
262	CCCC(C)CBr	0.0	314	-	1156.5	-	-	43.3	-	Br
263	CCCC(Br)CC	0.0	312	-	1149.7	-	42.5	42.9	0.5	Br
264	CC(C)CCCBr	1.0	293	1168.3	1174.7	6.4	-	44.8	-	Br
265	CC(C)CCCBr	0.0	316	-	1148.7	-	-	43.6	-	Br
266	CCCCC(C)Br	1.0	298	1159.7	1160.7	1.0	-	43.9	-	Br
267	CCCCC(C)Br	1.0	318	-	1138.6	-	43.8	42.9	-0.9	Br
268	CC(C)(Br)C(C)(C)Br	0.3	435	-	1474.4	-	-	47.1	-	Br
269	CC(C)C(C)(Br)CBr	0.1	400	1450.3	1509.0	58.6	-	49.5	-	Br
270	CC(C)(C)C(Br)CBr	0.1	400	1462.2	1504.4	42.1	-	51.6	-	Br
271	CCCCC(C)(Br)Br	1.0	295	1546.3	1582.4	36.1	-	54.4	-	Br
272	CCCCC(C)(Br)Br	0.1	400	-	1443.8	-	-	48.4	-	Br
273	CC(C)C(CBr)CBr	1.0	293	1605.0	1627.9	22.9	-	58.4	-	Br
274	CC(CBr)C(C)CBr	0.1	400	1465.9	1493.4	27.5	-	52.6	-	Br
275	CCC(Br)C(Br)CC	1.0	293	1602.7	1595.4	-7.3	-	55.5	-	Br
276	CCC(Br)C(Br)CC	0.1	400	-	1459.1	-	-	49.7	-	Br
277	CCCC(Br)C(C)Br	1.0	293	1581.2	1591.6	10.4	-	56.4	-	Br
278	CCCC(Br)C(C)Br	0.1	400	-	1453.8	-	-	49.8	-	Br
279	CC(Br)CCC(C)Br	1.0	293	1578.8	1581.2	2.4	-	58.1	-	Br
280	CC(Br)CCC(C)Br	0.0	365	-	1489.1	-	49.5	53.7	4.1	Br
281	CCCC(CBr)CBr	1.0	293	1577.1	1615.2	38.1	-	59.0	-	Br
282	CC(CCBr)CCBr	0.1	426	1395.4	1444.3	48.9	50.8	52.2	1.4	Br
283	CCC(Br)CCCBr	0.1	400	1443.8	1462.5	18.7	-	52.8	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
284	CCCCC(Br)CBr	1.0	293	1560.4	1593.3	32.9	56.5	57.9	1.4	Br
285	CC(Br)CCCCBr	0.1	400	1415.4	1455.8	40.5	-	53.1	-	Br
286	CCCCCC(Br)Br	0.1	400	1416.2	1437.3	21.1	-	50.9	-	Br
287	CCCCCC(Br)Br	1.0	393	-	1446.9	-	51.6	51.3	-0.3	Br
288	BrCCCCCCBr	1.0	298	1602.5	1599.0	-3.5	-	61.1	-	Br
289	BrCCCCCCBr	0.0	364	-	1516.2	-	57.1	56.8	-0.2	Br
290	CCC(CBr)(CBr)CBr	1.0	293	1912.2	2027.1	114.9	-	71.6	-	Br
291	CCCC(Br)CCC	1.0	296	1133.0	1136.8	3.8	-	48.4	-	Br
292	CCCC(Br)CCC	0.0	327	-	1103.4	-	-	46.6	-	Br
293	CCCCC(Br)CC	1.0	295	1134.1	1137.2	3.1	-	48.5	-	Br
294	CCCCCC(C)Br	0.0	320	1095.5	1106.4	10.8	46.2	47.3	1.1	Br
295	CCC(Br)(CBr)C(C)C	1.0	293	1526.1	1583.2	57.1	-	59.5	-	Br
296	CC(C)(C)CC(Br)CBr	1.0	293	1502.0	1544.2	42.2	-	59.4	-	Br
297	CCCC(Br)(CC)CBr	1.0	293	1492.9	1560.3	67.4	-	60.6	-	Br
298	CC(C)(CCBr)CCBr	1.0	293	1532.0	1572.6	40.6	-	64.6	-	Br
299	CCCC(Br)C(Br)CC	1.0	293	1516.2	1525.2	9.0	-	60.5	-	Br
300	CCCC(Br)C(Br)CC	0.1	418	-	1374.8	-	-	52.3	-	Br
301	CCCCC(Br)C(C)Br	1.0	293	1513.2	1519.9	6.7	-	60.4	-	Br
302	CCCCC(Br)C(C)Br	0.1	418	-	1367.1	-	-	52.6	-	Br
303	CCC(Br)CCCCBr	0.1	418	-	1376.2	-	-	55.6	-	Br
304	CCCCCC(Br)CBr	1.0	293	1518.0	1521.2	3.2	-	62.3	-	Br
305	CCCCCC(Br)CBr	1.0	300	-	1512.9	-	54.4	61.8	7.4	Br
306	CCCCCCC(Br)Br	1.0	294	1500.0	1507.0	7.0	-	61.9	-	Br
307	CCCCCCC(Br)Br	1.0	410	-	1365.6	-	54.4	54.4	0.0	Br
308	BrCCCCCCCBr	0.0	385	1469.2	1424.4	-44.8	57.8	59.7	1.9	Br
309	CC(C)CCCC(C)Br	1.0	293	1091.0	1106.0	15.0	-	52.4	-	Br
310	CCCCCCC(C)Br	1.0	298	1096.8	1104.5	7.7	-	53.3	-	Br
311	CCCCCCC(C)Br	1.0	358	-	1044.2	-	48.4	49.5	1.1	Br
312	CCC(C)(C)CC(Br)CBr	1.0	293	1468.9	1499.7	30.8	-	63.9	-	Br
313	CCCC(Br)C(Br)CCC	0.1	435	-	1303.1	-	-	55.0	-	Br
314	CCCCC(Br)CCCBr	0.1	435	-	1305.2	-	-	58.2	-	Br
315	CCCC(Br)CCCCBr	0.1	435	-	1305.4	-	-	58.2	-	Br
316	CCCCCCC(Br)CBr	1.0	293	1458.0	1461.9	3.9	-	66.8	-	Br
317	CCCCCCC(Br)CBr	0.1	435	-	1297.9	-	-	57.1	-	Br
318	CCCCCCCC(Br)Br	0.1	435	-	1286.6	-	-	56.8	-	Br
319	CCCCCCCC(Br)Br	1.0	427	-	1296.4	-	57.1	57.3	0.2	Br
320	BrCCCCCCCCBr	0.0	399	1413.1	1353.9	-59.1	59.6	62.7	3.1	Br
321	CCCCCCCC(C)Br	1.0	298	1076.0	1084.0	8.0	-	57.9	-	Br
322	CCCCCCCCCBr	1.0	298	1084.9	1091.9	7.1	-	59.6	-	Br
323	CCCCCCCCCBr	1.0	391	-	1002.7	-	53.1	53.2	0.1	Br
324	CCCCCCCC(Br)CBr	1.0	293	1398.0	1413.6	15.6	-	71.4	-	Br
325	CCCCCCCC(Br)CBr	0.1	451	-	1238.6	-	-	59.8	-	Br
326	CCCCCCCCC(Br)Br	0.1	451	-	1229.0	-	-	59.5	-	Br
327	CCCCCCCCC(Br)Br	1.0	442	-	1239.3	-	59.5	60.1	0.6	Br
328	BrCCCCCCCCCBr	1.0	298	1428.0	1417.5	-10.5	-	74.6	-	Br
329	BrCCCCCCCCCBr	0.0	415	-	1292.6	-	61.8	65.6	3.8	Br
330	CCCCCCCCC(C)Br	1.0	298	1047.0	1066.0	19.0	-	62.6	-	Br
331	CCCCCCCCC(C)Br	0.0	383	-	987.6	-	-	56.4	-	Br
332	CCCCCCCCCCBr	1.0	298	1062.5	1073.5	11.0	-	64.3	-	Br
333	CCCCCCCCCCBr	1.0	398	-	982.0	-	56.6	57.0	0.4	Br
334	CCCCCCCCC(Br)CBr	1.0	383	-	1278.5	-	67.0	68.9	1.9	Br
335	CCCCCCCCCC(Br)Br	1.0	457	-	1189.7	-	62.2	63.0	0.8	Br
336	CCC(C)CCl	0.0	298	-	874.6	-	36.3	36.3	-0.1	Cl
337	CC(Cl)C(C)(C)Cl	0.0	307	1080.9	1055.5	-25.4	-	40.2	-	Cl
338	CC(C)C(C)(Cl)Cl	0.0	333	1051.1	1018.2	-32.9	-	37.8	-	Cl
339	CC(C)(CCl)CCl	0.0	314	1066.8	1088.0	21.2	-	44.2	-	Cl
340	CCC(C)(Cl)CCl	0.0	306	1061.9	1070.2	8.3	35.9	41.3	5.4	Cl
341	CCC(Cl)(Cl)CC	0.0	303	1043.7	1046.9	3.2	40.3	39.5	-0.7	Cl
342	CC(C)(Cl)CCCl	1.0	293	1075.8	1083.6	7.8	-	44.8	-	Cl
343	CC(C)(Cl)CCCl	0.0	314	-	1062.8	-	-	43.7	-	Cl
344	CCCC(C)(Cl)Cl	0.0	299	1034.6	1040.6	6.0	40.0	40.0	0.0	Cl
345	CC(Cl)C(C)CCl	1.0	293	1093.8	1088.0	-5.8	-	46.5	-	Cl
346	CC(Cl)C(C)CCl	0.0	313	-	1069.2	-	-	45.3	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
347	CCC(C)C(Cl)Cl	0.0	302	1045.7	1054.5	8.8	-	42.1	-	Cl
348	CC(C)C(Cl)CCl	1.0	293	1080.5	1081.0	0.5	-	43.9	-	Cl
349	CC(C)C(Cl)CCl	0.0	312	-	1061.8	-	42.1	42.9	0.8	Cl
350	CCC(Cl)C(C)Cl	1.0	298	1075.0	1070.4	-4.6	-	46.8	-	Cl
351	CCC(Cl)C(C)Cl	0.0	309	-	1058.1	-	41.6	46.1	4.4	Cl
352	CC(C)CC(Cl)Cl	1.0	293	1047.3	1055.1	7.8	-	42.9	-	Cl
353	CC(C)CC(Cl)Cl	0.0	302	-	1045.6	-	40.1	42.4	2.3	Cl
354	CC(Cl)CC(C)Cl	1.0	291	1063.0	1063.0	0.0	-	44.8	-	Cl
355	CC(Cl)CC(C)Cl	0.0	317	-	1036.7	-	41.5	43.3	1.8	Cl
356	CC(CCl)CCCl	1.0	294	1103.0	1100.9	-2.1	-	50.4	-	Cl
357	CC(CCl)CCCl	0.0	324	-	1070.5	-	-	48.4	-	Cl
358	CCC(Cl)CCCl	1.0	293	1083.4	1084.5	1.1	-	46.6	-	Cl
359	CCC(Cl)CCCl	0.0	322	-	1055.5	-	-	45.0	-	Cl
360	CCCC(Cl)CCl	1.0	298	1074.1	1073.3	-0.8	43.9	44.7	0.8	Cl
361	CC(Cl)CCCCl	1.0	293	1073.4	1085.2	11.8	48.1	49.6	1.5	Cl
362	CCCCC(Cl)Cl	0.0	304	1041.7	1044.5	2.8	-	43.3	-	Cl
363	CCCCC(Cl)Cl	1.0	298	-	1051.0	-	44.3	43.7	-0.6	Cl
364	CC(C)(Cl)C(C)(Cl)Cl	0.0	342	1144.6	1205.2	60.6	-	48.0	-	Cl
365	CC(Cl)C(C)(Cl)CCl	0.0	343	1184.5	1214.9	30.3	-	50.4	-	Cl
366	CC(C)(Cl)C(Cl)CCl	1.0	293	1264.1	1257.8	-6.3	-	53.7	-	Cl
367	CC(CCl)(CCl)CCl	0.0	338	1215.5	1257.4	41.9	-	54.1	-	Cl
368	CCCCC(Cl)(Cl)Cl	0.0	298	1183.9	1189.9	6.0	-	46.4	-	Cl
369	CCC(C)(C)CCl	0.0	298	874.6	892.5	17.9	-	39.3	-	Cl
370	CC(C)(C)CCCl	0.0	298	863.1	884.8	21.7	38.5	40.0	1.5	Cl
371	CC(C)C(C)CCl	1.0	298	881.6	881.2	-0.4	-	40.1	-	Cl
372	CC(C)C(C)CCl	0.0	298	-	881.8	-	-	40.2	-	Cl
373	CCC(C)C(C)Cl	0.0	298	869.9	872.4	2.5	-	39.7	-	Cl
374	CCC(Cl)C(C)C	0.0	298	869.9	867.8	-2.0	-	39.4	-	Cl
375	CC(C)CC(C)Cl	0.0	298	855.9	860.6	4.7	-	39.6	-	Cl
376	CCC(CC)CCl	0.0	300	884.2	877.7	-6.4	-	40.5	-	Cl
377	CCC(C)CCCl	1.0	300	892.0	875.6	-16.4	-	41.0	-	Cl
378	CCC(C)CCCl	0.0	303	-	873.4	-	-	40.9	-	Cl
379	CCCC(C)CCl	0.0	298	869.9	874.4	4.5	-	40.8	-	Cl
380	CCCC(Cl)CC	1.0	297	871.0	865.5	-5.5	-	40.4	-	Cl
381	CCCC(Cl)CC	0.0	298	-	864.5	-	39.9	40.4	0.5	Cl
382	CC(C)CCCCl	0.0	300	868.5	870.2	1.7	-	41.1	-	Cl
383	CCCCC(C)Cl	0.0	299	864.8	861.2	-3.6	41.2	40.6	-0.6	Cl
384	CC(C)(C)C(C)(Cl)Cl	0.0	317	-	1053.5	-	-	43.0	-	Cl
385	CC(C)(C)CC(Cl)Cl	1.0	293	1027.1	1052.7	25.6	-	46.0	-	Cl
386	CC(C)(C)CC(Cl)Cl	0.0	322	-	1024.6	-	41.8	44.4	2.7	Cl
387	CC(Cl)CC(C)(C)Cl	1.0	293	1036.0	1050.4	14.4	-	46.7	-	Cl
388	CCCCC(C)(Cl)Cl	1.0	298	1015.0	1024.6	9.6	-	44.8	-	Cl
389	CCCCC(C)(Cl)Cl	0.0	338	-	984.0	-	-	42.5	-	Cl
390	CCC(Cl)C(Cl)CC	1.0	293	1061.7	1057.8	-3.9	-	52.4	-	Cl
391	CCCC(Cl)C(C)Cl	0.0	334	1015.7	1009.9	-5.8	-	46.9	-	Cl
392	CCCC(Cl)CCCl	0.0	343	-	1010.9	-	-	48.0	-	Cl
393	CCC(Cl)CCCCl	0.0	350	-	1008.3	-	-	49.9	-	Cl
394	CCCCC(Cl)CCl	1.0	293	1080.0	1053.5	-26.5	48.2	49.5	1.3	Cl
395	CC(Cl)CCCCCl	1.0	293	1108.6	1060.0	-48.6	-	54.2	-	Cl
396	CCCCCC(Cl)Cl	0.0	335	987.4	992.6	5.3	-	45.9	-	Cl
397	CCCCCC(Cl)Cl	1.0	298	-	1029.6	-	48.7	48.1	-0.6	Cl
398	CCCCCC(Cl)(Cl)Cl	0.1	390	1033.3	1056.4	23.1	-	45.5	-	Cl
399	CC(C)(C)C(C)(C)Cl	0.0	298	864.3	908.8	44.6	-	41.9	-	Cl
400	CCC(C)(Cl)C(C)C	0.0	301	861.7	887.8	26.1	-	42.1	-	Cl
401	CCC(C)C(C)(C)Cl	0.0	301	-	883.4	-	-	42.2	-	Cl
402	CC(Cl)CC(C)(C)C	0.0	302	852.3	872.5	20.2	-	42.6	-	Cl
403	CC(C)CC(C)(C)Cl	1.0	293	862.8	869.6	6.8	-	41.5	-	Cl
404	CC(C)CC(C)(C)Cl	0.0	302	-	861.6	-	-	41.0	-	Cl
405	CCC(Cl)(CC)CC	0.0	314	865.9	871.5	5.6	-	41.4	-	Cl
406	CCCC(C)(Cl)CC	0.0	308	865.5	867.5	2.1	-	42.0	-	Cl
407	CCCCC(C)(C)Cl	1.0	293	863.5	869.3	5.8	-	42.7	-	Cl
408	CCCCC(C)(C)Cl	0.0	309	-	855.2	-	-	41.9	-	Cl
409	CC(C)CCC(C)Cl	0.0	309	848.9	850.3	1.5	-	43.5	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
410	CCCC(C)CCCl	0.0	320	851.3	856.9	5.5	-	44.4	-	Cl
411	CCCC(Cl)CCC	1.0	295	869.4	867.9	-1.5	-	45.1	-	Cl
412	CCCC(Cl)CCC	0.0	315	-	850.4	-	-	44.0	-	Cl
413	CCCCC(Cl)CC	1.0	298	857.9	864.8	6.9	-	44.9	-	Cl
414	CCCCC(Cl)CC	0.0	315	-	850.0	-	-	43.9	-	Cl
415	CCCCCC(C)Cl	1.0	295	865.1	864.4	-0.7	-	45.3	-	Cl
416	CCCCCC(C)Cl	1.0	328	-	835.3	-	44.8	43.4	-1.4	Cl
417	CC(C)(Cl)CC(C)(C)Cl	0.0	339	986.3	1000.9	14.6	-	47.3	-	Cl
418	CCC(C)(C)CC(Cl)Cl	1.0	293	1032.1	1047.8	15.7	-	50.7	-	Cl
419	CC(C)(C)CC(Cl)CCl	1.0	293	1025.9	1049.4	23.5	-	51.1	-	Cl
420	CC(C)(C)CC(Cl)CCl	0.0	344	-	1002.4	-	45.1	48.2	3.1	Cl
421	CC(C)(CCCl)CCCl	1.0	293	1056.3	1079.4	23.1	-	58.9	-	Cl
422	CC(C)(CCCl)CCCl	0.0	339	-	1039.5	-	-	55.9	-	Cl
423	CCCC(Cl)(Cl)CCC	0.0	349	1021.9	969.6	-52.3	-	46.4	-	Cl
424	CCCCCC(C)(Cl)Cl	0.0	340	968.2	967.4	-0.8	-	46.7	-	Cl
425	CCCCCC(Cl)CCl	1.0	293	1062.5	1032.9	-29.6	53.2	53.8	0.6	Cl
426	CCCCCCC(Cl)Cl	0.0	353	995.8	959.6	-36.3	-	49.1	-	Cl
427	CCCCCCC(Cl)Cl	1.0	298	-	1013.0	-	53.5	52.7	-0.8	Cl
428	ClCCCCCCCCl	1.0	298	1040.8	1044.7	3.9	61.2	59.9	-1.3	Cl
429	CCCCCCC(Cl)(Cl)Cl	1.0	298	1121.2	1129.5	8.3	-	55.7	-	Cl
430	CCCCCCC(Cl)(Cl)Cl	0.1	410	-	1012.9	-	-	48.4	-	Cl
431	ClCCCCCCC(Cl)Cl	1.0	293	1174.4	1168.6	-5.8	-	66.5	-	Cl
432	CCC(C)(C)C(C)(C)Cl	1.0	298	906.5	921.0	14.5	-	47.0	-	Cl
433	CCC(C)(Cl)C(C)(C)C	1.0	293	906.6	923.0	16.4	-	47.0	-	Cl
434	CC(C)(C)CC(C)(C)Cl	1.0	293	874.1	885.1	11.0	-	44.8	-	Cl
435	CC(C)(C)CC(C)(C)Cl	0.0	332	-	852.1	-	-	42.7	-	Cl
436	CC(C)C(C)C(C)(C)Cl	1.0	293	888.0	896.9	8.9	-	46.2	-	Cl
437	CCCC(C)(Cl)C(C)C	0.0	332	834.5	859.9	25.4	-	44.9	-	Cl
438	CC(C)CCC(C)(C)Cl	0.0	332	-	832.7	-	-	43.7	-	Cl
439	CCCC(C)(Cl)CCC	0.0	332	834.8	846.2	11.3	-	45.2	-	Cl
440	CCCCC(C)(Cl)CC	0.0	328	845.6	848.8	3.2	-	45.2	-	Cl
441	CCCCCC(C)(C)Cl	1.0	298	856.8	864.8	8.0	-	47.0	-	Cl
442	CCCCCC(C)(C)Cl	0.0	328	-	838.3	-	-	45.2	-	Cl
443	CC(C)CCCC(C)Cl	0.0	328	-	833.6	-	-	46.7	-	Cl
444	CCCCC(CC)CCl	1.0	293	876.9	880.6	3.7	-	49.9	-	Cl
445	CCCCC(CC)CCl	0.0	337	-	843.1	-	47.4	47.1	-0.3	Cl
446	CCC(C)CCCCCl	0.0	336	-	842.2	-	-	47.8	-	Cl
447	CCCCCCC(C)Cl	1.0	298	861.5	862.1	0.6	-	49.8	-	Cl
448	CCCCCCC(C)Cl	1.0	345	-	822.1	-	47.8	46.8	-1.0	Cl
449	CC(C)(Cl)CCC(C)(C)Cl	0.0	363	-	954.4	-	-	49.4	-	Cl
450	CCC(C)(C)CC(Cl)CCl	1.0	293	1029.0	1044.3	15.3	-	55.4	-	Cl
451	CCCCCC(Cl)C(C)Cl	0.0	368	-	943.5	-	-	51.7	-	Cl
452	CCCCCCC(Cl)CCl	1.0	298	-	1011.8	-	57.6	58.0	0.4	Cl
453	CCCCCCCC(Cl)Cl	0.0	370	-	932.9	-	-	52.2	-	Cl
454	CCCCCCCC(Cl)Cl	1.0	298	-	999.1	-	57.7	57.3	-0.4	Cl
455	ClCCCCCCCCCl	1.0	298	1024.8	1026.3	1.5	65.6	64.1	-1.5	Cl
456	CCCCCCCC(Cl)(Cl)Cl	0.1	430	948.0	975.6	27.7	-	51.1	-	Cl
457	CCC(Cl)(CC)C(C)(C)C	0.0	344	-	886.5	-	-	48.2	-	Cl
458	CCCC(C)(Cl)C(C)(C)C	0.0	340	858.2	880.8	22.6	-	48.8	-	Cl
459	CCCCC(Cl)(CC)CC	0.0	351	836.3	838.9	2.7	-	47.9	-	Cl
460	CCCCC(C)(Cl)CCC	0.0	347	827.0	835.1	8.0	-	48.6	-	Cl
461	CCCCCC(C)(Cl)CC	0.0	347	826.8	833.0	6.1	-	48.4	-	Cl
462	CCCCCC(Cl)C(C)C	1.0	293	856.6	871.0	14.4	-	53.3	-	Cl
463	CCCCC(Cl)CCCC	0.0	351	815.6	821.5	5.9	-	50.5	-	Cl
464	CCCCCCC(Cl)CC	0.0	352	807.5	820.1	12.6	-	50.4	-	Cl
465	CCCCCCCC(C)Cl	1.0	293	879.0	866.4	-12.6	-	54.8	-	Cl
466	CCCCCCCCCCl	1.0	298	867.4	870.7	3.3	55.9	55.9	0.0	Cl
467	CC(C)(Cl)CCCC(C)(C)Cl	0.0	374	-	929.7	-	-	53.0	-	Cl
468	CCCCCCCC(Cl)CCl	1.0	298	-	999.1	-	62.1	62.5	0.4	Cl
469	CCCCCCCCC(Cl)Cl	0.1	436	-	862.8	-	-	51.7	-	Cl
470	CCCCCCCCC(Cl)Cl	1.0	298	-	987.7	-	62.3	61.9	-0.4	Cl
471	ClCCCCCCCCCCl	1.0	298	1017.3	1012.0	-5.3	-	68.6	-	Cl
472	ClCCCCCCCCCCl	0.1	453	-	876.6	-	54.6	56.2	1.6	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
473	CCCCCCCCC(Cl)(Cl)Cl	0.1	449	914.4	943.1	28.7	-	53.8	-	Cl
474	CCCCCCCCC(C)Cl	1.0	293	870.6	866.2	-4.4	-	59.4	-	Cl
475	CCCCCCCCCCCl	1.0	298	865.8	870.0	4.2	64.0	60.6	-3.4	Cl
476	CCCCCCCCCC(Cl)Cl	0.1	456	-	839.3	-	-	54.2	-	Cl
477	CCCCCCCCCC(Cl)Cl	1.0	430	-	864.1	-	56.9	56.2	-0.7	Cl
478	ClCCCCCCCCCCCl	1.0	298	992.9	999.6	6.7	73.1	73.0	-0.1	Cl
479	CCCCCCCCCC(Cl)(Cl)Cl	0.1	439	917.0	943.4	26.4	52.5	58.5	5.9	Cl
480	CCC(C)CF	1.0	302	-	778.2	-	30.7	30.8	0.1	F
481	CC(C)CCF	1.0	293	694.1	787.3	93.2	-	31.5	-	F
482	CC(C)CCF	0.4	298	-	781.8	-	-	31.2	-	F
483	CCCCCF	0.2	298	-	785.2	-	30.9	32.1	1.2	F
484	CC(F)C(C)(C)F	0.1	298	-	872.9	-	-	29.1	-	F
485	CC(C)C(C)(F)F	0.1	298	-	856.8	-	-	28.5	-	F
486	CC(C)(CF)CF	0.1	298	-	952.8	-	-	35.3	-	F
487	CCC(C)(F)CF	0.1	298	-	900.5	-	-	30.5	-	F
488	CCC(F)(F)CC	1.0	293	910.6	864.8	-45.8	-	29.4	-	F
489	CCC(F)(F)CC	1.0	277	-	884.3	-	33.8	30.2	-3.6	F
490	CC(C)(F)CCF	0.1	298	-	907.9	-	-	33.0	-	F
491	CCCC(C)(F)F	1.0	293	898.7	855.5	-43.2	-	29.3	-	F
492	CCCC(C)(F)F	1.0	277	-	875.1	-	33.7	30.1	-3.7	F
493	CC(F)C(C)CF	0.1	298	-	924.1	-	-	34.9	-	F
494	CCC(C)C(F)F	0.1	298	-	894.3	-	-	32.1	-	F
495	CC(C)C(F)CF	0.1	298	-	913.8	-	-	32.8	-	F
496	CCC(F)C(C)F	0.1	298	-	893.7	-	-	31.6	-	F
497	CC(C)CC(F)F	0.1	298	-	888.7	-	-	32.2	-	F
498	CC(F)CC(C)F	0.1	298	-	891.8	-	-	33.6	-	F
499	CC(CF)CCF	0.1	298	-	953.7	-	-	38.5	-	F
500	CCC(F)CCF	0.1	298	-	927.1	-	-	35.8	-	F
501	CCCC(F)CF	0.1	298	-	914.8	-	-	33.9	-	F
502	CC(F)CCCF	0.1	298	-	928.1	-	-	37.7	-	F
503	CCCCC(F)F	0.1	298	-	891.2	-	-	33.1	-	F
504	CCCCC(F)F	1.0	283	-	908.7	-	34.4	33.9	-0.5	F
505	FCCCCCF	1.0	298	957.2	958.5	1.3	-	40.3	-	F
506	FCCCCCF	0.0	298	-	958.1	-	-	40.3	-	F
507	CC(C)CC(F)(F)F	1.0	298	978.8	940.6	-38.2	-	28.6	-	F
508	CCCCC(F)(F)F	1.0	293	970.1	950.1	-20.0	-	29.9	-	F
509	CCCCC(F)(F)F	0.3	298	-	943.2	-	-	29.6	-	F
510	CCC(C)(C)CF	0.1	298	-	809.9	-	-	34.3	-	F
511	CC(C)(C)CCF	1.0	293	780.9	811.7	30.8	-	34.9	-	F
512	CC(C)(C)CCF	0.1	298	-	807.2	-	-	34.7	-	F
513	CC(C)C(C)CF	0.1	298	-	801.4	-	-	34.9	-	F
514	CCC(C)C(C)F	0.1	298	-	782.7	-	-	34.0	-	F
515	CCC(F)C(C)C	0.1	298	-	777.4	-	-	34.0	-	F
516	CC(C)CC(C)F	0.1	298	-	772.8	-	-	34.1	-	F
517	CCC(C)CCF	0.1	298	-	800.7	-	-	35.8	-	F
518	CCCC(C)CF	0.1	298	-	794.6	-	-	35.6	-	F
519	CCCC(F)CC	0.1	298	-	776.4	-	-	34.8	-	F
520	CCCC(F)CC	1.0	296	-	778.5	-	36.8	34.9	-1.9	F
521	CC(C)CCCF	0.1	298	-	793.6	-	-	35.9	-	F
522	CCCCC(C)F	0.1	298	-	773.7	-	-	34.8	-	F
523	CCCCCCF	0.1	298	-	796.2	-	35.6	36.7	1.2	F
524	CCCCCC(F)F	0.1	310	-	876.5	-	-	37.1	-	F
525	CCCCCC(F)F	1.0	305	-	882.1	-	37.7	37.4	-0.3	F
526	CCCCCC(F)(F)F	1.0	293	960.8	946.6	-14.2	-	34.6	-	F
527	CCCCCC(F)(F)F	0.1	298	-	939.9	-	-	34.3	-	F
528	CCCCCCC(F)F	1.0	293	-	892.7	-	-	42.7	-	F
529	CCCCCCC(F)F	1.0	326	-	860.3	-	41.1	40.8	-0.4	F
530	CCCCCCC(F)(F)F	0.1	317	-	913.9	-	-	37.9	-	F
531	CCCCCCCCF	1.0	322	-	791.0	-	44.1	44.5	0.4	F
532	CCCCCCCC(F)F	0.1	365	-	822.4	-	-	42.8	-	F
533	CCCCCCCC(F)F	1.0	344	-	842.8	-	44.2	44.1	-0.1	F
534	CCCCCCCC(F)(F)F	0.1	341	-	884.8	-	-	41.0	-	F
535	CCCCCCCCCF	1.0	293	-	820.1	-	-	51.0	-	F

Continued on next page (AT/EEM-G)

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
536	CCCCCCCCCF	1.0	348	-	776.0	-	46.8	47.4	0.6	F
537	CCCCCCCCC(F)F	0.1	389	-	801.1	-	-	45.4	-	F
538	CCCCCCCCC(F)F	1.0	362	-	826.8	-	47.2	47.2	0.0	F
539	CCCCCCCCC(F)(F)F	1.0	293	935.7	931.7	-4.0	-	48.8	-	F
540	CCCCCCCCC(F)(F)F	0.1	363	-	860.3	-	-	44.1	-	F
541	CCCCCCCCCCF	1.0	293	819.4	824.4	5.0	-	55.8	-	F
542	CCCCCCCCCCF	1.0	357	-	774.1	-	50.4	51.2	0.8	F
543	CCCCCCCCCC(F)F	0.1	412	-	782.1	-	-	48.0	-	F
544	CCCCCCCCCC(F)F	1.0	379	-	812.3	-	50.2	50.4	0.2	F
545	CCCCCCCCCC(F)(F)F	0.1	385	-	838.7	-	-	46.9	-	F
546	CCC(C)CI	0.0	310	1496.8	1500.0	3.2	43.1	42.3	-0.8	I
547	CC(I)C(C)(C)I	0.0	378	-	2070.4	-	-	54.0	-	I
548	CC(C)(CI)CI	0.0	385	-	2075.3	-	-	54.0	-	I
549	CCC(C)(I)CI	0.0	392	-	2048.1	-	-	53.0	-	I
550	CCC(I)(I)CC	0.0	386	-	2044.1	-	-	52.0	-	I
551	CC(C)(I)CCI	0.0	381	-	2046.7	-	-	55.1	-	I
552	CCCC(C)(I)I	0.0	386	-	2018.1	-	-	52.3	-	I
553	CCC(C)C(I)I	0.0	386	-	2021.5	-	-	53.3	-	I
554	CC(C)C(I)CI	0.0	378	-	2042.5	-	-	55.1	-	I
555	CCC(I)C(C)I	0.0	389	-	2017.7	-	-	53.8	-	I
556	CC(C)CC(I)I	0.0	389	-	1990.0	-	-	53.5	-	I
557	CC(I)CC(C)I	0.0	392	-	1989.6	-	-	53.6	-	I
558	CC(CI)CCI	0.0	398	-	2012.4	-	-	56.1	-	I
559	CCC(I)CCI	0.0	400	1966.0	2000.0	34.0	-	55.0	-	I
560	CCCC(I)CI	0.0	397	1961.6	1997.7	36.1	-	54.6	-	I
561	CC(I)CCCI	0.0	403	1970.4	1985.2	14.8	-	55.7	-	I
562	CCCCC(I)I	0.0	394	1962.8	1979.6	16.8	-	53.9	-	I
563	ICCCCCI	0.0	406	-	1991.0	-	59.7	56.8	-2.9	I
564	CCCCC(I)(I)I	0.0	469	-	2333.1	-	-	62.4	-	I
565	CCC(C)(C)CI	0.0	319	1393.3	1450.1	56.7	-	45.0	-	I
566	CC(C)(C)CCI	0.0	324	1387.2	1425.7	38.5	-	45.8	-	I
567	CC(C)C(C)CI	0.0	326	1385.2	1422.5	37.3	-	45.7	-	I
568	CCC(C)C(C)I	0.0	332	1376.8	1406.8	30.0	-	45.0	-	I
569	CCC(I)C(C)C	0.0	319	1393.3	1418.6	25.3	-	45.2	-	I
570	CC(C)CC(C)I	0.0	319	1393.3	1402.7	9.3	-	45.4	-	I
571	CCC(CC)CI	1.0	296	1440.0	1456.0	16.0	-	47.5	-	I
572	CCC(C)CCI	0.0	333	1349.7	1401.5	51.8	-	46.1	-	I
573	CCCC(C)CI	0.0	328	-	1404.8	-	-	45.8	-	I
574	CCCC(I)CC	0.0	328	1382.1	1398.8	16.8	-	45.6	-	I
575	CC(C)CCCI	1.0	293	1428.3	1442.9	14.6	-	48.2	-	I
576	CC(C)CCCI	0.0	332	-	1391.9	-	-	46.1	-	I
577	CCCCC(C)I	0.0	329	-	1390.5	-	-	45.8	-	I
578	CCCCCC(I)I	0.0	410	-	1838.9	-	-	56.9	-	I
579	ICCCCCCI	0.0	402	-	1880.6	-	-	61.1	-	I
580	CCCC(I)CCC	0.1	387	-	1270.3	-	-	46.6	-	I
581	CCCCC(I)CC	1.0	295	1365.6	1383.3	17.7	-	51.9	-	I
582	CCCCC(I)CC	0.0	349	-	1317.8	-	-	48.7	-	I
583	CCCCCC(C)I	0.0	349	1285.9	1311.0	25.1	-	49.0	-	I
584	CCCCCCC(I)I	0.1	491	-	1623.8	-	-	55.7	-	I
585	CCCCCCC(C)I	1.0	299	1316.4	1325.0	8.6	-	56.6	-	I
586	CCCCCCC(C)I	0.1	406	-	1201.0	-	-	49.9	-	I
587	CCCCCCCC(I)I	0.0	442	-	1627.2	-	-	62.8	-	I
588	ICCCCCCCCI	0.0	453	-	1634.9	-	-	65.4	-	I
589	CCCCCCCCCI	1.0	298	1283.6	1294.9	11.3	64.5	63.0	-1.5	I
590	CCCCCCCCC(C)I	1.0	298	1241.2	1255.5	14.3	-	66.0	-	I
591	CCCCCCCCCCI	1.0	293	1256.7	1266.6	9.9	69.8	68.1	-1.7	I
592	FCCCCCCl	0.0	325	1006.0	1003.3	-2.6	-	44.1	-	Mix
593	FCCCCCCCl	0.0	353	962.2	956.2	-6.1	-	46.7	-	Mix
594	FCCCCCCCCl	0.1	379	923.4	917.4	-6.0	-	49.0	-	Mix
595	FCCCCCCCCCCl	0.1	426	870.8	855.8	-15.0	-	53.3	-	Mix
596	FCCCCCCCCCCCl	0.1	447	851.5	831.6	-19.9	-	55.6	-	Mix

Table S17: Comparison of experimental and simulated properties validation using the SH/EEM-G scheme.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	BrCBr	0.1	298	2482.0	2464.3	-17.7	-	37.6	-	Br
2	BrCBr	1.0	298	-	2464.1	-	37.0	37.6	0.6	Br
3	BrC(Br)Br	1.0	298	2877.2	2874.8	-2.4	46.1	46.8	0.7	Br
4	BrC(Br)(Br)Br	1.0	374	2953.3	3001.5	48.2	-	51.5	-	Br
5	BrC(Br)(Br)Br	1.0	384	-	2979.2	-	48.2	51.0	2.8	Br
6	CC(Br)Br	1.0	316	-	2045.1	-	39.6	37.9	-1.7	Br
7	BrCC(Br)Br	1.0	321	-	2553.9	-	52.9	52.7	-0.2	Br
8	CC(C)(Br)Br	0.0	298	1820.0	1860.3	40.2	37.3	39.0	1.6	Br
9	CCC(Br)Br	0.0	302	1968.8	1891.1	-77.7	43.1	42.4	-0.6	Br
10	CC(Br)(Br)CBr	0.0	349	-	2259.3	-	47.5	51.4	3.9	Br
11	BrCC(Br)CBr	0.0	374	-	2273.3	-	52.1	56.4	4.3	Br
12	BrCCC(Br)Br	1.0	290	2350.0	2387.0	37.0	-	58.5	-	Br
13	CC(C)(Br)CBr	1.0	293	1760.4	1794.5	34.1	-	45.8	-	Br
14	CC(C)(Br)CBr	0.0	322	-	1750.9	-	41.8	44.2	2.4	Br
15	CCC(C)(Br)Br	0.0	318	1718.7	1727.7	9.1	41.0	42.5	1.4	Br
16	CC(C)C(Br)Br	0.0	321	1733.3	1727.2	-6.2	-	44.2	-	Br
17	CC(Br)C(C)Br	1.0	295	1789.3	1774.0	-15.3	-	46.0	-	Br
18	CC(Br)C(C)Br	0.0	325	-	1730.0	-	43.0	44.6	1.5	Br
19	CC(Br)CCBr	0.0	343	-	1722.1	-	45.1	47.2	2.1	Br
20	CCCC(Br)Br	1.0	298	1784.0	1756.9	-27.1	-	46.9	-	Br
21	CCCC(Br)Br	1.0	357	-	1666.2	-	45.8	43.8	-2.0	Br
22	BrCCCCBr	1.0	298	1818.8	1811.9	-7.0	52.6	53.4	0.8	Br
23	CC(Br)C(C)(Br)Br	1.0	293	2172.4	2187.0	14.6	-	56.2	-	Br
24	CC(Br)C(C)(Br)Br	1.0	326	-	2135.3	-	51.7	54.3	2.6	Br
25	CCC(Br)(Br)CBr	1.0	293	2168.5	2198.0	29.5	-	57.4	-	Br
26	CCC(Br)(Br)CBr	1.0	329	-	2140.2	-	50.7	55.2	4.5	Br
27	CC(Br)C(Br)CBr	1.0	293	2183.5	2210.2	26.7	-	63.6	-	Br
28	CC(Br)C(Br)CBr	1.0	333	-	2146.2	-	51.3	60.7	9.4	Br
29	CCC(Br)C(Br)Br	1.0	293	2183.5	2176.2	-7.3	-	59.0	-	Br
30	CCC(Br)C(Br)Br	0.0	369	-	2055.8	-	51.1	54.3	3.2	Br
31	BrCC(CBr)CBr	1.0	490	-	1938.0	-	66.1	53.3	-12.8	Br
32	BrCCC(Br)CBr	1.0	298	2210.0	2215.9	5.9	-	64.0	-	Br
33	BrCCC(Br)CBr	1.0	405	-	2049.4	-	53.5	57.6	4.1	Br
34	CC(C)(C)CBr	1.0	308	-	1212.5	-	35.6	37.8	2.2	Br
35	CC(C)C(C)Br	0.0	298	1215.6	1203.6	-12.0	-	37.9	-	Br
36	CC(C)C(C)Br	1.0	316	-	1181.7	-	37.2	37.0	-0.2	Br
37	CCC(Br)CC	0.0	298	-	1200.8	-	39.3	38.6	-0.7	Br
38	CC(Br)C(C)(C)C	0.0	298	1169.8	1194.9	25.2	-	41.9	-	Br
39	CC(Br)C(C)(C)C	1.0	330	-	1159.4	-	39.5	40.3	0.8	Br
40	CC(C)C(C)(C)Br	1.0	292	1187.4	1190.8	3.4	-	40.6	-	Br
41	CCCC(C)(C)Br	1.0	293	1180.4	1173.1	-7.3	-	41.3	-	Br
42	ClCCl	1.0	298	1316.4	1320.4	4.0	28.8	29.7	0.9	Cl
43	ClC(Cl)Cl	1.0	298	1479.5	1506.3	26.8	31.1	32.8	1.7	Cl
44	ClC(Cl)(Cl)Cl	1.0	298	1584.3	1617.2	32.9	-	34.5	-	Cl
45	ClC(Cl)(Cl)Cl	0.1	298	-	1616.5	-	32.4	34.5	2.1	Cl
46	CC(C)Cl	0.7	298	-	848.7	-	26.4	27.0	0.5	Cl
47	CCCCl	1.0	298	884.1	876.9	-7.2	28.5	28.6	0.1	Cl
48	CC(C)(Cl)Cl	0.2	298	1107.3	1076.0	-31.3	-	30.4	-	Cl
49	CC(C)(Cl)Cl	1.0	298	-	1076.5	-	32.1	30.4	-1.7	Cl
50	CCC(Cl)Cl	0.1	298	1126.0	1114.1	-11.9	-	34.7	-	Cl
51	CCC(Cl)Cl	1.0	298	-	1114.5	-	35.2	34.7	-0.5	Cl
52	CC(Cl)(Cl)CCl	0.0	298	1317.9	1327.6	9.8	40.5	41.9	1.4	Cl
53	CCC(Cl)(Cl)Cl	1.0	298	1283.6	1282.7	-0.9	-	36.7	-	Cl
54	CCC(Cl)(Cl)Cl	1.0	259	-	1334.7	-	38.8	38.5	-0.3	Cl
55	CC(Cl)C(Cl)Cl	1.0	289	1353.0	1343.0	-10.0	-	44.2	-	Cl
56	CC(Cl)C(Cl)Cl	0.0	302	-	1327.6	-	42.3	43.4	1.1	Cl
57	ClCC(Cl)CCl	1.0	298	1388.8	1388.8	0.0	46.8	50.4	3.6	Cl
58	ClCCC(Cl)Cl	1.0	293	1355.5	1366.4	10.8	-	45.9	-	Cl
59	ClCCC(Cl)Cl	0.0	313	-	1341.8	-	44.2	44.9	0.7	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
60	CC(C)(Cl)CCl	0.0	298	1089.0	1098.2	9.2	36.8	37.4	0.6	Cl
61	CCC(C)(Cl)Cl	0.1	298	1065.1	1065.9	0.8	-	34.9	-	Cl
62	CCC(C)(Cl)Cl	1.0	298	-	1065.9	-	36.7	34.9	-1.8	Cl
63	CC(C)C(Cl)Cl	0.0	298	1100.1	1080.8	-19.4	36.5	37.7	1.2	Cl
64	CC(Cl)C(C)Cl	0.0	298	-	1095.4	-	38.5	41.7	3.1	Cl
65	CC(CCl)CCl	0.0	307	1090.0	1117.3	27.2	-	42.5	-	Cl
66	CC(CCl)CCl	1.0	285	-	1140.8	-	45.1	44.0	-1.1	Cl
67	CC(Cl)CCCl	1.0	298	1108.3	1110.1	1.8	42.1	42.4	0.3	Cl
68	CCCC(Cl)Cl	0.0	298	1080.1	1078.7	-1.4	-	39.0	-	Cl
69	CCCC(Cl)Cl	1.0	298	-	1079.4	-	39.4	39.0	-0.4	Cl
70	CC(C)(Cl)C(Cl)Cl	1.0	298	1267.7	1276.9	9.2	-	44.5	-	Cl
71	CC(Cl)C(C)(Cl)Cl	1.0	291	1263.0	1276.4	13.4	-	44.4	-	Cl
72	CC(Cl)C(C)(Cl)Cl	0.0	310	-	1252.3	-	42.7	43.3	0.6	Cl
73	CC(Cl)(CCl)CCl	1.0	298	1301.2	1316.0	14.8	-	49.1	-	Cl
74	CC(Cl)(CCl)CCl	0.0	327	-	1284.2	-	45.9	47.1	1.2	Cl
75	CCCC(Cl)(Cl)Cl	0.0	298	1231.0	1231.1	0.2	-	41.4	-	Cl
76	CC(CCl)C(Cl)Cl	0.0	312	1251.1	1278.7	27.7	-	47.0	-	Cl
77	CC(Cl)C(Cl)CCl	1.0	293	1316.4	1308.1	-8.3	-	51.3	-	Cl
78	CC(Cl)C(Cl)CCl	1.0	288	-	1313.8	-	41.3	51.6	10.3	Cl
79	CC(Cl)CC(Cl)Cl	1.0	288	1317.0	1282.1	-34.9	-	47.9	-	Cl
80	CC(Cl)CC(Cl)Cl	0.0	318	-	1248.6	-	43.9	46.0	2.1	Cl
81	ClCCC(Cl)CCl	1.0	293	1317.5	1324.0	6.5	-	53.3	-	Cl
82	CC(C)(C)CCl	0.1	298	860.9	882.6	21.7	-	35.1	-	Cl
83	CC(C)(C)CCl	1.0	294	-	886.8	-	34.9	35.3	0.4	Cl
84	CC(C)C(C)Cl	0.1	298	857.0	864.0	6.9	-	34.6	-	Cl
85	CC(C)C(C)Cl	1.0	300	-	862.6	-	35.9	34.6	-1.3	Cl
86	CCC(Cl)CC	1.0	298	884.0	863.1	-20.9	-	35.5	-	Cl
87	CCC(Cl)CC	1.0	304	-	857.5	-	36.5	35.2	-1.3	Cl
88	CC(C)(C)C(Cl)Cl	0.0	312	1074.8	1063.9	-10.8	-	40.7	-	Cl
89	CC(C)C(C)(C)Cl	1.0	298	874.9	877.3	2.4	-	36.8	-	Cl
90	CC(C)C(C)(C)Cl	1.0	316	-	861.8	-	38.0	35.9	-2.1	Cl
91	CCC(C)(Cl)CC	1.0	293	883.9	878.4	-5.5	-	37.3	-	Cl
92	CCCC(C)(C)Cl	0.0	298	858.3	862.9	4.6	37.7	37.3	-0.4	Cl
93	FCF	1.0	221	1213.8	1238.1	24.3	20.9	22.6	1.8	F
94	FCF	17.6	298	891.6	1064.9	173.2	-	19.6	-	F
95	FCF	1.0	298	961.0	1059.3	98.3	-	19.5	-	F
96	FC(F)F	1.0	191	1442.9	1795.7	352.8	16.7	23.9	7.2	F
97	FC(F)(F)F	1.0	145	1605.2	1893.8	288.7	12.3	17.0	4.7	F
98	FCCF	1.0	283	1024.0	1046.0	22.0	-	23.9	-	F
99	FCCF	1.8	298	-	1019.5	-	22.5	23.3	0.8	F
100	CC(F)(F)F	12.9	298	-	915.8	-	13.1	14.8	1.7	F
101	FCC(F)F	1.0	314	1175.5	1152.2	-23.3	-	24.8	-	F
102	FCC(F)F	1.0	278	-	1230.2	-	23.2	26.8	3.6	F
103	FCC(F)F	2.0	296	-	1190.8	-	20.6	25.8	5.2	F
104	CC(C)F	1.0	293	723.8	710.0	-13.8	-	21.4	-	F
105	CC(C)F	1.0	249	-	769.7	-	23.7	23.2	-0.5	F
106	CC(C)(F)F	1.0	271	943.8	864.5	-79.2	22.6	20.8	-1.8	F
107	CC(C)(F)F	2.1	291	911.4	827.8	-83.6	21.6	20.0	-1.6	F
108	CC(F)CF	1.4	298	960.0	928.4	-31.6	-	24.6	-	F
109	CCC(F)F	1.3	298	920.1	898.2	-21.8	23.7	24.2	0.4	F
110	CCC(F)(F)F	0.9	259	1148.2	1019.7	-128.4	21.8	21.3	-0.4	F
111	CC(C)(C)F	1.0	237	-	783.8	-	27.6	25.3	-2.3	F
112	CC(C)CF	0.9	286	764.5	773.6	9.1	-	27.1	-	F
113	CC(C)CF	1.4	298	750.0	760.0	10.0	-	26.5	-	F
114	CCC(C)F	1.0	248	-	796.2	-	29.2	27.9	-1.3	F
115	CCCCF	1.0	237	-	835.8	-	30.1	30.4	0.3	F
116	CCC(C)(F)F	1.0	293	915.9	853.2	-62.7	-	24.6	-	F
117	CCC(C)(F)F	0.8	298	-	845.3	-	25.9	24.4	-1.5	F
118	CCCC(F)F	0.4	298	910.1	898.8	-11.3	-	28.7	-	F
119	CCCC(F)F	1.0	261	-	945.5	-	31.0	30.5	-0.5	F
120	FCCCCF	0.1	298	-	978.2	-	34.6	36.1	1.6	F
121	CCC(C)(C)F	0.4	298	-	750.4	-	29.4	27.5	-1.9	F
122	CC(C)(C)C(F)(F)F	1.0	293	990.5	997.4	6.9	-	29.1	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
123	IC(I)I	0.0	396	3685.6	3434.2	-251.4	47.9	56.8	8.9	I
124	IC(I)(I)I	0.0	447	3819.2	3687.7	-131.5	-	68.3	-	I
125	CCI	0.2	298	-	1907.7	-	31.7	30.9	-0.8	I
126	CC(I)I	0.0	336	2682.9	2650.0	-32.9	-	45.6	-	I
127	ICCI	0.0	356	2551.8	2678.4	126.6	48.1	47.9	-0.2	I
128	CCCI	0.1	298	-	1731.0	-	36.0	35.4	-0.6	I
129	CC(C)(I)I	0.0	352	2379.7	2340.9	-38.8	-	46.3	-	I
130	CC(I)CI	0.0	330	2506.9	2441.1	-65.9	-	50.7	-	I
131	CCC(I)I	0.0	357	2370.2	2380.7	10.5	-	48.5	-	I
132	CC(C)CI	1.0	298	-	1598.8	-	38.8	38.6	-0.2	I
133	CC(C)(I)CI	0.0	370	2163.1	2211.4	48.4	-	51.2	-	I
134	CCC(C)(I)I	0.0	370	2163.1	2198.7	35.6	-	50.0	-	I
135	CC(C)C(I)I	0.0	365	2171.2	2191.5	20.3	-	50.6	-	I
136	CC(I)C(C)I	0.0	374	2155.0	2167.5	12.5	-	50.2	-	I
137	CC(CI)CI	0.0	374	2155.0	2198.6	43.6	-	52.7	-	I
138	CCC(I)CI	0.0	371	2160.5	2186.3	25.8	-	52.1	-	I
139	CC(I)CCI	0.0	382	2141.4	2164.4	23.1	-	52.4	-	I
140	CCCC(I)I	0.0	373	2144.3	2165.5	21.3	-	51.7	-	I
141	CCC(C)(C)I	1.0	323	-	1488.3	-	40.4	40.1	-0.3	I
142	CC(I)C(C)(C)C	0.0	320	1392.3	1448.1	55.7	-	44.5	-	I
143	CC(C)C(C)(C)I	1.0	293	1448.0	1478.3	30.3	-	45.3	-	I
144	CCC(C)(I)CC	0.0	319	1393.3	1441.9	48.6	-	44.5	-	I
145	CCCC(C)(C)I	0.0	332	1376.8	1407.8	31.0	-	44.2	-	I
146	ClCBr	1.0	298	1924.9	1924.7	-0.2	-	33.7	-	Mix
147	ClCBr	1.0	304	-	1912.5	-	33.5	33.5	-0.0	Mix
148	FCCl	1.0	260	1282.1	1291.0	8.8	21.9	26.2	4.3	Mix
149	BrCI	1.0	290	2926.0	2879.8	-46.2	-	42.5	-	Mix
150	ClCI	1.0	293	2422.0	2408.5	-13.5	-	38.8	-	Mix
151	FC(F)Br	1.0	298	1775.5	2012.1	236.7	-	27.2	-	Mix
152	FC(F)Br	1.0	244	-	2208.0	-	24.0	30.2	6.2	Mix
153	FC(F)Cl	1.0	233	1408.0	1567.4	159.4	20.2	25.7	5.5	Mix
154	FC(F)Cl	10.8	298	1193.0	1351.9	158.9	-	22.0	-	Mix
155	FC(Cl)Cl	1.8	298	1367.0	1438.8	71.8	-	27.6	-	Mix
156	FC(Cl)Cl	1.0	267	-	1506.9	-	26.1	29.1	3.0	Mix
157	FC(I)I	1.0	295	3196.9	3242.4	45.5	-	48.7	-	Mix
158	FC(I)I	1.0	314	-	3191.6	-	32.9	47.8	14.9	Mix
159	FC(F)I	1.0	272	-	2619.7	-	26.0	35.1	9.1	Mix
160	FC(Br)Br	1.0	293	2421.0	2551.2	130.2	-	37.9	-	Mix
161	ClC(Cl)Br	1.0	298	1983.5	2001.5	18.0	-	37.6	-	Mix
162	ClC(Br)Br	1.0	293	2451.0	2472.6	21.6	-	42.7	-	Mix
163	ClC(Cl)(Cl)Br	1.0	298	2002.1	2045.8	43.7	-	39.8	-	Mix
164	ClC(Cl)(Cl)Br	0.1	298	-	2047.7	-	36.1	39.8	3.7	Mix
165	ClC(Cl)(Br)Br	1.0	298	2420.0	2445.3	25.3	-	44.9	-	Mix
166	ClC(Br)(Br)Br	1.0	288	2710.0	2841.4	131.4	-	50.6	-	Mix
167	FC(F)(F)Br	1.0	215	1989.9	2548.1	558.2	17.5	28.7	11.2	Mix
168	FC(F)(F)Br	16.6	298	1536.1	1942.9	406.8	-	22.2	-	Mix
169	FC(Br)(Br)Br	1.0	330	-	2781.9	-	34.4	43.0	8.6	Mix
170	FC(F)(Br)Br	1.0	298	2251.2	2482.9	231.7	25.0	33.7	8.7	Mix
171	FC(F)(F)Cl	1.0	190	1527.8	1942.8	415.0	15.4	23.3	7.9	Mix
172	FC(F)(F)Cl	36.7	298	840.9	1323.0	482.1	-	16.5	-	Mix
173	FC(F)(Cl)Cl	1.0	243	1488.0	1570.7	82.7	20.1	24.6	4.5	Mix
174	FC(F)(Cl)Cl	6.7	298	1307.0	1432.9	125.9	-	22.4	-	Mix
175	FC(Cl)(Cl)Cl	1.1	298	1477.0	1539.7	62.7	24.9	28.6	3.7	Mix
176	FC(F)(F)I	20.0	298	2046.8	2462.2	415.4	-	29.1	-	Mix
177	FC(F)(F)I	1.0	281	-	2527.7	-	22.5	29.9	7.4	Mix
178	FC(Cl)Br	1.0	273	1977.1	2070.5	93.4	-	33.7	-	Mix
179	FC(F)(Cl)Br	1.0	269	1899.6	2051.4	151.8	23.1	29.2	6.1	Mix
180	FC(F)(Cl)Br	2.6	298	1810.0	1968.1	158.2	-	28.0	-	Mix
181	FC(Cl)(Cl)Br	1.0	295	1950.0	2017.8	67.8	-	34.0	-	Mix
182	FC(Cl)(Cl)Br	0.4	298	-	2009.0	-	29.1	33.9	4.8	Mix
183	FC(Cl)(Br)Br	1.0	295	2317.3	2456.5	139.2	-	39.3	-	Mix
184	CC(Cl)Br	1.0	305	-	1628.6	-	33.1	34.4	1.3	Mix
185	CC(F)Cl	1.4	298	-	1048.3	-	23.7	25.2	1.5	Mix

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
186	FCCCl	1.0	303	-	1138.0	-	32.1	28.8	-3.3	Mix
187	CC(F)(F)Cl	1.0	263	-	1178.2	-	22.7	22.3	-0.4	Mix
188	FCC(F)Cl	0.8	298	-	1293.8	-	26.6	30.9	4.3	Mix
189	FC(F)CCl	1.0	288	1312.0	1304.8	-7.2	-	31.7	-	Mix
190	FC(F)CCl	0.7	298	-	1287.1	-	26.6	31.2	4.6	Mix
191	CC(F)(Cl)Cl	0.8	298	-	1233.2	-	26.0	26.6	0.6	Mix
192	FC(Cl)CCl	0.1	298	-	1369.4	-	32.8	36.5	3.8	Mix
193	ClC(Cl)(Br)CBr	1.0	273	2298.0	2320.4	22.4	-	54.3	-	Mix
194	ClC(Cl)(Br)CBr	1.0	369	-	2148.9	-	45.9	48.5	2.6	Mix
195	ClC(Br)C(Cl)Br	1.0	293	2135.0	2318.0	183.0	-	56.4	-	Mix
196	ClC(Br)C(Cl)Br	1.0	335	-	2245.2	-	45.9	53.9	8.0	Mix
197	FC(F)(Cl)CCl	0.4	298	-	1422.0	-	28.3	32.9	4.6	Mix
198	FC(Cl)C(F)Cl	0.4	298	1405.4	1488.6	83.2	-	35.9	-	Mix
199	FC(F)(F)CBr	1.0	293	1788.1	1779.1	-9.0	-	30.5	-	Mix
200	FC(F)(F)CCl	1.9	298	-	1313.5	-	22.3	27.0	4.7	Mix
201	FC(Cl)(Cl)CCl	0.1	298	-	1503.1	-	34.7	38.7	4.1	Mix
202	FCC(Cl)(Cl)Cl	0.1	298	1575.0	1522.1	-52.9	-	38.7	-	Mix
203	FC(Cl)C(Cl)Cl	0.0	298	-	1541.8	-	36.9	41.2	4.3	Mix
204	ClCCCBr	1.0	341	-	1526.9	-	42.0	42.3	0.3	Mix
205	CC(C)(F)Cl	0.1	298	-	959.2	-	31.5	25.0	-6.4	Mix
206	CC(F)(F)CCl	0.4	298	1191.6	1145.9	-45.7	-	30.4	-	Mix
207	FC(F)(F)CCCl	0.5	298	1290.1	1266.7	-23.3	-	31.6	-	Mix
208	FC(F)(F)CCCl	1.0	306	-	1252.2	-	29.9	31.1	1.2	Mix
209	FCCCCCl	0.0	298	1062.7	1061.5	-1.3	-	41.6	-	Mix
210	CC(Cl)C(F)(F)F	1.0	313	-	1821.8	-	30.4	41.2	10.8	Mix
211	CC(I)CC(F)(F)F	1.0	312	-	1793.8	-	32.4	40.4	8.0	Mix
212	CCC(C)CBr	1.0	321	-	1185.7	-	37.9	38.2	0.3	Br
213	CC(C)CCBr	0.0	298	-	1208.8	-	39.7	39.8	0.1	Br
214	CC(Br)C(C)(C)Br	1.0	298	1663.0	1688.7	25.7	-	49.9	-	Br
215	CC(Br)C(C)(C)Br	0.0	335	-	1638.0	-	-	47.9	-	Br
216	CC(C)C(C)(Br)Br	0.0	337	1622.0	1620.1	-1.9	-	45.1	-	Br
217	CC(C)(CBr)CBr	1.0	293	1693.4	1726.0	32.6	-	52.2	-	Br
218	CC(C)(CBr)CBr	0.0	345	-	1658.2	-	-	49.2	-	Br
219	CCC(C)(Br)CBr	1.0	294	1663.8	1698.6	34.8	-	49.1	-	Br
220	CCC(C)(Br)CBr	0.0	337	-	1640.1	-	-	46.9	-	Br
221	CCC(Br)(Br)CC	0.0	332	1610.0	1620.9	10.9	-	45.6	-	Br
222	CC(C)(Br)CCBr	1.0	273	1696.0	1720.0	24.0	-	52.8	-	Br
223	CC(C)(Br)CCBr	0.0	337	-	1633.2	-	-	49.3	-	Br
224	CCCC(C)(Br)Br	1.0	289	1645.2	1665.0	19.8	-	48.4	-	Br
225	CCCC(C)(Br)Br	0.0	335	-	1602.0	-	-	46.1	-	Br
226	CC(Br)C(C)CBr	0.0	337	1751.0	1636.6	-114.4	-	50.2	-	Br
227	CCC(C)C(Br)Br	0.0	337	1602.8	1609.8	7.1	-	47.4	-	Br
228	CC(C)C(Br)CBr	1.0	293	1677.0	1686.8	9.8	-	50.9	-	Br
229	CC(C)C(Br)CBr	0.0	337	-	1627.4	-	-	48.7	-	Br
230	CCC(Br)C(C)Br	1.0	293	1673.0	1677.2	4.2	-	52.7	-	Br
231	CCC(Br)C(C)Br	0.0	341	-	1610.2	-	-	49.3	-	Br
232	CC(C)CC(Br)Br	0.0	337	1602.8	1595.4	-7.3	-	47.9	-	Br
233	CC(Br)CC(C)Br	1.0	293	1665.9	1659.6	-6.3	-	51.0	-	Br
234	CC(Br)CC(C)Br	0.0	344	-	1589.5	-	-	48.0	-	Br
235	CC(CBr)CCBr	1.0	293	1711.5	1704.7	-6.8	-	56.4	-	Br
236	CC(CBr)CCBr	0.0	337	-	1645.1	-	-	53.5	-	Br
237	CCC(Br)CCBr	1.0	293	1665.3	1688.1	22.8	-	53.4	-	Br
238	CCC(Br)CCBr	0.0	351	-	1609.4	-	-	50.2	-	Br
239	CCCC(Br)CBr	1.0	293	1670.8	1679.8	9.0	49.0	52.4	3.4	Br
240	CC(Br)CCCBr	1.0	293	1683.0	1685.3	2.3	-	55.7	-	Br
241	CC(Br)CCCBr	1.0	392	-	1549.1	-	51.8	49.7	-2.1	Br
242	CCCCC(Br)Br	0.0	343	1588.3	1588.8	0.5	-	48.7	-	Br
243	CCCCC(Br)Br	1.0	375	-	1542.8	-	48.8	46.9	-1.9	Br
244	BrCCCCCBr	1.0	298	1694.0	1693.2	-0.8	-	57.4	-	Br
245	BrCCCCCBr	1.0	411	-	1539.8	-	54.4	50.5	-3.9	Br
246	CC(Br)C(C)(Br)CBr	1.0	293	2082.1	2099.5	17.4	-	63.6	-	Br
247	CC(CBr)(CBr)CBr	1.0	293	2091.7	2134.1	42.4	-	67.1	-	Br
248	CCCCC(Br)(Br)Br	1.0	293	1988.2	2013.3	25.1	-	59.8	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
249	CCCCC(Br)(Br)Br	0.1	427	-	1810.9	-	-	51.9	-	Br
250	BrCCC(Br)CCBr	1.0	292	2065.0	2079.5	14.5	-	69.3	-	Br
251	BrCCCC(Br)CBr	1.0	295	2073.0	2069.3	-3.7	-	69.6	-	Br
252	CCC(C)(C)CBr	0.0	311	1150.8	1186.4	35.6	-	41.9	-	Br
253	CC(C)(C)CCBr	1.0	293	1155.6	1195.4	39.8	-	43.9	-	Br
254	CC(C)(C)CCBr	0.0	308	-	1178.6	-	-	43.1	-	Br
255	CC(C)C(C)CBr	1.0	298	1190.0	1181.7	-8.3	-	42.9	-	Br
256	CC(C)C(C)CBr	0.0	311	-	1168.0	-	-	42.3	-	Br
257	CCC(C)C(C)Br	0.0	303	1163.1	1166.8	3.7	-	42.1	-	Br
258	CCC(Br)C(C)C	0.0	303	1163.1	1161.7	-1.4	-	41.7	-	Br
259	CC(C)CC(C)Br	0.0	303	1144.3	1151.5	7.2	40.9	42.1	1.2	Br
260	CCC(CC)CBr	0.0	313	1159.9	1161.8	1.9	42.7	42.6	-0.1	Br
261	CCC(C)CCBr	1.0	296	1171.0	1178.4	7.4	-	44.2	-	Br
262	CCC(C)CCBr	0.0	317	-	1155.4	-	-	43.2	-	Br
263	CCCC(C)CBr	1.0	293	1177.9	1178.0	0.1	-	44.0	-	Br
264	CCCC(C)CBr	0.0	314	-	1154.8	-	-	42.9	-	Br
265	CCCC(Br)CC	0.0	312	-	1147.6	-	42.5	42.4	-0.1	Br
266	CC(C)CCCBr	1.0	293	1168.3	1175.0	6.7	-	44.6	-	Br
267	CC(C)CCCBr	0.0	316	-	1148.9	-	-	43.3	-	Br
268	CCCCC(C)Br	1.0	298	1159.7	1159.3	-0.4	-	43.5	-	Br
269	CCCCC(C)Br	1.0	318	-	1137.4	-	43.8	42.4	-1.4	Br
270	CC(C)(Br)C(C)(C)Br	0.3	435	-	1462.3	-	-	45.2	-	Br
271	CC(C)C(C)(Br)CBr	0.1	400	1450.3	1496.7	46.4	-	47.3	-	Br
272	CC(C)(C)C(Br)CBr	0.1	400	1462.2	1500.0	37.8	-	51.0	-	Br
273	CCCCC(C)(Br)Br	1.0	295	1546.3	1574.4	28.1	-	52.6	-	Br
274	CCCCC(C)(Br)Br	0.1	400	-	1435.1	-	-	46.7	-	Br
275	CC(C)C(CBr)CBr	1.0	293	1605.0	1625.7	20.7	-	57.8	-	Br
276	CC(CBr)C(C)CBr	0.1	400	1465.9	1492.2	26.3	-	52.3	-	Br
277	CCC(Br)C(Br)CC	1.0	293	1602.7	1589.2	-13.5	-	53.8	-	Br
278	CCC(Br)C(Br)CC	0.1	400	-	1450.2	-	-	47.8	-	Br
279	CCCC(Br)C(C)Br	1.0	293	1581.2	1587.1	5.9	-	54.6	-	Br
280	CCCC(Br)C(C)Br	0.1	400	-	1446.9	-	-	48.1	-	Br
281	CC(Br)CCC(C)Br	1.0	293	1578.8	1581.6	2.8	-	57.7	-	Br
282	CC(Br)CCC(C)Br	0.0	365	-	1490.2	-	49.5	53.1	3.6	Br
283	CCCC(CBr)CBr	1.0	293	1577.1	1614.7	37.6	-	58.7	-	Br
284	CC(CCBr)CCBr	0.1	426	1395.4	1446.4	50.9	50.8	52.1	1.3	Br
285	CCC(Br)CCCBr	0.1	400	1443.8	1462.7	18.9	-	52.5	-	Br
286	CCCCC(Br)CBr	1.0	293	1560.4	1591.4	31.0	56.5	56.5	0.0	Br
287	CC(Br)CCCCBr	0.1	400	1415.4	1457.7	42.3	-	52.9	-	Br
288	CCCCCC(Br)Br	0.1	400	1416.2	1432.0	15.8	-	49.4	-	Br
289	CCCCCC(Br)Br	1.0	393	-	1442.4	-	51.6	49.8	-1.8	Br
290	BrCCCCCCBr	1.0	298	1602.5	1602.6	0.1	-	61.7	-	Br
291	BrCCCCCCBr	0.0	364	-	1520.4	-	57.1	57.3	0.2	Br
292	CCC(CBr)(CBr)CBr	1.0	293	1912.2	2024.4	112.2	-	70.4	-	Br
293	CCCC(Br)CCC	1.0	296	1133.0	1134.3	1.3	-	47.7	-	Br
294	CCCC(Br)CCC	0.0	327	-	1100.5	-	-	45.8	-	Br
295	CCCCC(Br)CC	1.0	295	1134.1	1135.3	1.2	-	47.8	-	Br
296	CCCCCC(C)Br	0.0	320	1095.5	1105.1	9.5	46.2	46.7	0.5	Br
297	CCC(Br)(CBr)C(C)C	1.0	293	1526.1	1572.3	46.2	-	57.3	-	Br
298	CC(C)(C)CC(Br)CBr	1.0	293	1502.0	1542.3	40.3	-	58.1	-	Br
299	CCCC(Br)(CC)CBr	1.0	293	1492.9	1552.3	59.4	-	58.7	-	Br
300	CC(C)(CCBr)CCBr	1.0	293	1532.0	1573.5	41.5	-	65.0	-	Br
301	CCCC(Br)C(Br)CC	1.0	293	1516.2	1519.9	3.7	-	58.4	-	Br
302	CCCC(Br)C(Br)CC	0.1	418	-	1365.5	-	-	50.3	-	Br
303	CCCCC(Br)C(C)Br	1.0	293	1513.2	1516.6	3.4	-	58.6	-	Br
304	CCCCC(Br)C(C)Br	0.1	418	-	1362.5	-	-	50.7	-	Br
305	CCC(Br)CCCCBr	0.1	418	-	1377.6	-	-	55.2	-	Br
306	CCCCCC(Br)CBr	1.0	293	1518.0	1519.6	1.6	-	60.9	-	Br
307	CCCCCC(Br)CBr	1.0	300	-	1511.2	-	54.4	60.4	6.0	Br
308	CCCCCCC(Br)Br	1.0	294	1500.0	1503.8	3.8	-	60.4	-	Br
309	CCCCCCC(Br)Br	1.0	410	-	1362.3	-	54.4	52.8	-1.6	Br
310	BrCCCCCCCBr	0.0	385	1469.2	1428.7	-40.5	57.8	59.9	2.1	Br
311	CC(C)CCCC(C)Br	1.0	293	1091.0	1105.4	14.4	-	51.5	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
312	CCCCCCC(C)Br	1.0	298	1096.8	1104.1	7.3	-	52.5	-	Br
313	CCCCCCC(C)Br	1.0	358	-	1044.2	-	48.4	48.8	0.4	Br
314	CCC(C)(C)CC(Br)CBr	1.0	293	1468.9	1495.7	26.8	-	62.1	-	Br
315	CCCC(Br)C(Br)CCC	0.1	435	-	1295.7	-	-	52.7	-	Br
316	CCCCC(Br)CCCBr	0.1	435	-	1305.8	-	-	57.4	-	Br
317	CCCC(Br)CCCCBr	0.1	435	-	1306.2	-	-	57.6	-	Br
318	CCCCCCC(Br)CBr	1.0	293	1458.0	1461.7	3.7	-	65.3	-	Br
319	CCCCCCC(Br)CBr	0.1	435	-	1297.3	-	-	55.5	-	Br
320	CCCCCCCC(Br)Br	0.1	435	-	1283.4	-	-	54.9	-	Br
321	CCCCCCCC(Br)Br	1.0	427	-	1294.5	-	57.1	55.5	-1.6	Br
322	BrCCCCCCCCBr	0.0	399	1413.1	1357.7	-55.3	59.6	62.7	3.1	Br
323	CCCCCCCC(C)Br	1.0	298	1076.0	1084.0	8.0	-	57.0	-	Br
324	CCCCCCCCCBr	1.0	298	1084.9	1093.0	8.2	-	59.1	-	Br
325	CCCCCCCCCBr	1.0	391	-	1004.6	-	53.1	52.7	-0.4	Br
326	CCCCCCCC(Br)CBr	1.0	293	1398.0	1413.4	15.4	-	69.8	-	Br
327	CCCCCCCC(Br)CBr	0.1	451	-	1238.0	-	-	58.1	-	Br
328	CCCCCCCCC(Br)Br	0.1	451	-	1227.2	-	-	57.4	-	Br
329	CCCCCCCCC(Br)Br	1.0	442	-	1238.3	-	59.5	58.1	-1.4	Br
330	BrCCCCCCCCCBr	1.0	298	1428.0	1420.5	-7.5	-	74.6	-	Br
331	BrCCCCCCCCCBr	0.0	415	-	1296.6	-	61.8	65.3	3.5	Br
332	CCCCCCCCC(C)Br	1.0	298	1047.0	1067.1	20.1	-	61.4	-	Br
333	CCCCCCCCC(C)Br	0.0	383	-	988.6	-	-	55.2	-	Br
334	CCCCCCCCCCBr	1.0	298	1062.5	1074.9	12.4	-	63.5	-	Br
335	CCCCCCCCCCBr	1.0	398	-	983.8	-	56.6	56.1	-0.5	Br
336	CCCCCCCCC(Br)CBr	1.0	383	-	1278.9	-	67.0	67.0	-0.0	Br
337	CCCCCCCCCC(Br)Br	1.0	457	-	1189.0	-	62.2	60.7	-1.5	Br
338	CCC(C)CCl	0.0	298	-	875.2	-	36.3	36.1	-0.2	Cl
339	CC(Cl)C(C)(C)Cl	0.0	307	1080.9	1060.6	-20.3	-	39.9	-	Cl
340	CC(C)C(C)(Cl)Cl	0.0	333	1051.1	1019.8	-31.3	-	37.2	-	Cl
341	CC(C)(CCl)CCl	0.0	314	1066.8	1094.1	27.3	-	44.7	-	Cl
342	CCC(C)(Cl)CCl	0.0	306	1061.9	1072.8	10.9	35.9	40.8	4.9	Cl
343	CCC(Cl)(Cl)CC	0.0	303	1043.7	1047.5	3.8	40.3	38.9	-1.3	Cl
344	CC(C)(Cl)CCCl	1.0	293	1075.8	1085.7	9.9	-	44.3	-	Cl
345	CC(C)(Cl)CCCl	0.0	314	-	1064.3	-	-	43.1	-	Cl
346	CCCC(C)(Cl)Cl	0.0	299	1034.6	1041.3	6.6	40.0	39.5	-0.5	Cl
347	CC(Cl)C(C)CCl	1.0	293	1093.8	1092.4	-1.4	-	46.2	-	Cl
348	CC(Cl)C(C)CCl	0.0	313	-	1071.8	-	-	45.0	-	Cl
349	CCC(C)C(Cl)Cl	0.0	302	1045.7	1055.7	10.0	-	41.7	-	Cl
350	CC(C)C(Cl)CCl	1.0	293	1080.5	1083.3	2.8	-	43.4	-	Cl
351	CC(C)C(Cl)CCl	0.0	312	-	1064.6	-	42.1	42.5	0.4	Cl
352	CCC(Cl)C(C)Cl	1.0	298	1075.0	1072.2	-2.8	-	46.6	-	Cl
353	CCC(Cl)C(C)Cl	0.0	309	-	1060.2	-	41.6	45.9	4.3	Cl
354	CC(C)CC(Cl)Cl	1.0	293	1047.3	1057.1	9.8	-	42.5	-	Cl
355	CC(C)CC(Cl)Cl	0.0	302	-	1047.6	-	40.1	42.1	2.0	Cl
356	CC(Cl)CC(C)Cl	1.0	291	1063.0	1064.2	1.2	-	44.3	-	Cl
357	CC(Cl)CC(C)Cl	0.0	317	-	1039.6	-	41.5	42.9	1.3	Cl
358	CC(CCl)CCCl	1.0	294	1103.0	1102.7	-0.3	-	50.3	-	Cl
359	CC(CCl)CCCl	0.0	324	-	1073.1	-	-	48.4	-	Cl
360	CCC(Cl)CCCl	1.0	293	1083.4	1086.5	3.1	-	46.3	-	Cl
361	CCC(Cl)CCCl	0.0	322	-	1057.7	-	-	44.7	-	Cl
362	CCCC(Cl)CCl	1.0	298	1074.1	1073.1	-1.0	43.9	44.4	0.5	Cl
363	CC(Cl)CCCCl	1.0	293	1073.4	1087.1	13.7	48.1	49.4	1.3	Cl
364	CCCCC(Cl)Cl	0.0	304	1041.7	1046.4	4.7	-	43.1	-	Cl
365	CCCCC(Cl)Cl	1.0	298	-	1053.1	-	44.3	43.4	-0.9	Cl
366	CC(C)(Cl)C(C)(Cl)Cl	0.0	342	1144.6	1207.6	63.0	-	46.1	-	Cl
367	CC(Cl)C(C)(Cl)CCl	0.0	343	1184.5	1219.9	35.3	-	49.4	-	Cl
368	CC(C)(Cl)C(Cl)CCl	1.0	293	1264.1	1265.7	1.6	-	53.3	-	Cl
369	CC(CCl)(CCl)CCl	0.0	338	1215.5	1266.5	50.9	-	54.2	-	Cl
370	CCCCC(Cl)(Cl)Cl	0.0	298	1183.9	1192.4	8.6	-	46.0	-	Cl
371	CCC(C)(C)CCl	0.0	298	874.6	894.4	19.8	-	39.3	-	Cl
372	CC(C)(C)CCCl	0.0	298	863.1	887.9	24.8	38.5	40.1	1.7	Cl
373	CC(C)C(C)CCl	1.0	298	881.6	881.0	-0.7	-	39.7	-	Cl
374	CC(C)C(C)CCl	0.0	298	-	880.4	-	-	39.6	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
375	CCC(C)C(C)Cl	0.0	298	869.9	871.9	2.1	-	39.2	-	Cl
376	CCC(Cl)C(C)C	0.0	298	869.9	867.1	-2.8	-	38.9	-	Cl
377	CC(C)CC(C)Cl	0.0	298	855.9	860.8	4.9	-	39.2	-	Cl
378	CCC(CC)CCl	0.0	300	884.2	877.0	-7.2	-	40.1	-	Cl
379	CCC(C)CCCl	1.0	300	892.0	875.5	-16.5	-	40.7	-	Cl
380	CCC(C)CCCl	0.0	303	-	873.4	-	-	40.5	-	Cl
381	CCCC(C)CCl	0.0	298	869.9	873.9	4.1	-	40.5	-	Cl
382	CCCC(Cl)CC	1.0	297	871.0	865.0	-6.0	-	39.9	-	Cl
383	CCCC(Cl)CC	0.0	298	-	864.3	-	39.9	39.9	0.0	Cl
384	CC(C)CCCCl	0.0	300	868.5	870.7	2.2	-	40.9	-	Cl
385	CCCCC(C)Cl	0.0	299	864.8	861.4	-3.4	41.2	40.2	-1.0	Cl
386	CC(C)(C)C(C)(Cl)Cl	0.0	317	-	1054.5	-	-	42.4	-	Cl
387	CC(C)(C)CC(Cl)Cl	1.0	293	1027.1	1055.0	27.9	-	45.8	-	Cl
388	CC(C)(C)CC(Cl)Cl	0.0	322	-	1026.6	-	41.8	44.1	2.4	Cl
389	CC(Cl)CC(C)(C)Cl	1.0	293	1036.0	1050.7	14.7	-	46.1	-	Cl
390	CCCCC(C)(Cl)Cl	1.0	298	1015.0	1024.8	9.8	-	44.1	-	Cl
391	CCCCC(C)(Cl)Cl	0.0	338	-	985.0	-	-	41.9	-	Cl
392	CCC(Cl)C(Cl)CC	1.0	293	1061.7	1057.8	-3.9	-	51.7	-	Cl
393	CCCC(Cl)C(C)Cl	0.0	334	1015.7	1010.5	-5.2	-	46.6	-	Cl
394	CCCC(Cl)CCCl	0.0	343	-	1012.4	-	-	47.6	-	Cl
395	CCC(Cl)CCCCl	0.0	350	-	1010.0	-	-	49.5	-	Cl
396	CCCCC(Cl)CCl	1.0	293	1080.0	1053.6	-26.4	48.2	48.9	0.6	Cl
397	CC(Cl)CCCCCl	1.0	293	1108.6	1060.5	-48.1	-	53.8	-	Cl
398	CCCCCC(Cl)Cl	0.0	335	987.4	995.1	7.8	-	45.6	-	Cl
399	CCCCCC(Cl)Cl	1.0	298	-	1031.2	-	48.7	47.8	-0.9	Cl
400	CCCCCC(Cl)(Cl)Cl	0.1	390	1033.3	1060.3	27.0	-	45.0	-	Cl
401	CC(C)(C)C(C)(C)Cl	0.0	298	864.3	977.4	113.1	-	46.2	-	Cl
402	CCC(C)(Cl)C(C)C	0.0	301	861.7	885.6	23.9	-	41.1	-	Cl
403	CCC(C)C(C)(C)Cl	0.0	301	-	881.3	-	-	41.3	-	Cl
404	CC(Cl)CC(C)(C)C	0.0	302	852.3	873.2	20.9	-	42.3	-	Cl
405	CC(C)CC(C)(C)Cl	1.0	293	862.8	868.1	5.3	-	40.7	-	Cl
406	CC(C)CC(C)(C)Cl	0.0	302	-	860.9	-	-	40.2	-	Cl
407	CCC(Cl)(CC)CC	0.0	314	865.9	868.9	2.9	-	40.5	-	Cl
408	CCCC(C)(Cl)CC	0.0	308	865.5	865.8	0.3	-	41.2	-	Cl
409	CCCCC(C)(C)Cl	1.0	293	863.5	869.0	5.5	-	42.1	-	Cl
410	CCCCC(C)(C)Cl	0.0	309	-	855.6	-	-	41.2	-	Cl
411	CC(C)CCC(C)Cl	0.0	309	848.9	851.0	2.1	-	43.0	-	Cl
412	CCCC(C)CCCl	0.0	320	851.3	856.7	5.4	-	43.9	-	Cl
413	CCCC(Cl)CCC	1.0	295	869.4	867.1	-2.3	-	44.6	-	Cl
414	CCCC(Cl)CCC	0.0	315	-	849.7	-	-	43.4	-	Cl
415	CCCCC(Cl)CC	1.0	298	857.9	864.8	7.0	-	44.4	-	Cl
416	CCCCC(Cl)CC	0.0	315	-	850.1	-	-	43.4	-	Cl
417	CCCCCC(C)Cl	1.0	295	865.1	864.8	-0.3	-	44.8	-	Cl
418	CCCCCC(C)Cl	1.0	328	-	836.3	-	44.8	42.9	-1.9	Cl
419	CC(C)(Cl)CC(C)(C)Cl	0.0	339	986.3	997.3	11.1	-	45.8	-	Cl
420	CCC(C)(C)CC(Cl)Cl	1.0	293	1032.1	1048.0	15.9	-	50.1	-	Cl
421	CC(C)(C)CC(Cl)CCl	1.0	293	1025.9	1050.4	24.5	-	50.6	-	Cl
422	CC(C)(C)CC(Cl)CCl	0.0	344	-	1004.2	-	45.1	47.6	2.5	Cl
423	CC(C)(CCCl)CCCl	1.0	293	1056.3	1080.0	23.7	-	58.7	-	Cl
424	CC(C)(CCCl)CCCl	0.0	339	-	1040.6	-	-	55.6	-	Cl
425	CCCC(Cl)(Cl)CCC	0.0	349	1021.9	968.9	-53.0	-	45.5	-	Cl
426	CCCCCC(C)(Cl)Cl	0.0	340	968.2	968.9	0.7	-	46.1	-	Cl
427	CCCCCC(Cl)CCl	1.0	293	1062.5	1033.7	-28.8	53.2	53.3	0.1	Cl
428	CCCCCCC(Cl)Cl	0.0	353	995.8	963.0	-32.8	-	48.7	-	Cl
429	CCCCCCC(Cl)Cl	1.0	298	-	1014.7	-	53.5	52.3	-1.2	Cl
430	ClCCCCCCCCl	1.0	298	1040.8	1046.2	5.4	61.2	59.8	-1.4	Cl
431	CCCCCCC(Cl)(Cl)Cl	1.0	298	1121.2	1132.0	10.8	-	55.1	-	Cl
432	CCCCCCC(Cl)(Cl)Cl	0.1	410	-	1018.4	-	-	47.9	-	Cl
433	ClCCCCCCC(Cl)Cl	1.0	293	1174.4	1171.1	-3.3	-	66.4	-	Cl
434	CCC(C)(C)C(C)(C)Cl	1.0	298	906.5	918.9	12.4	-	46.1	-	Cl
435	CCC(C)(Cl)C(C)(C)C	1.0	293	906.6	920.4	13.8	-	46.1	-	Cl
436	CC(C)(C)CC(C)(C)Cl	1.0	293	874.1	884.6	10.5	-	44.2	-	Cl
437	CC(C)(C)CC(C)(C)Cl	0.0	332	-	852.6	-	-	42.1	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
438	CC(C)C(C)C(C)(C)Cl	1.0	293	888.0	893.0	5.0	-	44.9	-	Cl
439	CCCC(C)(Cl)C(C)C	0.0	332	834.5	857.3	22.7	-	43.8	-	Cl
440	CC(C)CCC(C)(C)Cl	0.0	332	-	834.6	-	-	43.1	-	Cl
441	CCCC(C)(Cl)CCC	0.0	332	834.8	845.5	10.7	-	44.4	-	Cl
442	CCCCC(C)(Cl)CC	0.0	328	845.6	848.8	3.2	-	44.4	-	Cl
443	CCCCCC(C)(C)Cl	1.0	298	856.8	865.1	8.3	-	46.3	-	Cl
444	CCCCCC(C)(C)Cl	0.0	328	-	839.7	-	-	44.5	-	Cl
445	CC(C)CCCC(C)Cl	0.0	328	-	835.3	-	-	46.1	-	Cl
446	CCCCC(CC)CCl	1.0	293	876.9	879.6	2.7	-	49.3	-	Cl
447	CCCCC(CC)CCl	0.0	337	-	842.6	-	47.4	46.4	-1.0	Cl
448	CCC(C)CCCCCl	0.0	336	-	843.1	-	-	47.3	-	Cl
449	CCCCCCC(C)Cl	1.0	298	861.5	863.3	1.8	-	49.2	-	Cl
450	CCCCCCC(C)Cl	1.0	345	-	824.2	-	47.8	46.2	-1.6	Cl
451	CC(C)(Cl)CCC(C)(C)Cl	0.0	363	-	954.3	-	-	48.1	-	Cl
452	CCC(C)(C)CC(Cl)CCl	1.0	293	1029.0	1042.9	13.9	-	54.6	-	Cl
453	CCCCCC(Cl)C(C)Cl	0.0	368	-	946.7	-	-	50.8	-	Cl
454	CCCCCCC(Cl)CCl	1.0	298	-	1013.7	-	57.6	57.3	-0.3	Cl
455	CCCCCCCC(Cl)Cl	0.0	370	-	936.7	-	-	51.6	-	Cl
456	CCCCCCCC(Cl)Cl	1.0	298	-	1001.6	-	57.7	56.7	-1.0	Cl
457	ClCCCCCCCCCl	1.0	298	1024.8	1028.3	3.5	65.6	63.9	-1.7	Cl
458	CCCCCCCC(Cl)(Cl)Cl	0.1	430	948.0	981.4	33.4	-	50.3	-	Cl
459	CCC(Cl)(CC)C(C)(C)C	0.0	344	-	883.5	-	-	47.0	-	Cl
460	CCCC(C)(Cl)C(C)(C)C	0.0	340	858.2	879.0	20.7	-	47.8	-	Cl
461	CCCCC(Cl)(CC)CC	0.0	351	836.3	837.9	1.6	-	46.9	-	Cl
462	CCCCC(C)(Cl)CCC	0.0	347	827.0	834.3	7.3	-	47.6	-	Cl
463	CCCCCC(C)(Cl)CC	0.0	347	826.8	833.4	6.5	-	47.5	-	Cl
464	CCCCCC(Cl)C(C)C	1.0	293	856.6	871.2	14.6	-	52.5	-	Cl
465	CCCCC(Cl)CCCC	0.0	351	815.6	822.6	7.0	-	49.5	-	Cl
466	CCCCCCC(Cl)CC	0.0	352	807.5	821.7	14.1	-	49.6	-	Cl
467	CCCCCCCC(C)Cl	1.0	293	879.0	867.5	-11.5	-	54.0	-	Cl
468	CCCCCCCCCCl	1.0	298	867.4	871.8	4.4	55.9	55.5	-0.4	Cl
469	CC(C)(Cl)CCCC(C)(C)Cl	0.0	374	-	930.4	-	-	51.6	-	Cl
470	CCCCCCCC(Cl)CCl	1.0	298	-	1000.7	-	62.1	61.7	-0.4	Cl
471	CCCCCCCCCC(Cl)Cl	0.1	436	-	867.8	-	-	50.8	-	Cl
472	CCCCCCCCCC(Cl)Cl	1.0	298	-	990.3	-	62.3	60.9	-1.4	Cl
473	ClCCCCCCCCCCl	1.0	298	1017.3	1014.2	-3.1	-	68.1	-	Cl
474	ClCCCCCCCCCCl	0.1	453	-	881.2	-	54.6	55.8	1.2	Cl
475	CCCCCCCCC(Cl)(Cl)Cl	0.1	449	914.4	948.5	34.1	-	52.7	-	Cl
476	CCCCCCCCCC(C)Cl	1.0	293	870.6	867.5	-3.1	-	58.2	-	Cl
477	CCCCCCCCCCCl	1.0	298	865.8	871.7	5.8	64.0	59.9	-4.1	Cl
478	CCCCCCCCCC(Cl)Cl	0.1	456	-	844.0	-	-	52.9	-	Cl
479	CCCCCCCCCC(Cl)Cl	1.0	430	-	868.2	-	56.9	54.9	-2.0	Cl
480	ClCCCCCCCCCCCl	1.0	298	992.9	1002.4	9.5	73.1	72.4	-0.7	Cl
481	CCCCCCCCCC(Cl)(Cl)Cl	0.1	439	917.0	948.4	31.4	52.5	56.9	4.4	Cl
482	CCC(C)CF	1.0	302	-	779.8	-	30.7	30.8	0.1	F
483	CC(C)CCF	1.0	293	694.1	789.1	95.0	-	31.4	-	F
484	CC(C)CCF	0.4	298	-	783.2	-	-	31.2	-	F
485	CCCCCF	0.2	298	-	786.4	-	30.9	32.2	1.3	F
486	CC(F)C(C)(C)F	0.1	298	-	882.2	-	-	29.3	-	F
487	CC(C)C(C)(F)F	0.1	298	-	869.4	-	-	28.7	-	F
488	CC(C)(CF)CF	0.1	298	-	959.9	-	-	35.9	-	F
489	CCC(C)(F)CF	0.1	298	-	905.2	-	-	30.5	-	F
490	CCC(F)(F)CC	1.0	293	910.6	869.8	-40.8	-	29.3	-	F
491	CCC(F)(F)CC	1.0	277	-	888.9	-	33.8	30.1	-3.7	F
492	CC(C)(F)CCF	0.1	298	-	915.5	-	-	33.3	-	F
493	CCCC(C)(F)F	1.0	293	898.7	861.9	-36.8	-	29.3	-	F
494	CCCC(C)(F)F	1.0	277	-	881.1	-	33.7	30.1	-3.6	F
495	CC(F)C(C)CF	0.1	298	-	928.1	-	-	35.0	-	F
496	CCC(C)C(F)F	0.1	298	-	899.9	-	-	32.1	-	F
497	CC(C)C(F)CF	0.1	298	-	915.6	-	-	32.2	-	F
498	CCC(F)C(C)F	0.1	298	-	894.3	-	-	31.2	-	F
499	CC(C)CC(F)F	0.1	298	-	895.4	-	-	32.2	-	F
500	CC(F)CC(C)F	0.1	298	-	893.1	-	-	33.4	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
501	CC(CF)CCF	0.1	298	-	957.9	-	-	38.8	-	F
502	CCC(F)CCF	0.1	298	-	927.3	-	-	35.6	-	F
503	CCCC(F)CF	0.1	298	-	915.0	-	-	33.3	-	F
504	CC(F)CCCF	0.1	298	-	931.9	-	-	37.9	-	F
505	CCCCC(F)F	0.1	298	-	897.0	-	-	33.2	-	F
506	CCCCC(F)F	1.0	283	-	914.6	-	34.4	34.0	-0.4	F
507	FCCCCCF	1.0	298	957.2	960.9	3.7	-	40.7	-	F
508	FCCCCCF	0.0	298	-	960.7	-	-	40.6	-	F
509	CC(C)CC(F)(F)F	1.0	298	978.8	951.3	-27.5	-	28.4	-	F
510	CCCCC(F)(F)F	1.0	293	970.1	958.9	-11.2	-	29.6	-	F
511	CCCCC(F)(F)F	0.3	298	-	951.7	-	-	29.3	-	F
512	CCC(C)(C)CF	0.1	298	-	812.7	-	-	34.5	-	F
513	CC(C)(C)CCF	1.0	293	780.9	815.8	34.9	-	35.2	-	F
514	CC(C)(C)CCF	0.1	298	-	810.5	-	-	34.9	-	F
515	CC(C)C(C)CF	0.1	298	-	801.7	-	-	34.6	-	F
516	CCC(C)C(C)F	0.1	298	-	783.6	-	-	33.7	-	F
517	CCC(F)C(C)C	0.1	298	-	778.3	-	-	33.8	-	F
518	CC(C)CC(C)F	0.1	298	-	774.7	-	-	33.9	-	F
519	CCC(C)CCF	0.1	298	-	800.8	-	-	35.6	-	F
520	CCCC(C)CF	0.1	298	-	795.0	-	-	35.5	-	F
521	CCCC(F)CC	0.1	298	-	777.3	-	-	34.7	-	F
522	CCCC(F)CC	1.0	296	-	780.0	-	36.8	34.8	-2.0	F
523	CC(C)CCCF	0.1	298	-	795.2	-	-	35.8	-	F
524	CCCCC(C)F	0.1	298	-	776.3	-	-	34.8	-	F
525	CCCCCCF	0.1	298	-	797.7	-	35.6	36.6	1.1	F
526	CCCCCC(F)F	0.1	310	-	881.8	-	-	37.0	-	F
527	CCCCCC(F)F	1.0	305	-	887.7	-	37.7	37.3	-0.4	F
528	CCCCCC(F)(F)F	1.0	293	960.8	953.8	-7.0	-	34.2	-	F
529	CCCCCC(F)(F)F	0.1	298	-	947.4	-	-	33.9	-	F
530	CCCCCCC(F)F	1.0	293	-	897.2	-	-	42.5	-	F
531	CCCCCCC(F)F	1.0	326	-	865.5	-	41.1	40.5	-0.6	F
532	CCCCCCC(F)(F)F	0.1	317	-	922.6	-	-	37.4	-	F
533	CCCCCCCCF	1.0	322	-	792.7	-	44.1	44.3	0.2	F
534	CCCCCCCC(F)F	0.1	365	-	828.0	-	-	42.2	-	F
535	CCCCCCCC(F)F	1.0	344	-	848.1	-	44.2	43.5	-0.7	F
536	CCCCCCCC(F)(F)F	0.1	341	-	893.7	-	-	40.1	-	F
537	CCCCCCCCCF	1.0	293	-	822.0	-	-	50.6	-	F
538	CCCCCCCCCF	1.0	348	-	777.8	-	46.8	46.9	0.1	F
539	CCCCCCCCC(F)F	0.1	389	-	806.6	-	-	44.4	-	F
540	CCCCCCCCC(F)F	1.0	362	-	832.0	-	47.2	46.2	-1.0	F
541	CCCCCCCCC(F)(F)F	1.0	293	935.7	939.2	3.5	-	47.3	-	F
542	CCCCCCCCC(F)(F)F	0.1	363	-	868.3	-	-	42.6	-	F
543	CCCCCCCCCCF	1.0	293	819.4	825.9	6.5	-	55.0	-	F
544	CCCCCCCCCCF	1.0	357	-	776.5	-	50.4	50.5	0.1	F
545	CCCCCCCCCC(F)F	0.1	412	-	787.5	-	-	46.7	-	F
546	CCCCCCCCCC(F)F	1.0	379	-	817.4	-	50.2	49.0	-1.2	F
547	CCCCCCCCCC(F)(F)F	0.1	385	-	846.6	-	-	44.8	-	F
548	CCC(C)CI	0.0	310	1496.8	1499.6	2.9	43.1	42.2	-0.9	I
549	CC(I)C(C)(C)I	0.0	378	-	2065.4	-	-	53.2	-	I
550	CC(C)(CI)CI	0.0	385	-	2077.2	-	-	54.4	-	I
551	CCC(C)(I)CI	0.0	392	-	2051.5	-	-	53.6	-	I
552	CCC(I)(I)CC	0.0	386	-	2046.5	-	-	52.6	-	I
553	CC(C)(I)CCI	0.0	381	-	2051.6	-	-	55.6	-	I
554	CCCC(C)(I)I	0.0	386	-	2024.6	-	-	53.3	-	I
555	CCC(C)C(I)I	0.0	386	-	2023.9	-	-	53.4	-	I
556	CC(C)C(I)CI	0.0	378	-	2038.3	-	-	54.6	-	I
557	CCC(I)C(C)I	0.0	389	-	2012.6	-	-	53.2	-	I
558	CC(C)CC(I)I	0.0	389	-	1993.7	-	-	53.8	-	I
559	CC(I)CC(C)I	0.0	392	-	1985.6	-	-	53.1	-	I
560	CC(CI)CCI	0.0	398	-	2012.8	-	-	55.8	-	I
561	CCC(I)CCI	0.0	400	1966.0	1998.8	32.8	-	54.8	-	I
562	CCCC(I)CI	0.0	397	1961.6	1995.7	34.1	-	54.4	-	I
563	CC(I)CCCI	0.0	403	1970.4	1985.3	14.9	-	55.2	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
564	CCCCC(I)I	0.0	394	1962.8	1988.0	25.2	-	54.5	-	I
565	ICCCCCI	0.0	406	-	1996.7	-	59.7	57.0	-2.7	I
566	CCCCC(I)(I)I	0.0	469	-	2346.7	-	-	63.7	-	I
567	CCC(C)(C)CI	0.0	319	1393.3	1451.8	58.4	-	45.2	-	I
568	CC(C)(C)CCI	0.0	324	1387.2	1429.8	42.5	-	46.2	-	I
569	CC(C)C(C)CI	0.0	326	1385.2	1421.1	36.0	-	45.4	-	I
570	CCC(C)C(C)I	0.0	332	1376.8	1404.7	28.0	-	44.2	-	I
571	CCC(I)C(C)C	0.0	319	1393.3	1416.1	22.8	-	44.5	-	I
572	CC(C)CC(C)I	0.0	319	1393.3	1400.4	7.1	-	44.7	-	I
573	CCC(CC)CI	1.0	296	1440.0	1452.9	12.9	-	47.2	-	I
574	CCC(C)CCI	0.0	333	1349.7	1402.9	53.2	-	46.1	-	I
575	CCCC(C)CI	0.0	328	-	1405.8	-	-	45.8	-	I
576	CCCC(I)CC	0.0	328	1382.1	1397.1	15.1	-	45.1	-	I
577	CC(C)CCCI	1.0	293	1428.3	1444.5	16.2	-	48.3	-	I
578	CC(C)CCCI	0.0	332	-	1394.9	-	-	46.1	-	I
579	CCCCC(C)I	0.0	329	-	1390.6	-	-	45.4	-	I
580	CCCCCC(I)I	0.0	410	-	1848.3	-	-	57.4	-	I
581	ICCCCCCI	0.0	402	-	1886.9	-	-	61.2	-	I
582	CCCC(I)CCC	0.1	387	-	1271.8	-	-	46.1	-	I
583	CCCCC(I)CC	1.0	295	1365.6	1382.2	16.6	-	51.3	-	I
584	CCCCC(I)CC	0.0	349	-	1317.8	-	-	48.2	-	I
585	CCCCCC(C)I	0.0	349	1285.9	1313.2	27.3	-	48.7	-	I
586	CCCCCCC(I)I	0.1	491	-	1638.4	-	-	56.2	-	I
587	CCCCCCC(C)I	1.0	299	1316.4	1326.2	9.8	-	56.1	-	I
588	CCCCCCC(C)I	0.1	406	-	1205.9	-	-	49.6	-	I
589	CCCCCCCC(I)I	0.0	442	-	1636.9	-	-	63.1	-	I
590	ICCCCCCCCI	0.0	453	-	1643.6	-	-	65.5	-	I
591	CCCCCCCCCI	1.0	298	1283.6	1297.1	13.5	64.5	62.9	-1.6	I
592	CCCCCCCCC(C)I	1.0	298	1241.2	1256.4	15.2	-	65.2	-	I
593	CCCCCCCCCI	1.0	293	1256.7	1268.7	12.0	69.8	67.9	-1.9	I
594	FCCCCCCl	0.0	325	1006.0	1006.0	-0.0	-	44.3	-	Mix
595	FCCCCCCCl	0.0	353	962.2	958.4	-3.8	-	46.6	-	Mix
596	FCCCCCCCCl	0.1	379	923.4	920.3	-3.2	-	48.9	-	Mix
597	FCCCCCCCCCCl	0.1	426	870.8	860.6	-10.1	-	53.0	-	Mix
598	FCCCCCCCCCCCl	0.1	447	851.5	835.9	-15.5	-	55.0	-	Mix

Table S18: Comparison of experimental and simulated properties validation using the SH/EEM-M scheme.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	BrCBr	0.1	298	2482.0	2435.4	-46.6	-	35.4	-	Br
2	BrCBr	1.0	298	-	2436.4	-	37.0	35.4	-1.6	Br
3	BrC(Br)Br	1.0	298	2877.2	2856.8	-20.4	46.1	45.0	-1.1	Br
4	BrC(Br)(Br)Br	1.0	374	2953.3	2959.1	5.8	-	50.1	-	Br
5	BrC(Br)(Br)Br	1.0	384	-	2934.8	-	48.2	49.6	1.4	Br
6	CC(Br)Br	1.0	316	-	2035.4	-	39.6	37.0	-2.6	Br
7	BrCC(Br)Br	1.0	321	-	2547.5	-	52.9	52.0	-0.9	Br
8	CC(C)(Br)Br	0.0	298	1820.0	1844.9	24.9	37.3	39.4	2.0	Br
9	CCC(Br)Br	0.0	302	1968.8	1887.6	-81.2	43.1	41.8	-1.3	Br
10	CC(Br)(Br)CBr	0.0	349	-	2247.8	-	47.5	52.0	4.5	Br
11	BrCC(Br)CBr	0.0	374	-	2262.1	-	52.1	55.0	2.9	Br
12	BrCCC(Br)Br	1.0	290	2350.0	2363.4	13.4	-	56.2	-	Br
13	CC(C)(Br)CBr	1.0	293	1760.4	1778.3	17.9	-	45.2	-	Br
14	CC(C)(Br)CBr	0.0	322	-	1736.0	-	41.8	43.6	1.8	Br
15	CCC(C)(Br)Br	0.0	318	1718.7	1718.3	-0.4	41.0	43.0	2.0	Br
16	CC(C)C(Br)Br	0.0	321	1733.3	1730.8	-2.6	-	44.4	-	Br
17	CC(Br)C(C)Br	1.0	295	1789.3	1777.3	-12.0	-	45.8	-	Br
18	CC(Br)C(C)Br	0.0	325	-	1731.9	-	43.0	44.3	1.3	Br
19	CC(Br)CCBr	0.0	343	-	1708.8	-	45.1	45.8	0.8	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
20	CCCC(Br)Br	1.0	298	1784.0	1757.0	-27.0	-	47.0	-	Br
21	CCCC(Br)Br	1.0	357	-	1667.1	-	45.8	44.0	-1.8	Br
22	BrCCCCBr	1.0	298	1818.8	1801.7	-17.2	52.6	51.7	-0.9	Br
23	CC(Br)C(C)(Br)Br	1.0	293	2172.4	2185.6	13.2	-	57.1	-	Br
24	CC(Br)C(C)(Br)Br	1.0	326	-	2134.7	-	51.7	55.2	3.5	Br
25	CCC(Br)(Br)CBr	1.0	293	2168.5	2193.7	25.2	-	58.4	-	Br
26	CCC(Br)(Br)CBr	1.0	329	-	2135.7	-	50.7	55.9	5.2	Br
27	CC(Br)C(Br)CBr	1.0	293	2183.5	2207.5	24.0	-	62.9	-	Br
28	CC(Br)C(Br)CBr	1.0	333	-	2143.5	-	51.3	59.7	8.4	Br
29	CCC(Br)C(Br)Br	1.0	293	2183.5	2177.4	-6.1	-	59.0	-	Br
30	CCC(Br)C(Br)Br	0.0	369	-	2057.3	-	51.1	54.5	3.4	Br
31	BrCC(CBr)CBr	1.0	490	-	1902.8	-	66.1	50.3	-15.8	Br
32	BrCCC(Br)CBr	1.0	298	2210.0	2201.4	-8.6	-	61.9	-	Br
33	BrCCC(Br)CBr	1.0	405	-	2031.0	-	53.5	55.6	2.1	Br
34	CC(C)(C)CBr	1.0	308	-	1208.6	-	35.6	38.6	3.0	Br
35	CC(C)C(C)Br	0.0	298	1215.6	1205.3	-10.2	-	37.9	-	Br
36	CC(C)C(C)Br	1.0	316	-	1182.4	-	37.2	37.0	-0.2	Br
37	CCC(Br)CC	0.0	298	-	1200.8	-	39.3	38.3	-1.0	Br
38	CC(Br)C(C)(C)C	0.0	298	1169.8	1192.9	23.2	-	42.7	-	Br
39	CC(Br)C(C)(C)C	1.0	330	-	1157.5	-	39.5	41.1	1.6	Br
40	CC(C)C(C)(C)Br	1.0	292	1187.4	1189.0	1.6	-	41.4	-	Br
41	CCCC(C)(C)Br	1.0	293	1180.4	1167.4	-13.0	-	41.8	-	Br
42	ClCCl	1.0	298	1316.4	1296.4	-20.0	28.8	26.9	-1.9	Cl
43	ClC(Cl)Cl	1.0	298	1479.5	1494.6	15.1	31.1	31.4	0.3	Cl
44	ClC(Cl)(Cl)Cl	1.0	298	1584.3	1599.2	14.9	-	34.4	-	Cl
45	ClC(Cl)(Cl)Cl	0.1	298	-	1597.5	-	32.4	34.4	2.0	Cl
46	CC(C)Cl	0.7	298	-	851.4	-	26.4	26.9	0.5	Cl
47	CCCCl	1.0	298	884.1	877.4	-6.7	28.5	28.3	-0.2	Cl
48	CC(C)(Cl)Cl	0.2	298	1107.3	1079.0	-28.3	-	32.7	-	Cl
49	CC(C)(Cl)Cl	1.0	298	-	1077.0	-	32.1	32.6	0.5	Cl
50	CCC(Cl)Cl	0.1	298	1126.0	1118.8	-7.2	-	34.8	-	Cl
51	CCC(Cl)Cl	1.0	298	-	1119.4	-	35.2	34.9	-0.3	Cl
52	CC(Cl)(Cl)CCl	0.0	298	1317.9	1329.3	11.5	40.5	43.4	2.9	Cl
53	CCC(Cl)(Cl)Cl	1.0	298	1283.6	1284.6	1.0	-	38.6	-	Cl
54	CCC(Cl)(Cl)Cl	1.0	259	-	1334.0	-	38.8	40.5	1.7	Cl
55	CC(Cl)C(Cl)Cl	1.0	289	1353.0	1351.7	-1.3	-	44.9	-	Cl
56	CC(Cl)C(Cl)Cl	0.0	302	-	1336.5	-	42.3	44.1	1.7	Cl
57	ClCC(Cl)CCl	1.0	298	1388.8	1385.0	-3.8	46.8	48.9	2.1	Cl
58	ClCCC(Cl)Cl	1.0	293	1355.5	1352.7	-2.8	-	44.3	-	Cl
59	ClCCC(Cl)Cl	0.0	313	-	1328.2	-	44.2	43.3	-0.9	Cl
60	CC(C)(Cl)CCl	0.0	298	1089.0	1092.8	3.8	36.8	37.4	0.6	Cl
61	CCC(C)(Cl)Cl	0.1	298	1065.1	1069.8	4.8	-	37.3	-	Cl
62	CCC(C)(Cl)Cl	1.0	298	-	1069.3	-	36.7	37.3	0.6	Cl
63	CC(C)C(Cl)Cl	0.0	298	1100.1	1091.8	-8.3	36.5	39.4	2.9	Cl
64	CC(Cl)C(C)Cl	0.0	298	-	1098.8	-	38.5	41.6	3.1	Cl
65	CC(CCl)CCl	0.0	307	1090.0	1111.8	21.7	-	41.7	-	Cl
66	CC(CCl)CCl	1.0	285	-	1136.8	-	45.1	43.0	-2.1	Cl
67	CC(Cl)CCCl	1.0	298	1108.3	1105.2	-3.1	42.1	41.4	-0.7	Cl
68	CCCC(Cl)Cl	0.0	298	1080.1	1087.0	6.9	-	40.6	-	Cl
69	CCCC(Cl)Cl	1.0	298	-	1087.4	-	39.4	40.6	1.2	Cl
70	CC(C)(Cl)C(Cl)Cl	1.0	298	1267.7	1281.5	13.8	-	46.5	-	Cl
71	CC(Cl)C(C)(Cl)Cl	1.0	291	1263.0	1285.4	22.4	-	47.5	-	Cl
72	CC(Cl)C(C)(Cl)Cl	0.0	310	-	1264.2	-	42.7	46.3	3.6	Cl
73	CC(Cl)(CCl)CCl	1.0	298	1301.2	1308.4	7.2	-	49.0	-	Cl
74	CC(Cl)(CCl)CCl	0.0	327	-	1276.8	-	45.9	47.1	1.2	Cl
75	CCCC(Cl)(Cl)Cl	0.0	298	1231.0	1239.1	8.2	-	45.3	-	Cl
76	CC(CCl)C(Cl)Cl	0.0	312	1251.1	1277.1	26.0	-	46.9	-	Cl
77	CC(Cl)C(Cl)CCl	1.0	293	1316.4	1308.5	-7.9	-	50.7	-	Cl
78	CC(Cl)C(Cl)CCl	1.0	288	-	1313.8	-	41.3	51.0	9.7	Cl
79	CC(Cl)CC(Cl)Cl	1.0	288	1317.0	1282.9	-34.1	-	48.2	-	Cl
80	CC(Cl)CC(Cl)Cl	0.0	318	-	1248.4	-	43.9	46.6	2.7	Cl
81	ClCCC(Cl)CCl	1.0	293	1317.5	1314.5	-3.0	-	51.0	-	Cl
82	CC(C)(C)CCl	0.1	298	860.9	881.0	20.2	-	36.1	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
83	CC(C)(C)CCl	1.0	294	-	885.8	-	34.9	36.4	1.5	Cl
84	CC(C)C(C)Cl	0.1	298	857.0	868.2	11.1	-	35.0	-	Cl
85	CC(C)C(C)Cl	1.0	300	-	866.4	-	35.9	34.9	-1.0	Cl
86	CCC(Cl)CC	1.0	298	884.0	864.3	-19.7	-	35.4	-	Cl
87	CCC(Cl)CC	1.0	304	-	858.1	-	36.5	35.0	-1.5	Cl
88	CC(C)(C)C(Cl)Cl	0.0	312	1074.8	1076.6	1.8	-	44.6	-	Cl
89	CC(C)C(C)(C)Cl	1.0	298	874.9	881.9	7.0	-	38.7	-	Cl
90	CC(C)C(C)(C)Cl	1.0	316	-	866.1	-	38.0	37.8	-0.2	Cl
91	CCC(C)(Cl)CC	1.0	293	883.9	878.8	-5.1	-	38.5	-	Cl
92	CCCC(C)(C)Cl	0.0	298	858.3	862.3	4.0	37.7	38.7	0.9	Cl
93	FCF	1.0	221	1213.8	1198.0	-15.8	20.9	19.0	-1.9	F
94	FCF	17.6	298	891.6	986.7	95.1	-	15.9	-	F
95	FCF	1.0	298	961.0	977.2	16.2	-	15.8	-	F
96	FC(F)F	1.0	191	1442.9	1576.9	134.0	16.7	18.8	2.1	F
97	FC(F)F	1.0	298	666.7	4.7	-662.0	-	-0.2	-	F
98	FC(F)(F)F	1.0	145	1605.2	1742.3	137.1	12.3	12.8	0.5	F
99	FCCF	1.0	283	1024.0	1051.7	27.7	-	23.7	-	F
100	FCCF	1.8	298	-	1025.5	-	22.5	23.1	0.6	F
101	CC(F)(F)F	12.9	298	-	839.6	-	13.1	14.9	1.8	F
102	FCC(F)F	1.0	314	1175.5	1171.9	-3.6	-	25.5	-	F
103	FCC(F)F	1.0	278	-	1248.0	-	23.2	27.4	4.2	F
104	FCC(F)F	2.0	296	-	1210.7	-	20.6	26.4	5.9	F
105	CC(C)F	1.0	293	723.8	716.0	-7.8	-	21.7	-	F
106	CC(C)F	1.0	249	-	772.9	-	23.7	23.5	-0.2	F
107	CC(C)(F)F	1.0	271	943.8	843.1	-100.6	22.6	22.4	-0.2	F
108	CC(C)(F)F	2.1	291	911.4	813.1	-98.3	21.6	21.6	0.1	F
109	CC(F)CF	1.4	298	960.0	933.2	-26.8	-	24.5	-	F
110	CCC(F)F	1.3	298	920.1	907.3	-12.8	23.7	25.0	1.2	F
111	CCC(F)(F)F	0.9	259	1148.2	984.0	-164.2	21.8	22.0	0.2	F
112	CC(C)(C)F	1.0	237	-	770.1	-	27.6	25.7	-1.9	F
113	CC(C)CF	0.9	286	764.5	778.3	13.9	-	27.5	-	F
114	CC(C)CF	1.4	298	750.0	765.1	15.1	-	27.0	-	F
115	CCC(C)F	1.0	248	-	799.5	-	29.2	28.1	-1.1	F
116	CCCCF	1.0	237	-	839.1	-	30.1	30.8	0.7	F
117	CCC(C)(F)F	1.0	293	915.9	845.0	-70.9	-	26.2	-	F
118	CCC(C)(F)F	0.8	298	-	838.2	-	25.9	25.9	0.0	F
119	CCCC(F)F	0.4	298	910.1	916.9	6.8	-	31.5	-	F
120	CCCC(F)F	1.0	261	-	962.3	-	31.0	33.3	2.3	F
121	FCCCCF	0.1	298	-	972.0	-	34.6	34.4	-0.2	F
122	CCC(C)(C)F	0.4	298	-	740.6	-	29.4	27.8	-1.5	F
123	CC(C)(C)C(F)(F)F	1.0	293	990.5	1007.7	17.2	-	36.7	-	F
124	IC(I)I	0.0	396	3685.6	3416.8	-268.8	47.9	54.9	7.0	I
125	IC(I)(I)I	0.0	447	3819.2	3647.0	-172.2	-	65.7	-	I
126	CCI	0.2	298	-	1911.7	-	31.7	31.1	-0.6	I
127	CC(I)I	0.0	336	2682.9	2645.9	-37.0	-	44.8	-	I
128	ICCI	0.0	356	2551.8	2682.7	130.8	48.1	48.1	-0.0	I
129	CCCI	0.1	298	-	1731.1	-	36.0	35.4	-0.6	I
130	CC(C)(I)I	0.0	352	2379.7	2307.6	-72.1	-	45.1	-	I
131	CC(I)CI	0.0	330	2506.9	2447.2	-59.8	-	50.9	-	I
132	CCC(I)I	0.0	357	2370.2	2374.9	4.7	-	47.7	-	I
133	CC(C)CI	1.0	298	-	1601.0	-	38.8	38.6	-0.1	I
134	CC(C)(I)CI	0.0	370	2163.1	2192.6	29.5	-	50.1	-	I
135	CCC(C)(I)I	0.0	370	2163.1	2179.1	16.0	-	49.1	-	I
136	CC(C)C(I)I	0.0	365	2171.2	2189.9	18.8	-	50.1	-	I
137	CC(I)C(C)I	0.0	374	2155.0	2172.0	17.0	-	50.6	-	I
138	CC(CI)CI	0.0	374	2155.0	2195.9	40.9	-	52.4	-	I
139	CCC(I)CI	0.0	371	2160.5	2188.4	28.0	-	52.1	-	I
140	CC(I)CCI	0.0	382	2141.4	2162.4	21.0	-	51.9	-	I
141	CCCC(I)I	0.0	373	2144.3	2161.0	16.7	-	51.1	-	I
142	CCC(C)(C)I	1.0	323	-	1475.3	-	40.4	39.6	-0.8	I
143	CC(I)C(C)(C)C	0.0	320	1392.3	1441.3	49.0	-	44.6	-	I
144	CC(C)C(C)(C)I	1.0	293	1448.0	1470.2	22.2	-	45.0	-	I
145	CCC(C)(I)CC	0.0	319	1393.3	1433.7	40.4	-	44.0	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
146	CCCC(C)(C)I	0.0	332	1376.8	1396.8	20.0	-	43.7	-	I
147	ClCBr	1.0	298	1924.9	1898.1	-26.7	-	31.3	-	Mix
148	ClCBr	1.0	304	-	1885.5	-	33.5	31.1	-2.4	Mix
149	FCCl	1.0	260	1282.1	1260.9	-21.2	21.9	23.1	1.2	Mix
150	BrCI	1.0	290	2926.0	2859.5	-66.5	-	40.7	-	Mix
151	ClCI	1.0	293	2422.0	2389.8	-32.2	-	36.8	-	Mix
152	FC(F)Br	1.0	298	1775.5	1969.7	194.2	-	25.7	-	Mix
153	FC(F)Br	1.0	244	-	2140.7	-	24.0	28.1	4.1	Mix
154	FC(F)Cl	1.0	233	1408.0	1474.2	66.2	20.2	22.5	2.3	Mix
155	FC(F)Cl	10.8	298	1193.0	1290.3	97.3	-	19.7	-	Mix
156	FC(Cl)Cl	1.8	298	1367.0	1415.3	48.3	-	25.8	-	Mix
157	FC(Cl)Cl	1.0	267	-	1481.1	-	26.1	27.1	1.0	Mix
158	FC(I)I	1.0	295	3196.9	3221.5	24.6	-	46.6	-	Mix
159	FC(I)I	1.0	314	-	3169.5	-	32.9	45.7	12.8	Mix
160	FC(F)I	1.0	272	-	2584.6	-	26.0	33.5	7.5	Mix
161	FC(Br)Br	1.0	293	2421.0	2509.5	88.5	-	35.9	-	Mix
162	ClC(Cl)Br	1.0	298	1983.5	1991.4	7.9	-	36.3	-	Mix
163	ClC(Br)Br	1.0	293	2451.0	2455.5	4.5	-	41.0	-	Mix
164	ClC(Cl)(Cl)Br	1.0	298	2002.1	2019.2	17.0	-	39.4	-	Mix
165	ClC(Cl)(Cl)Br	0.1	298	-	2019.2	-	36.1	39.4	3.2	Mix
166	ClC(Cl)(Br)Br	1.0	298	2420.0	2413.3	-6.7	-	44.2	-	Mix
167	ClC(Br)(Br)Br	1.0	288	2710.0	2803.3	93.3	-	49.5	-	Mix
168	FC(F)(F)Br	1.0	215	1989.9	2389.7	399.8	17.5	25.0	7.5	Mix
169	FC(F)(F)Br	16.6	298	1536.1	1786.5	250.4	-	19.2	-	Mix
170	FC(Br)(Br)Br	1.0	330	-	2709.5	-	34.4	40.8	6.4	Mix
171	FC(F)(Br)Br	1.0	298	2251.2	2370.1	118.8	25.0	30.9	6.0	Mix
172	FC(F)(F)Cl	1.0	190	1527.8	1800.5	272.7	15.4	19.6	4.2	Mix
173	FC(F)(Cl)Cl	1.0	243	1488.0	1492.2	4.2	20.1	22.5	2.4	Mix
174	FC(F)(Cl)Cl	6.7	298	1307.0	1342.3	35.3	-	20.3	-	Mix
175	FC(Cl)(Cl)Cl	1.1	298	1477.0	1493.2	16.2	24.9	27.4	2.6	Mix
176	FC(F)(F)I	20.0	298	2046.8	2305.4	258.6	-	26.0	-	Mix
177	FC(F)(F)I	1.0	281	-	2388.5	-	22.5	26.9	4.4	Mix
178	FC(Cl)Br	1.0	273	1977.1	2043.7	66.6	-	32.0	-	Mix
179	FC(F)(Cl)Br	1.0	269	1899.6	1949.8	50.2	23.1	26.8	3.7	Mix
180	FC(F)(Cl)Br	2.6	298	1810.0	1867.8	57.9	-	25.7	-	Mix
181	FC(Cl)(Cl)Br	1.0	295	1950.0	1960.8	10.8	-	32.6	-	Mix
182	FC(Cl)(Cl)Br	0.4	298	-	1954.2	-	29.1	32.5	3.4	Mix
183	FC(Cl)(Br)Br	1.0	295	2317.3	2394.3	77.0	-	37.6	-	Mix
184	CC(Cl)Br	1.0	305	-	1623.6	-	33.1	33.8	0.7	Mix
185	CC(F)Cl	1.4	298	-	1052.5	-	23.7	25.3	1.6	Mix
186	FCCCl	1.0	303	-	1142.5	-	32.1	28.7	-3.4	Mix
187	CC(F)(F)Cl	1.0	263	-	1147.4	-	22.7	22.9	0.2	Mix
188	FCC(F)Cl	0.8	298	-	1304.2	-	26.6	30.9	4.4	Mix
189	FC(F)CCl	1.0	288	1312.0	1323.9	11.9	-	32.7	-	Mix
190	FC(F)CCl	0.7	298	-	1308.5	-	26.6	32.3	5.7	Mix
191	CC(F)(Cl)Cl	0.8	298	-	1214.1	-	26.0	27.5	1.4	Mix
192	FC(Cl)CCl	0.1	298	-	1380.1	-	32.8	36.9	4.2	Mix
193	ClC(Cl)(Br)CBr	1.0	273	2298.0	2316.3	18.3	-	56.0	-	Mix
194	ClC(Cl)(Br)CBr	1.0	369	-	2149.8	-	45.9	50.1	4.2	Mix
195	ClC(Br)C(Cl)Br	1.0	293	2135.0	2314.9	179.9	-	55.3	-	Mix
196	ClC(Br)C(Cl)Br	1.0	335	-	2239.7	-	45.9	52.8	6.9	Mix
197	FC(F)(Cl)CCl	0.4	298	-	1408.2	-	28.3	34.3	6.0	Mix
198	FC(Cl)C(F)Cl	0.4	298	1405.4	1492.5	87.1	-	35.3	-	Mix
199	FC(F)(F)CBr	1.0	293	1788.1	1758.0	-30.1	-	32.9	-	Mix
200	FC(F)(F)CCl	1.9	298	-	1292.4	-	22.3	28.4	6.1	Mix
201	FC(Cl)(Cl)CCl	0.1	298	-	1497.9	-	34.7	40.3	5.6	Mix
202	FCC(Cl)(Cl)Cl	0.1	298	1575.0	1523.7	-51.3	-	40.3	-	Mix
203	FC(Cl)C(Cl)Cl	0.0	298	-	1544.9	-	36.9	40.6	3.7	Mix
204	ClCCCBr	1.0	341	-	1507.3	-	42.0	40.0	-2.0	Mix
205	CC(C)(F)Cl	0.1	298	-	952.8	-	31.5	26.9	-4.6	Mix
206	CC(F)(F)CCl	0.4	298	1191.6	1131.9	-59.7	-	31.4	-	Mix
207	FC(F)(F)CCCl	0.5	298	1290.1	1205.9	-84.1	-	28.7	-	Mix
208	FC(F)(F)CCCl	1.0	306	-	1192.4	-	29.9	28.4	-1.5	Mix

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
209	FCCCCCl	0.0	298	1062.7	1055.8	-7.0	-	39.7	-	Mix
210	CC(CI)C(F)(F)F	1.0	313	-	1817.1	-	30.4	45.1	14.7	Mix
211	CC(I)CC(F)(F)F	1.0	312	-	1781.5	-	32.4	44.5	12.1	Mix
212	CCC(C)CBr	1.0	321	-	1187.1	-	37.9	38.4	0.5	Br
213	CC(C)CCBr	0.0	298	-	1210.7	-	39.7	40.1	0.4	Br
214	CC(Br)C(C)(C)Br	1.0	298	1663.0	1685.8	22.8	-	50.8	-	Br
215	CC(Br)C(C)(C)Br	0.0	335	-	1633.6	-	-	48.6	-	Br
216	CC(C)C(C)(Br)Br	0.0	337	1622.0	1623.0	1.0	-	46.7	-	Br
217	CC(C)(CBr)CBr	1.0	293	1693.4	1719.0	25.6	-	52.9	-	Br
218	CC(C)(CBr)CBr	0.0	345	-	1650.3	-	-	49.8	-	Br
219	CCC(C)(Br)CBr	1.0	294	1663.8	1690.6	26.8	-	48.8	-	Br
220	CCC(C)(Br)CBr	0.0	337	-	1632.4	-	-	46.8	-	Br
221	CCC(Br)(Br)CC	0.0	332	1610.0	1617.5	7.5	-	46.4	-	Br
222	CC(C)(Br)CCBr	1.0	273	1696.0	1704.2	8.2	-	52.0	-	Br
223	CC(C)(Br)CCBr	0.0	337	-	1617.5	-	-	48.4	-	Br
224	CCCC(C)(Br)Br	1.0	289	1645.2	1660.0	14.8	-	49.7	-	Br
225	CCCC(C)(Br)Br	0.0	335	-	1598.0	-	-	47.3	-	Br
226	CC(Br)C(C)CBr	0.0	337	1751.0	1631.7	-119.4	-	49.3	-	Br
227	CCC(C)C(Br)Br	0.0	337	1602.8	1615.8	13.1	-	48.3	-	Br
228	CC(C)C(Br)CBr	1.0	293	1677.0	1690.8	13.8	-	50.7	-	Br
229	CC(C)C(Br)CBr	0.0	337	-	1630.7	-	-	48.5	-	Br
230	CCC(Br)C(C)Br	1.0	293	1673.0	1679.1	6.1	-	52.6	-	Br
231	CCC(Br)C(C)Br	0.0	341	-	1612.9	-	-	49.5	-	Br
232	CC(C)CC(Br)Br	0.0	337	1602.8	1601.8	-0.9	-	49.1	-	Br
233	CC(Br)CC(C)Br	1.0	293	1665.9	1656.5	-9.4	-	50.3	-	Br
234	CC(Br)CC(C)Br	0.0	344	-	1586.0	-	-	47.5	-	Br
235	CC(CBr)CCBr	1.0	293	1711.5	1700.9	-10.6	-	55.2	-	Br
236	CC(CBr)CCBr	0.0	337	-	1640.4	-	-	52.5	-	Br
237	CCC(Br)CCBr	1.0	293	1665.3	1680.3	15.0	-	52.3	-	Br
238	CCC(Br)CCBr	0.0	351	-	1600.2	-	-	49.1	-	Br
239	CC(Br)CCCBr	1.0	293	1683.0	1679.2	-3.8	-	54.4	-	Br
240	CC(Br)CCCBr	1.0	392	-	1541.7	-	51.8	48.5	-3.3	Br
241	CCCCC(Br)Br	0.0	343	1588.3	1590.1	1.7	-	49.3	-	Br
242	CCCCC(Br)Br	1.0	375	-	1545.3	-	48.8	47.6	-1.2	Br
243	BrCCCCCBr	1.0	298	1694.0	1687.3	-6.7	-	56.2	-	Br
244	BrCCCCCBr	1.0	411	-	1531.9	-	54.4	49.5	-4.9	Br
245	CC(Br)C(C)(Br)CBr	1.0	293	2082.1	2091.9	9.8	-	63.2	-	Br
246	CC(CBr)(CBr)CBr	1.0	293	2091.7	2115.9	24.2	-	65.1	-	Br
247	CCCCC(Br)(Br)Br	1.0	293	1988.2	2009.0	20.8	-	61.6	-	Br
248	CCCCC(Br)(Br)Br	0.1	427	-	1809.8	-	-	53.5	-	Br
249	BrCCC(Br)CCBr	1.0	292	2065.0	2060.8	-4.2	-	66.6	-	Br
250	BrCCCC(Br)CBr	1.0	295	2073.0	2061.7	-11.3	-	67.9	-	Br
251	CCC(C)(C)CBr	0.0	311	1150.8	1183.3	32.5	-	42.7	-	Br
252	CC(C)(C)CCBr	1.0	293	1155.6	1189.9	34.3	-	44.8	-	Br
253	CC(C)(C)CCBr	0.0	308	-	1173.9	-	-	44.0	-	Br
254	CC(C)C(C)CBr	1.0	298	1190.0	1184.6	-5.4	-	43.3	-	Br
255	CC(C)C(C)CBr	0.0	311	-	1171.2	-	-	42.7	-	Br
256	CCC(C)C(C)Br	0.0	303	1163.1	1169.4	6.3	-	42.3	-	Br
257	CCC(Br)C(C)C	0.0	303	1163.1	1162.9	-0.1	-	41.7	-	Br
258	CC(C)CC(C)Br	0.0	303	1144.3	1153.6	9.3	40.9	42.1	1.2	Br
259	CCC(CC)CBr	0.0	313	1159.9	1163.8	3.9	42.7	43.0	0.3	Br
260	CCC(C)CCBr	1.0	296	1171.0	1180.1	9.1	-	44.7	-	Br
261	CCC(C)CCBr	0.0	317	-	1157.0	-	-	43.5	-	Br
262	CCCC(C)CBr	1.0	293	1177.9	1179.6	1.7	-	44.4	-	Br
263	CCCC(C)CBr	0.0	314	-	1156.3	-	-	43.2	-	Br
264	CCCC(Br)CC	0.0	312	-	1147.2	-	42.5	42.3	-0.2	Br
265	CC(C)CCCBr	1.0	293	1168.3	1176.6	8.3	-	45.2	-	Br
266	CC(C)CCCBr	0.0	316	-	1151.2	-	-	43.9	-	Br
267	CCCCC(C)Br	1.0	298	1159.7	1160.0	0.3	-	43.6	-	Br
268	CCCCC(C)Br	1.0	318	-	1137.7	-	43.8	42.5	-1.3	Br
269	CC(C)(Br)C(C)(C)Br	0.3	435	-	1465.4	-	-	47.2	-	Br
270	CC(C)C(C)(Br)CBr	0.1	400	1450.3	1498.5	48.1	-	47.6	-	Br
271	CC(C)(C)C(Br)CBr	0.1	400	1462.2	1503.9	41.7	-	53.4	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
272	CCCCC(C)(Br)Br	1.0	295	1546.3	1572.9	26.6	-	54.4	-	Br
273	CCCCC(C)(Br)Br	0.1	400	-	1434.8	-	-	48.1	-	Br
274	CC(C)C(CBr)CBr	1.0	293	1605.0	1624.2	19.2	-	57.6	-	Br
275	CC(CBr)C(C)CBr	0.1	400	1465.9	1489.2	23.3	-	51.6	-	Br
276	CCC(Br)C(Br)CC	1.0	293	1602.7	1590.1	-12.6	-	53.7	-	Br
277	CCC(Br)C(Br)CC	0.1	400	-	1451.0	-	-	47.5	-	Br
278	CCCC(Br)C(C)Br	1.0	293	1581.2	1588.7	7.5	-	54.4	-	Br
279	CCCC(Br)C(C)Br	0.1	400	-	1449.9	-	-	48.0	-	Br
280	CC(Br)CCC(C)Br	1.0	293	1578.8	1578.1	-0.7	-	56.5	-	Br
281	CC(Br)CCC(C)Br	0.0	365	-	1485.6	-	49.5	52.0	2.5	Br
282	CCCC(CBr)CBr	1.0	293	1577.1	1611.1	34.0	-	58.3	-	Br
283	CC(CCBr)CCBr	0.1	426	1395.4	1442.1	46.6	50.8	51.7	0.9	Br
284	CCC(Br)CCCBr	0.1	400	1443.8	1455.7	11.9	-	51.2	-	Br
285	CCCCC(Br)CBr	1.0	293	1560.4	1592.7	32.3	56.5	56.5	0.0	Br
286	CC(Br)CCCCBr	0.1	400	1415.4	1453.0	37.6	-	52.2	-	Br
287	CCCCCC(Br)Br	0.1	400	1416.2	1435.4	19.2	-	50.4	-	Br
288	CCCCCC(Br)Br	1.0	393	-	1446.0	-	51.6	50.9	-0.7	Br
289	BrCCCCCCBr	1.0	298	1602.5	1597.0	-5.5	-	60.8	-	Br
290	BrCCCCCCBr	0.0	364	-	1515.1	-	57.1	56.4	-0.6	Br
291	CCC(CBr)(CBr)CBr	1.0	293	1912.2	2013.8	101.6	-	69.8	-	Br
292	CCCC(Br)CCC	1.0	296	1133.0	1134.7	1.7	-	47.7	-	Br
293	CCCC(Br)CCC	0.0	327	-	1101.3	-	-	45.9	-	Br
294	CCCCC(Br)CC	1.0	295	1134.1	1135.2	1.1	-	47.7	-	Br
295	CCCCCC(C)Br	0.0	320	1095.5	1105.2	9.6	46.2	46.7	0.5	Br
296	CCC(Br)(CBr)C(C)C	1.0	293	1526.1	1575.0	48.9	-	58.2	-	Br
297	CC(C)(C)CC(Br)CBr	1.0	293	1502.0	1538.9	36.9	-	58.1	-	Br
298	CCCC(Br)(CC)CBr	1.0	293	1492.9	1550.7	57.8	-	59.2	-	Br
299	CC(C)(CCBr)CCBr	1.0	293	1532.0	1567.7	35.7	-	65.5	-	Br
300	CCCC(Br)C(Br)CC	1.0	293	1516.2	1521.6	5.4	-	58.1	-	Br
301	CCCC(Br)C(Br)CC	0.1	418	-	1367.7	-	-	50.3	-	Br
302	CCCCC(Br)C(C)Br	1.0	293	1513.2	1518.6	5.4	-	58.6	-	Br
303	CCCCC(Br)C(C)Br	0.1	418	-	1364.4	-	-	50.6	-	Br
304	CCC(Br)CCCCBr	0.1	418	-	1372.7	-	-	54.4	-	Br
305	CCCCCC(Br)CBr	1.0	293	1518.0	1520.5	2.5	-	60.9	-	Br
306	CCCCCC(Br)CBr	1.0	300	-	1512.0	-	54.4	60.5	6.1	Br
307	CCCCCCC(Br)Br	1.0	294	1500.0	1506.6	6.6	-	61.9	-	Br
308	CCCCCCC(Br)Br	1.0	410	-	1366.0	-	54.4	54.2	-0.2	Br
309	BrCCCCCCCBr	0.0	385	1469.2	1423.6	-45.6	57.8	59.4	1.6	Br
310	CC(C)CCCC(C)Br	1.0	293	1091.0	1107.9	16.9	-	51.9	-	Br
311	CCCCCCC(C)Br	1.0	298	1096.8	1104.5	7.7	-	52.6	-	Br
312	CCCCCCC(C)Br	1.0	358	-	1044.1	-	48.4	48.8	0.4	Br
313	CCC(C)(C)CC(Br)CBr	1.0	293	1468.9	1494.5	25.6	-	62.4	-	Br
314	CCCC(Br)C(Br)CCC	0.1	435	-	1297.4	-	-	52.7	-	Br
315	CCCCC(Br)CCCBr	0.1	435	-	1301.4	-	-	56.7	-	Br
316	CCCC(Br)CCCCBr	0.1	435	-	1301.9	-	-	57.0	-	Br
317	CCCCCCC(Br)CBr	1.0	293	1458.0	1461.7	3.7	-	65.4	-	Br
318	CCCCCCC(Br)CBr	0.1	435	-	1299.2	-	-	55.9	-	Br
319	CCCCCCCC(Br)Br	0.1	435	-	1289.2	-	-	56.8	-	Br
320	CCCCCCCC(Br)Br	1.0	427	-	1299.4	-	57.1	57.3	0.2	Br
321	BrCCCCCCCCBr	0.0	399	1413.1	1353.4	-59.6	59.6	62.2	2.7	Br
322	CCCCCCCC(C)Br	1.0	298	1076.0	1083.8	7.8	-	57.2	-	Br
323	CCCCCCCCCBr	1.0	298	1084.9	1091.8	6.9	-	59.3	-	Br
324	CCCCCCCCCBr	1.0	391	-	1003.9	-	53.1	52.9	-0.2	Br
325	CCCCCCCC(Br)CBr	1.0	293	1398.0	1413.9	15.9	-	69.9	-	Br
326	CCCCCCCC(Br)CBr	0.1	451	-	1239.8	-	-	58.5	-	Br
327	CCCCCCCCC(Br)Br	0.1	451	-	1231.4	-	-	59.5	-	Br
328	CCCCCCCCC(Br)Br	1.0	442	-	1242.3	-	59.5	60.1	0.6	Br
329	BrCCCCCCCCCBr	1.0	298	1428.0	1417.4	-10.6	-	74.6	-	Br
330	BrCCCCCCCCCBr	0.0	415	-	1293.0	-	61.8	65.2	3.4	Br
331	CCCCCCCCC(C)Br	1.0	298	1047.0	1066.4	19.4	-	61.5	-	Br
332	CCCCCCCCC(C)Br	0.0	383	-	988.3	-	-	55.4	-	Br
333	CCCCCCCCCCBr	1.0	298	1062.5	1073.3	10.9	-	63.8	-	Br
334	CCCCCCCCCCBr	1.0	398	-	982.6	-	56.6	56.4	-0.2	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
335	CCCCCCCCC(Br)CBr	1.0	383	-	1279.9	-	67.0	67.4	0.4	Br
336	CCCCCCCCCC(Br)Br	1.0	457	-	1193.1	-	62.2	63.0	0.8	Br
337	CCC(C)CCl	0.0	298	-	878.4	-	36.3	36.6	0.3	Cl
338	CC(Cl)C(C)(C)Cl	0.0	307	1080.9	1059.9	-21.0	-	40.4	-	Cl
339	CC(C)C(C)(Cl)Cl	0.0	333	1051.1	1033.3	-17.8	-	41.0	-	Cl
340	CC(C)(CCl)CCl	0.0	314	1066.8	1091.9	25.0	-	45.8	-	Cl
341	CCC(C)(Cl)CCl	0.0	306	1061.9	1071.3	9.4	35.9	41.1	5.2	Cl
342	CCC(Cl)(Cl)CC	0.0	303	1043.7	1053.0	9.3	40.3	41.5	1.2	Cl
343	CC(C)(Cl)CCCl	1.0	293	1075.8	1076.1	0.3	-	44.0	-	Cl
344	CC(C)(Cl)CCCl	0.0	314	-	1054.9	-	-	42.9	-	Cl
345	CCCC(C)(Cl)Cl	0.0	299	1034.6	1047.8	13.2	40.0	43.0	3.0	Cl
346	CC(Cl)C(C)CCl	1.0	293	1093.8	1090.9	-2.9	-	45.4	-	Cl
347	CC(Cl)C(C)CCl	0.0	313	-	1071.6	-	-	44.3	-	Cl
348	CCC(C)C(Cl)Cl	0.0	302	1045.7	1068.7	23.0	-	44.5	-	Cl
349	CC(C)C(Cl)CCl	1.0	293	1080.5	1087.9	7.4	-	43.1	-	Cl
350	CC(C)C(Cl)CCl	0.0	312	-	1069.3	-	42.1	42.3	0.1	Cl
351	CCC(Cl)C(C)Cl	1.0	298	1075.0	1075.7	0.7	-	46.9	-	Cl
352	CCC(Cl)C(C)Cl	0.0	309	-	1064.2	-	41.6	46.1	4.5	Cl
353	CC(C)CC(Cl)Cl	1.0	293	1047.3	1070.9	23.6	-	45.9	-	Cl
354	CC(C)CC(Cl)Cl	0.0	302	-	1061.8	-	40.1	45.4	5.3	Cl
355	CC(Cl)CC(C)Cl	1.0	291	1063.0	1066.2	3.2	-	44.2	-	Cl
356	CC(Cl)CC(C)Cl	0.0	317	-	1039.1	-	41.5	42.8	1.2	Cl
357	CC(CCl)CCCl	1.0	294	1103.0	1100.6	-2.4	-	48.9	-	Cl
358	CC(CCl)CCCl	0.0	324	-	1071.0	-	-	47.0	-	Cl
359	CCC(Cl)CCCl	1.0	293	1083.4	1081.9	-1.5	-	45.7	-	Cl
360	CCC(Cl)CCCl	0.0	322	-	1052.5	-	-	44.1	-	Cl
361	CCCC(Cl)CCl	1.0	298	1074.1	1077.2	3.1	43.9	44.6	0.7	Cl
362	CC(Cl)CCCCl	1.0	293	1073.4	1083.5	10.1	48.1	47.9	-0.2	Cl
363	CCCCC(Cl)Cl	0.0	304	1041.7	1055.9	14.2	-	45.6	-	Cl
364	CCCCC(Cl)Cl	1.0	298	-	1062.4	-	44.3	46.0	1.7	Cl
365	CC(C)(Cl)C(C)(Cl)Cl	0.0	342	1144.6	1225.9	81.2	-	53.1	-	Cl
366	CC(Cl)C(C)(Cl)CCl	0.0	343	1184.5	1219.0	34.4	-	49.2	-	Cl
367	CC(C)(Cl)C(Cl)CCl	1.0	293	1264.1	1261.6	-2.5	-	53.0	-	Cl
368	CC(CCl)(CCl)CCl	0.0	338	1215.5	1253.2	37.7	-	52.3	-	Cl
369	CCCCC(Cl)(Cl)Cl	0.0	298	1183.9	1202.1	18.2	-	51.6	-	Cl
370	CCC(C)(C)CCl	0.0	298	874.6	894.2	19.6	-	40.5	-	Cl
371	CC(C)(C)CCCl	0.0	298	863.1	886.6	23.6	38.5	41.7	3.2	Cl
372	CC(C)C(C)CCl	1.0	298	881.6	885.5	3.9	-	40.4	-	Cl
373	CC(C)C(C)CCl	0.0	298	-	885.1	-	-	40.3	-	Cl
374	CCC(C)C(C)Cl	0.0	298	869.9	875.3	5.5	-	39.6	-	Cl
375	CCC(Cl)C(C)C	0.0	298	869.9	870.1	0.2	-	39.1	-	Cl
376	CC(C)CC(C)Cl	0.0	298	855.9	864.1	8.2	-	39.6	-	Cl
377	CCC(CC)CCl	0.0	300	884.2	880.4	-3.8	-	40.8	-	Cl
378	CCC(C)CCCl	1.0	300	892.0	879.4	-12.6	-	41.5	-	Cl
379	CCC(C)CCCl	0.0	303	-	877.1	-	-	41.3	-	Cl
380	CCCC(C)CCl	0.0	298	869.9	876.9	7.0	-	41.2	-	Cl
381	CCCC(Cl)CC	1.0	297	871.0	866.4	-4.6	-	40.0	-	Cl
382	CCCC(Cl)CC	0.0	298	-	865.5	-	39.9	40.0	0.0	Cl
383	CC(C)CCCCl	0.0	300	868.5	875.1	6.6	-	41.9	-	Cl
384	CCCCC(C)Cl	0.0	299	864.8	863.6	-1.2	41.2	40.5	-0.7	Cl
385	CC(C)(C)C(C)(Cl)Cl	0.0	317	-	1074.9	-	-	49.0	-	Cl
386	CC(C)(C)CC(Cl)Cl	1.0	293	1027.1	1065.2	38.1	-	50.6	-	Cl
387	CC(C)(C)CC(Cl)Cl	0.0	322	-	1037.4	-	41.8	48.8	7.1	Cl
388	CC(Cl)CC(C)(C)Cl	1.0	293	1036.0	1044.6	8.6	-	45.7	-	Cl
389	CCCCC(C)(Cl)Cl	1.0	298	1015.0	1031.6	16.6	-	48.3	-	Cl
390	CCCCC(C)(Cl)Cl	0.0	338	-	993.5	-	-	46.0	-	Cl
391	CCC(Cl)C(Cl)CC	1.0	293	1061.7	1061.7	-0.0	-	52.3	-	Cl
392	CCCC(Cl)C(C)Cl	0.0	334	1015.7	1015.1	-0.6	-	47.3	-	Cl
393	CCCC(Cl)CCCl	0.0	343	-	1010.0	-	-	47.6	-	Cl
394	CCC(Cl)CCCCl	0.0	350	-	1006.8	-	-	48.2	-	Cl
395	CCCCC(Cl)CCl	1.0	293	1080.0	1056.6	-23.4	48.2	49.3	1.1	Cl
396	CC(Cl)CCCCCl	1.0	293	1108.6	1058.8	-49.8	-	52.9	-	Cl
397	CCCCCC(Cl)Cl	0.0	335	987.4	1005.8	18.4	-	48.8	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
398	CCCCCC(Cl)Cl	1.0	298	-	1041.1	-	48.7	51.2	2.5	Cl
399	CCCCCC(Cl)(Cl)Cl	0.1	390	1033.3	1078.0	44.7	-	51.7	-	Cl
400	CC(C)(C)C(C)(C)Cl	0.0	298	864.3	977.4	113.1	-	49.0	-	Cl
401	CCC(C)(Cl)C(C)C	0.0	301	861.7	889.6	27.9	-	42.8	-	Cl
402	CCC(C)C(C)(C)Cl	0.0	301	-	884.4	-	-	43.2	-	Cl
403	CC(Cl)CC(C)(C)C	0.0	302	852.3	871.4	19.1	-	42.8	-	Cl
404	CC(C)CC(C)(C)Cl	1.0	293	862.8	868.6	5.8	-	42.0	-	Cl
405	CC(C)CC(C)(C)Cl	0.0	302	-	861.0	-	-	41.5	-	Cl
406	CCC(Cl)(CC)CC	0.0	314	865.9	871.0	5.1	-	41.8	-	Cl
407	CCCC(C)(Cl)CC	0.0	308	865.5	866.2	0.8	-	42.5	-	Cl
408	CCCCC(C)(C)Cl	1.0	293	863.5	868.2	4.7	-	43.6	-	Cl
409	CCCCC(C)(C)Cl	0.0	309	-	854.7	-	-	42.7	-	Cl
410	CC(C)CCC(C)Cl	0.0	309	848.9	855.4	6.6	-	43.9	-	Cl
411	CCCC(C)CCCl	0.0	320	851.3	859.9	8.6	-	44.8	-	Cl
412	CCCC(Cl)CCC	1.0	295	869.4	869.0	-0.4	-	44.9	-	Cl
413	CCCC(Cl)CCC	0.0	315	-	851.8	-	-	43.8	-	Cl
414	CCCCC(Cl)CC	1.0	298	857.9	866.0	8.1	-	44.6	-	Cl
415	CCCCC(Cl)CC	0.0	315	-	851.4	-	-	43.6	-	Cl
416	CCCCCC(C)Cl	1.0	295	865.1	866.7	1.6	-	45.3	-	Cl
417	CCCCCC(C)Cl	1.0	328	-	838.3	-	44.8	43.3	-1.5	Cl
418	CC(C)(Cl)CC(C)(C)Cl	0.0	339	986.3	993.7	7.4	-	46.9	-	Cl
419	CCC(C)(C)CC(Cl)Cl	1.0	293	1032.1	1058.3	26.2	-	55.4	-	Cl
420	CC(C)(C)CC(Cl)CCl	1.0	293	1025.9	1050.4	24.5	-	51.5	-	Cl
421	CC(C)(C)CC(Cl)CCl	0.0	344	-	1005.9	-	45.1	48.6	3.5	Cl
422	CC(C)(CCCl)CCCl	1.0	293	1056.3	1079.0	22.7	-	59.9	-	Cl
423	CC(C)(CCCl)CCCl	0.0	339	-	1040.0	-	-	56.9	-	Cl
424	CCCC(Cl)(Cl)CCC	0.0	349	1021.9	978.9	-43.0	-	49.4	-	Cl
425	CCCCCC(C)(Cl)Cl	0.0	340	968.2	978.2	10.1	-	50.9	-	Cl
426	CCCCCC(Cl)CCl	1.0	293	1062.5	1037.3	-25.2	53.2	54.0	0.8	Cl
427	CCCCCCC(Cl)Cl	0.0	353	995.8	974.1	-21.7	-	52.7	-	Cl
428	CCCCCCC(Cl)Cl	1.0	298	-	1024.0	-	53.5	56.4	2.9	Cl
429	ClCCCCCCCCl	1.0	298	1040.8	1044.5	3.7	61.2	59.4	-1.8	Cl
430	CCCCCCC(Cl)(Cl)Cl	1.0	298	1121.2	1143.2	22.0	-	63.7	-	Cl
431	CCCCCCC(Cl)(Cl)Cl	0.1	410	-	1037.7	-	-	55.9	-	Cl
432	ClCCCCCCC(Cl)Cl	1.0	293	1174.4	1174.9	0.5	-	67.9	-	Cl
433	CCC(C)(C)C(C)(C)Cl	1.0	298	906.5	922.0	15.5	-	49.0	-	Cl
434	CCC(C)(Cl)C(C)(C)C	1.0	293	906.6	924.4	17.8	-	48.8	-	Cl
435	CC(C)(C)CC(C)(C)Cl	1.0	293	874.1	881.9	7.8	-	45.8	-	Cl
436	CC(C)(C)CC(C)(C)Cl	0.0	332	-	850.5	-	-	43.7	-	Cl
437	CC(C)C(C)C(C)(C)Cl	1.0	293	888.0	895.7	7.7	-	46.7	-	Cl
438	CCCC(C)(Cl)C(C)C	0.0	332	834.5	862.3	27.8	-	45.5	-	Cl
439	CC(C)CCC(C)(C)Cl	0.0	332	-	835.9	-	-	45.0	-	Cl
440	CCCC(C)(Cl)CCC	0.0	332	834.8	847.4	12.6	-	45.9	-	Cl
441	CCCCC(C)(Cl)CC	0.0	328	845.6	849.5	3.9	-	45.8	-	Cl
442	CCCCCC(C)(C)Cl	1.0	298	856.8	863.9	7.1	-	47.9	-	Cl
443	CCCCCC(C)(C)Cl	0.0	328	-	839.6	-	-	46.1	-	Cl
444	CC(C)CCCC(C)Cl	0.0	328	-	838.7	-	-	46.9	-	Cl
445	CCCCC(CC)CCl	1.0	293	876.9	882.3	5.4	-	50.0	-	Cl
446	CCCCC(CC)CCl	0.0	337	-	845.2	-	47.4	47.1	-0.2	Cl
447	CCC(C)CCCCCl	0.0	336	-	846.1	-	-	48.5	-	Cl
448	CCCCCCC(C)Cl	1.0	298	861.5	864.7	3.3	-	49.8	-	Cl
449	CCCCCCC(C)Cl	1.0	345	-	825.7	-	47.8	46.8	-1.0	Cl
450	CC(C)(Cl)CCC(C)(C)Cl	0.0	363	-	949.6	-	-	49.3	-	Cl
451	CCC(C)(C)CC(Cl)CCl	1.0	293	1029.0	1044.9	15.9	-	55.8	-	Cl
452	CCCCCC(Cl)C(C)Cl	0.0	368	-	951.7	-	-	52.0	-	Cl
453	CCCCCCC(Cl)CCl	1.0	298	-	1016.5	-	57.6	58.2	0.6	Cl
454	CCCCCCCC(Cl)Cl	0.0	370	-	948.1	-	-	56.2	-	Cl
455	CCCCCCCC(Cl)Cl	1.0	298	-	1010.0	-	57.7	61.3	3.6	Cl
456	ClCCCCCCCCCl	1.0	298	1024.8	1027.6	2.8	65.6	63.8	-1.8	Cl
457	CCCCCCCC(Cl)(Cl)Cl	0.1	430	948.0	1002.2	54.2	-	59.6	-	Cl
458	CCC(Cl)(CC)C(C)(C)C	0.0	344	-	887.5	-	-	49.2	-	Cl
459	CCCC(C)(Cl)C(C)(C)C	0.0	340	858.2	882.2	24.0	-	50.2	-	Cl
460	CCCCC(Cl)(CC)CC	0.0	351	836.3	840.2	4.0	-	48.3	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
461	CCCCC(C)(Cl)CCC	0.0	347	827.0	835.8	8.8	-	49.1	-	Cl
462	CCCCCC(C)(Cl)CC	0.0	347	826.8	834.4	7.5	-	49.0	-	Cl
463	CCCCCC(Cl)C(C)C	1.0	293	856.6	872.8	16.2	-	52.9	-	Cl
464	CCCCC(Cl)CCCC	0.0	351	815.6	824.0	8.4	-	50.0	-	Cl
465	CCCCCCC(Cl)CC	0.0	352	807.5	823.3	15.7	-	50.1	-	Cl
466	CCCCCCCC(C)Cl	1.0	293	879.0	868.5	-10.5	-	54.4	-	Cl
467	CCCCCCCCCCl	1.0	298	867.4	872.7	5.3	55.9	56.2	0.3	Cl
468	CC(C)(Cl)CCCC(C)(C)Cl	0.0	374	-	927.9	-	-	53.5	-	Cl
469	CCCCCCCC(Cl)CCl	1.0	298	-	1004.1	-	62.1	62.9	0.8	Cl
470	CCCCCCCCC(Cl)Cl	0.1	436	-	880.9	-	-	55.8	-	Cl
471	CCCCCCCCC(Cl)Cl	1.0	298	-	998.6	-	62.3	66.2	3.9	Cl
472	ClCCCCCCCCCCl	1.0	298	1017.3	1013.4	-3.9	-	68.6	-	Cl
473	ClCCCCCCCCCCl	0.1	453	-	882.8	-	54.6	56.5	1.9	Cl
474	CCCCCCCCC(Cl)(Cl)Cl	0.1	449	914.4	970.7	56.4	-	63.1	-	Cl
475	CCCCCCCCC(C)Cl	1.0	293	870.6	868.4	-2.2	-	58.8	-	Cl
476	CCCCCCCCCCCl	1.0	298	865.8	872.2	6.4	64.0	60.7	-3.3	Cl
477	CCCCCCCCCC(Cl)Cl	0.1	456	-	857.1	-	-	58.3	-	Cl
478	CCCCCCCCCC(Cl)Cl	1.0	430	-	880.2	-	56.9	60.4	3.5	Cl
479	ClCCCCCCCCCCCl	1.0	298	992.9	1001.8	8.8	73.1	73.0	-0.1	Cl
480	CCCCCCCCCC(Cl)(Cl)Cl	0.1	439	917.0	969.0	52.0	52.5	68.5	16.0	Cl
481	CCC(C)CF	1.0	302	-	784.7	-	30.7	31.4	0.7	F
482	CC(C)CCF	1.0	293	694.1	794.7	100.6	-	32.3	-	F
483	CC(C)CCF	0.4	298	-	789.1	-	-	32.0	-	F
484	CCCCCF	0.2	298	-	789.4	-	30.9	32.7	1.8	F
485	CC(F)C(C)(C)F	0.1	298	-	870.1	-	-	29.0	-	F
486	CC(C)C(C)(F)F	0.1	298	-	873.9	-	-	32.2	-	F
487	CC(C)(CF)CF	0.1	298	-	959.7	-	-	37.2	-	F
488	CCC(C)(F)CF	0.1	298	-	891.9	-	-	30.0	-	F
489	CCC(F)(F)CC	1.0	293	910.6	864.8	-45.8	-	30.8	-	F
490	CCC(F)(F)CC	1.0	277	-	883.1	-	33.8	31.5	-2.3	F
491	CC(C)(F)CCF	0.1	298	-	902.1	-	-	33.1	-	F
492	CCCC(C)(F)F	1.0	293	898.7	860.8	-37.9	-	32.2	-	F
493	CCCC(C)(F)F	1.0	277	-	878.5	-	33.7	32.9	-0.8	F
494	CC(F)C(C)CF	0.1	298	-	934.2	-	-	35.7	-	F
495	CCC(C)C(F)F	0.1	298	-	922.4	-	-	36.0	-	F
496	CC(C)C(F)CF	0.1	298	-	920.4	-	-	32.2	-	F
497	CCC(F)C(C)F	0.1	298	-	899.2	-	-	31.0	-	F
498	CC(C)CC(F)F	0.1	298	-	920.2	-	-	37.0	-	F
499	CC(F)CC(C)F	0.1	298	-	901.0	-	-	34.6	-	F
500	CC(CF)CCF	0.1	298	-	957.9	-	-	37.6	-	F
501	CCC(F)CCF	0.1	298	-	928.4	-	-	35.8	-	F
502	CCCC(F)CF	0.1	298	-	921.1	-	-	33.7	-	F
503	CC(F)CCCF	0.1	298	-	931.6	-	-	37.0	-	F
504	CCCCC(F)F	0.1	298	-	915.6	-	-	37.1	-	F
505	CCCCC(F)F	1.0	283	-	932.2	-	34.4	37.9	3.5	F
506	FCCCCCF	1.0	298	957.2	959.4	2.2	-	39.9	-	F
507	FCCCCCF	0.0	298	-	959.6	-	-	39.9	-	F
508	CC(C)CC(F)(F)F	1.0	298	978.8	960.7	-18.1	-	34.4	-	F
509	CCCCC(F)(F)F	1.0	293	970.1	960.4	-9.7	-	35.6	-	F
510	CCCCC(F)(F)F	0.3	298	-	954.3	-	-	35.3	-	F
511	CCC(C)(C)CF	0.1	298	-	812.6	-	-	35.5	-	F
512	CC(C)(C)CCF	1.0	293	780.9	816.1	35.2	-	36.8	-	F
513	CC(C)(C)CCF	0.1	298	-	811.7	-	-	36.6	-	F
514	CC(C)C(C)CF	0.1	298	-	806.8	-	-	35.4	-	F
515	CCC(C)C(C)F	0.1	298	-	787.8	-	-	34.4	-	F
516	CCC(F)C(C)C	0.1	298	-	782.1	-	-	34.1	-	F
517	CC(C)CC(C)F	0.1	298	-	779.0	-	-	34.4	-	F
518	CCC(C)CCF	0.1	298	-	805.6	-	-	36.5	-	F
519	CCCC(C)CF	0.1	298	-	799.3	-	-	36.1	-	F
520	CCCC(F)CC	0.1	298	-	780.0	-	-	34.9	-	F
521	CCCC(F)CC	1.0	296	-	782.0	-	36.8	35.0	-1.8	F
522	CC(C)CCCF	0.1	298	-	800.8	-	-	37.0	-	F
523	CCCCC(C)F	0.1	298	-	779.5	-	-	35.3	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
524	CCCCCCF	0.1	298	-	800.1	-	35.6	37.3	1.7	F
525	CCCCCC(F)F	0.1	310	-	900.8	-	-	42.0	-	F
526	CCCCCC(F)F	1.0	305	-	906.3	-	37.7	42.3	4.6	F
527	CCCCCC(F)(F)F	1.0	293	960.8	959.5	-1.3	-	42.3	-	F
528	CCCCCC(F)(F)F	0.1	298	-	953.4	-	-	42.0	-	F
529	CCCCCCC(F)F	1.0	293	-	914.5	-	-	48.5	-	F
530	CCCCCCC(F)F	1.0	326	-	884.7	-	41.1	46.4	5.3	F
531	CCCCCCC(F)(F)F	0.1	317	-	932.3	-	-	47.3	-	F
532	CCCCCCCCF	1.0	322	-	795.2	-	44.1	45.1	1.0	F
533	CCCCCCCC(F)F	0.1	365	-	847.8	-	-	48.6	-	F
534	CCCCCCCC(F)F	1.0	344	-	866.3	-	44.2	50.0	5.8	F
535	CCCCCCCC(F)(F)F	0.1	341	-	907.1	-	-	51.6	-	F
536	CCCCCCCCCF	1.0	293	-	823.0	-	-	51.5	-	F
537	CCCCCCCCCF	1.0	348	-	779.5	-	46.8	47.9	1.1	F
538	CCCCCCCCC(F)F	0.1	389	-	826.9	-	-	51.5	-	F
539	CCCCCCCCC(F)F	1.0	362	-	850.3	-	47.2	53.5	6.3	F
540	CCCCCCCCC(F)(F)F	1.0	293	935.7	948.0	12.3	-	61.0	-	F
541	CCCCCCCCC(F)(F)F	0.1	363	-	885.6	-	-	55.8	-	F
542	CCCCCCCCCCF	1.0	293	819.4	826.7	7.3	-	55.9	-	F
543	CCCCCCCCCCF	1.0	357	-	777.9	-	50.4	51.5	1.1	F
544	CCCCCCCCCC(F)F	0.1	412	-	807.5	-	-	54.4	-	F
545	CCCCCCCCCC(F)F	1.0	379	-	835.5	-	50.2	56.8	6.6	F
546	CCCCCCCCCC(F)(F)F	0.1	385	-	865.9	-	-	59.1	-	F
547	CCC(C)CI	0.0	310	1496.8	1501.0	4.2	43.1	42.3	-0.8	I
548	CC(I)C(C)(C)I	0.0	378	-	2056.9	-	-	53.2	-	I
549	CC(C)(CI)CI	0.0	385	-	2066.7	-	-	54.6	-	I
550	CCC(C)(I)CI	0.0	392	-	2039.0	-	-	52.7	-	I
551	CCC(I)(I)CC	0.0	386	-	2033.9	-	-	51.9	-	I
552	CC(C)(I)CCI	0.0	381	-	2032.9	-	-	54.5	-	I
553	CCCC(C)(I)I	0.0	386	-	2010.4	-	-	52.6	-	I
554	CCC(C)C(I)I	0.0	386	-	2022.1	-	-	53.0	-	I
555	CC(C)C(I)CI	0.0	378	-	2042.1	-	-	54.4	-	I
556	CCC(I)C(C)I	0.0	389	-	2012.8	-	-	52.9	-	I
557	CC(C)CC(I)I	0.0	389	-	1993.9	-	-	53.5	-	I
558	CC(I)CC(C)I	0.0	392	-	1982.1	-	-	52.5	-	I
559	CC(CI)CCI	0.0	398	-	2014.0	-	-	56.0	-	I
560	CCC(I)CCI	0.0	400	1966.0	1994.8	28.8	-	54.2	-	I
561	CCCC(I)CI	0.0	397	1961.6	1997.0	35.4	-	54.3	-	I
562	CC(I)CCCI	0.0	403	1970.4	1983.5	13.1	-	55.0	-	I
563	CCCCC(I)I	0.0	394	1962.8	1984.3	21.5	-	54.0	-	I
564	ICCCCCI	0.0	406	-	1993.2	-	59.7	57.1	-2.6	I
565	CCCCC(I)(I)I	0.0	469	-	2331.0	-	-	62.8	-	I
566	CCC(C)(C)CI	0.0	319	1393.3	1444.4	51.1	-	45.4	-	I
567	CC(C)(C)CCI	0.0	324	1387.2	1419.4	32.2	-	46.3	-	I
568	CC(C)C(C)CI	0.0	326	1385.2	1422.5	37.3	-	45.3	-	I
569	CCC(C)C(C)I	0.0	332	1376.8	1406.0	29.2	-	44.2	-	I
570	CCC(I)C(C)C	0.0	319	1393.3	1417.0	23.7	-	44.3	-	I
571	CC(C)CC(C)I	0.0	319	1393.3	1402.2	8.9	-	44.7	-	I
572	CCC(CC)CI	1.0	296	1440.0	1454.7	14.7	-	47.4	-	I
573	CCC(C)CCI	0.0	333	1349.7	1402.3	52.7	-	46.0	-	I
574	CCCC(C)CI	0.0	328	-	1405.3	-	-	45.7	-	I
575	CCCC(I)CC	0.0	328	1382.1	1396.6	14.6	-	44.9	-	I
576	CC(C)CCCI	1.0	293	1428.3	1444.5	16.2	-	48.4	-	I
577	CC(C)CCCI	0.0	332	-	1395.4	-	-	46.2	-	I
578	CCCCC(C)I	0.0	329	-	1390.2	-	-	45.3	-	I
579	CCCCCC(I)I	0.0	410	-	1845.1	-	-	57.0	-	I
580	ICCCCCCI	0.0	402	-	1884.1	-	-	61.2	-	I
581	CCCC(I)CCC	0.1	387	-	1269.7	-	-	45.9	-	I
582	CCCCC(I)CC	1.0	295	1365.6	1381.1	15.5	-	51.0	-	I
583	CCCCC(I)CC	0.0	349	-	1317.0	-	-	48.0	-	I
584	CCCCCC(C)I	0.0	349	1285.9	1311.9	26.0	-	48.5	-	I
585	CCCCCCC(I)I	0.1	491	-	1632.8	-	-	55.8	-	I
586	CCCCCCC(C)I	1.0	299	1316.4	1325.2	8.8	-	55.9	-	I

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
587	CCCCCCC(C)I	0.1	406	-	1203.7	-	-	49.3	-	I
588	CCCCCCCC(I)I	0.0	442	-	1633.4	-	-	62.8	-	I
589	ICCCCCCCCI	0.0	453	-	1639.9	-	-	65.4	-	I
590	CCCCCCCCCI	1.0	298	1283.6	1295.3	11.7	64.5	62.7	-1.8	I
591	CCCCCCCCC(C)I	1.0	298	1241.2	1254.8	13.6	-	64.9	-	I
592	CCCCCCCCCCI	1.0	293	1256.7	1266.5	9.8	69.8	67.6	-2.2	I
593	FCCCCCCl	0.0	325	1006.0	1003.2	-2.8	-	43.3	-	Mix
594	FCCCCCCCl	0.0	353	962.2	957.2	-5.1	-	46.0	-	Mix
595	FCCCCCCCCl	0.1	379	923.4	920.3	-3.1	-	48.8	-	Mix
596	FCCCCCCCCCCl	0.1	426	870.8	861.9	-8.9	-	53.7	-	Mix
597	FCCCCCCCCCCCl	0.1	447	851.5	837.8	-13.6	-	55.9	-	Mix

Table S19: Comparison of experimental and simulated properties validation using the SH/SQE-M scheme.

	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
1	BrCBr	0.1	298	2482.0	2442.9	-39.1	-	36.0	-	Br
2	BrCBr	1.0	298	-	2443.3	-	37.0	36.0	-1.0	Br
3	BrC(Br)Br	1.0	298	2877.2	2870.6	-6.6	46.1	46.2	0.1	Br
4	BrC(Br)(Br)Br	1.0	374	2953.3	2993.0	39.7	-	52.0	-	Br
5	BrC(Br)(Br)Br	1.0	384	-	2971.1	-	48.2	51.5	3.3	Br
6	CC(Br)Br	1.0	316	-	2041.2	-	39.6	37.3	-2.3	Br
7	BrCC(Br)Br	1.0	321	-	2548.9	-	52.9	51.9	-1.0	Br
8	CC(C)(Br)Br	0.0	298	1820.0	1859.6	39.6	37.3	40.1	2.7	Br
9	CCC(Br)Br	0.0	302	1968.8	1889.5	-79.3	43.1	42.1	-1.0	Br
10	CC(Br)(Br)CBr	0.0	349	-	2260.5	-	47.5	52.5	5.0	Br
11	BrCC(Br)CBr	0.0	374	-	2263.4	-	52.1	55.3	3.1	Br
12	BrCCC(Br)Br	1.0	290	2350.0	2372.0	22.0	-	57.4	-	Br
13	CC(C)(Br)CBr	1.0	293	1760.4	1787.7	27.3	-	45.6	-	Br
14	CC(C)(Br)CBr	0.0	322	-	1744.9	-	41.8	44.3	2.5	Br
15	CCC(C)(Br)Br	0.0	318	1718.7	1725.4	6.7	41.0	43.4	2.4	Br
16	CC(C)C(Br)Br	0.0	321	1733.3	1731.0	-2.4	-	44.3	-	Br
17	CC(Br)C(C)Br	1.0	295	1789.3	1775.5	-13.8	-	45.8	-	Br
18	CC(Br)C(C)Br	0.0	325	-	1731.6	-	43.0	44.3	1.3	Br
19	CC(Br)CCBr	0.0	343	-	1716.1	-	45.1	46.6	1.5	Br
20	CCCC(Br)Br	1.0	298	1784.0	1758.2	-25.8	-	46.8	-	Br
21	CCCC(Br)Br	1.0	357	-	1668.4	-	45.8	43.9	-1.9	Br
22	BrCCCCBr	1.0	298	1818.8	1806.9	-12.0	52.6	52.5	-0.1	Br
23	CC(Br)C(C)(Br)Br	1.0	293	2172.4	2186.1	13.7	-	56.9	-	Br
24	CC(Br)C(C)(Br)Br	1.0	326	-	2138.0	-	51.7	55.1	3.4	Br
25	CCC(Br)(Br)CBr	1.0	293	2168.5	2197.9	29.4	-	58.6	-	Br
26	CCC(Br)(Br)CBr	1.0	329	-	2141.2	-	50.7	56.2	5.5	Br
27	CC(Br)C(Br)CBr	1.0	293	2183.5	2206.9	23.4	-	62.8	-	Br
28	CC(Br)C(Br)CBr	1.0	333	-	2142.6	-	51.3	59.9	8.6	Br
29	CCC(Br)C(Br)Br	1.0	293	2183.5	2175.2	-8.3	-	58.5	-	Br
30	CCC(Br)C(Br)Br	0.0	369	-	2055.5	-	51.1	54.1	3.0	Br
31	BrCC(CBr)CBr	1.0	490	-	1921.3	-	66.1	52.0	-14.1	Br
32	BrCCC(Br)CBr	1.0	298	2210.0	2206.4	-3.6	-	63.0	-	Br
33	BrCCC(Br)CBr	1.0	405	-	2039.1	-	53.5	56.8	3.3	Br
34	CC(C)(C)CBr	1.0	308	-	1203.9	-	35.6	37.6	2.0	Br
35	CC(C)C(C)Br	0.0	298	1215.6	1203.8	-11.8	-	37.9	-	Br
36	CC(C)C(C)Br	1.0	316	-	1182.6	-	37.2	37.0	-0.2	Br
37	CCC(Br)CC	0.0	298	-	1200.3	-	39.3	38.4	-0.9	Br
38	CC(Br)C(C)(C)C	0.0	298	1169.8	1190.0	20.3	-	41.7	-	Br
39	CC(Br)C(C)(C)C	1.0	330	-	1154.6	-	39.5	40.1	0.6	Br
40	CC(C)C(C)(C)Br	1.0	292	1187.4	1189.9	2.5	-	41.3	-	Br
41	CCCC(C)(C)Br	1.0	293	1180.4	1170.2	-10.2	-	41.9	-	Br
42	ClCCl	1.0	298	1316.4	1287.9	-28.5	28.8	26.4	-2.4	Cl
43	ClC(Cl)Cl	1.0	298	1479.5	1487.3	7.8	31.1	30.7	-0.4	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
44	ClC(Cl)(Cl)Cl	1.0	298	1584.3	1608.9	24.6	-	34.4	-	Cl
45	ClC(Cl)(Cl)Cl	0.1	298	-	1609.3	-	32.4	34.4	2.0	Cl
46	CC(C)Cl	0.7	298	-	850.4	-	26.4	27.1	0.7	Cl
47	CCCCl	1.0	298	884.1	876.6	-7.4	28.5	28.4	-0.1	Cl
48	CC(C)(Cl)Cl	0.2	298	1107.3	1086.6	-20.7	-	33.1	-	Cl
49	CC(C)(Cl)Cl	1.0	298	-	1087.0	-	32.1	33.2	1.1	Cl
50	CCC(Cl)Cl	0.1	298	1126.0	1114.6	-11.4	-	34.2	-	Cl
51	CCC(Cl)Cl	1.0	298	-	1115.5	-	35.2	34.2	-1.0	Cl
52	CC(Cl)(Cl)CCl	0.0	298	1317.9	1334.9	17.1	40.5	43.5	3.0	Cl
53	CCC(Cl)(Cl)Cl	1.0	298	1283.6	1286.6	3.0	-	38.0	-	Cl
54	CCC(Cl)(Cl)Cl	1.0	259	-	1336.6	-	38.8	39.9	1.1	Cl
55	CC(Cl)C(Cl)Cl	1.0	289	1353.0	1343.2	-9.8	-	43.3	-	Cl
56	CC(Cl)C(Cl)Cl	0.0	302	-	1327.5	-	42.3	42.5	0.2	Cl
57	ClCC(Cl)CCl	1.0	298	1388.8	1385.9	-2.9	46.8	48.8	2.0	Cl
58	ClCCC(Cl)Cl	1.0	293	1355.5	1353.5	-2.0	-	44.4	-	Cl
59	ClCCC(Cl)Cl	0.0	313	-	1329.6	-	44.2	43.4	-0.8	Cl
60	CC(C)(Cl)CCl	0.0	298	1089.0	1098.8	9.9	36.8	37.6	0.8	Cl
61	CCC(C)(Cl)Cl	0.1	298	1065.1	1073.0	7.9	-	37.4	-	Cl
62	CCC(C)(Cl)Cl	1.0	298	-	1073.0	-	36.7	37.4	0.7	Cl
63	CC(C)C(Cl)Cl	0.0	298	1100.1	1086.4	-13.7	36.5	38.2	1.8	Cl
64	CC(Cl)C(C)Cl	0.0	298	-	1098.2	-	38.5	41.6	3.1	Cl
65	CC(CCl)CCl	0.0	307	1090.0	1117.9	27.8	-	42.8	-	Cl
66	CC(CCl)CCl	1.0	285	-	1141.0	-	45.1	44.1	-1.0	Cl
67	CC(Cl)CCCl	1.0	298	1108.3	1108.0	-0.3	42.1	42.1	0.0	Cl
68	CCCC(Cl)Cl	0.0	298	1080.1	1081.8	1.7	-	39.1	-	Cl
69	CCCC(Cl)Cl	1.0	298	-	1081.8	-	39.4	39.2	-0.2	Cl
70	CC(C)(Cl)C(Cl)Cl	1.0	298	1267.7	1282.0	14.3	-	45.9	-	Cl
71	CC(Cl)C(C)(Cl)Cl	1.0	291	1263.0	1285.0	22.0	-	46.8	-	Cl
72	CC(Cl)C(C)(Cl)Cl	0.0	310	-	1263.6	-	42.7	45.7	3.0	Cl
73	CC(Cl)(CCl)CCl	1.0	298	1301.2	1316.5	15.3	-	49.7	-	Cl
74	CC(Cl)(CCl)CCl	0.0	327	-	1284.0	-	45.9	47.9	2.0	Cl
75	CCCC(Cl)(Cl)Cl	0.0	298	1231.0	1236.3	5.3	-	43.3	-	Cl
76	CC(CCl)C(Cl)Cl	0.0	312	1251.1	1280.1	29.1	-	47.1	-	Cl
77	CC(Cl)C(Cl)CCl	1.0	293	1316.4	1308.9	-7.5	-	50.6	-	Cl
78	CC(Cl)C(Cl)CCl	1.0	288	-	1314.2	-	41.3	50.8	9.5	Cl
79	CC(Cl)CC(Cl)Cl	1.0	288	1317.0	1281.3	-35.7	-	47.7	-	Cl
80	CC(Cl)CC(Cl)Cl	0.0	318	-	1246.0	-	43.9	45.9	2.0	Cl
81	ClCCC(Cl)CCl	1.0	293	1317.5	1319.8	2.3	-	51.8	-	Cl
82	CC(C)(C)CCl	0.1	298	860.9	879.7	18.8	-	35.5	-	Cl
83	CC(C)(C)CCl	1.0	294	-	884.3	-	34.9	35.7	0.8	Cl
84	CC(C)C(C)Cl	0.1	298	857.0	868.5	11.4	-	35.2	-	Cl
85	CC(C)C(C)Cl	1.0	300	-	867.2	-	35.9	35.2	-0.7	Cl
86	CCC(Cl)CC	1.0	298	884.0	864.9	-19.1	-	35.6	-	Cl
87	CCC(Cl)CC	1.0	304	-	859.1	-	36.5	35.3	-1.2	Cl
88	CC(C)(C)C(Cl)Cl	0.0	312	1074.8	1066.4	-8.4	-	41.6	-	Cl
89	CC(C)C(C)(C)Cl	1.0	298	874.9	881.2	6.3	-	38.5	-	Cl
90	CC(C)C(C)(C)Cl	1.0	316	-	865.4	-	38.0	37.6	-0.4	Cl
91	CCC(C)(Cl)CC	1.0	293	883.9	880.5	-3.4	-	38.8	-	Cl
92	CCCC(C)(C)Cl	0.0	298	858.3	864.5	6.2	37.7	38.9	1.1	Cl
93	FCF	1.0	221	1213.8	1204.3	-9.5	20.9	18.2	-2.7	F
94	FCF	17.6	298	891.6	955.7	64.0	-	14.9	-	F
95	FCF	1.0	298	961.0	942.7	-18.3	-	14.7	-	F
96	FC(F)F	1.0	191	1442.9	1613.0	170.1	16.7	16.7	-0.0	F
97	FC(F)F	47.1	298	636.7	252.9	-383.7	-	5.2	-	F
98	FC(F)F	1.0	298	666.7	4.6	-662.1	-	-0.2	-	F
99	FC(F)(F)F	1.0	145	1605.2	1821.8	216.7	12.3	11.1	-1.2	F
100	FCCF	1.0	283	1024.0	1053.8	29.8	-	22.6	-	F
101	FCCF	1.8	298	-	1024.2	-	22.5	21.9	-0.6	F
102	CC(F)(F)F	12.9	298	-	850.1	-	13.1	15.0	1.9	F
103	FCC(F)F	1.0	314	1175.5	1156.5	-19.0	-	23.1	-	F
104	FCC(F)F	1.0	278	-	1244.2	-	23.2	25.0	1.8	F
105	FCC(F)F	2.0	296	-	1200.8	-	20.6	24.1	3.5	F
106	CC(C)F	1.0	293	723.8	709.7	-14.1	-	21.3	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
107	CC(C)F	1.0	249	-	772.2	-	23.7	23.2	-0.5	F
108	CC(C)(F)F	1.0	271	943.8	862.1	-81.7	22.6	22.8	0.2	F
109	CC(C)(F)F	2.1	291	911.4	826.1	-85.3	21.6	21.9	0.3	F
110	CC(F)CF	1.4	298	960.0	929.8	-30.2	-	23.3	-	F
111	CCC(F)F	1.3	298	920.1	906.5	-13.6	23.7	24.2	0.5	F
112	CC(F)(F)CF	0.4	262	-	1087.5	-	27.3	25.0	-2.3	F
113	CCC(F)(F)F	0.9	259	1148.2	989.3	-158.8	21.8	20.8	-1.0	F
114	CC(C)(C)F	1.0	237	-	775.4	-	27.6	25.5	-2.1	F
115	CC(C)CF	0.9	286	764.5	776.9	12.4	-	26.8	-	F
116	CC(C)CF	1.4	298	750.0	762.2	12.2	-	26.3	-	F
117	CCC(C)F	1.0	248	-	798.5	-	29.2	27.7	-1.5	F
118	CCCCF	1.0	237	-	837.8	-	30.1	29.9	-0.2	F
119	CCC(C)(F)F	1.0	293	915.9	852.1	-63.8	-	26.0	-	F
120	CCC(C)(F)F	0.8	298	-	847.2	-	25.9	25.9	-0.0	F
121	CCCC(F)F	0.4	298	910.1	911.6	1.5	-	29.4	-	F
122	CCCC(F)F	1.0	261	-	959.7	-	31.0	31.2	0.2	F
123	FCCCCF	0.1	298	-	981.5	-	34.6	34.1	-0.5	F
124	CCC(C)(C)F	0.4	298	-	742.6	-	29.4	27.6	-1.8	F
125	CC(C)(C)C(F)(F)F	1.0	293	990.5	982.2	-8.3	-	29.5	-	F
126	ICI	1.0	298	3307.8	3171.9	-135.9	49.0	44.3	-4.7	I
127	IC(I)I	0.0	396	3685.6	3421.9	-263.7	47.9	54.1	6.2	I
128	IC(I)(I)I	0.0	447	3819.2	3655.6	-163.6	-	64.6	-	I
129	CCI	0.2	298	-	1907.5	-	31.7	30.9	-0.8	I
130	CC(I)I	0.0	336	2682.9	2645.2	-37.7	-	44.3	-	I
131	ICCI	0.0	356	2551.8	2689.0	137.1	48.1	47.9	-0.2	I
132	CCCI	0.1	298	-	1730.2	-	36.0	35.3	-0.7	I
133	CC(C)(I)I	0.0	352	2379.7	2312.4	-67.2	-	44.7	-	I
134	CC(I)CI	0.0	330	2506.9	2449.6	-57.4	-	50.6	-	I
135	CCC(I)I	0.0	357	2370.2	2375.1	4.9	-	47.2	-	I
136	CC(C)CI	1.0	298	-	1600.0	-	38.8	38.5	-0.3	I
137	CC(C)(I)CI	0.0	370	2163.1	2199.4	36.4	-	50.0	-	I
138	CCC(C)(I)I	0.0	370	2163.1	2180.4	17.4	-	48.6	-	I
139	CC(C)C(I)I	0.0	365	2171.2	2187.9	16.8	-	49.5	-	I
140	CC(I)C(C)I	0.0	374	2155.0	2173.7	18.7	-	50.3	-	I
141	CC(Cl)CI	0.0	374	2155.0	2201.8	46.9	-	52.5	-	I
142	CCC(I)CI	0.0	371	2160.5	2191.0	30.5	-	51.9	-	I
143	CC(I)CCI	0.0	382	2141.4	2167.7	26.3	-	51.9	-	I
144	CCCC(I)I	0.0	373	2144.3	2160.6	16.3	-	50.5	-	I
145	CCC(C)(C)I	1.0	323	-	1475.9	-	40.4	39.4	-1.0	I
146	CC(I)C(C)(C)C	0.0	320	1392.3	1439.8	47.5	-	44.0	-	I
147	CC(C)C(C)(C)I	1.0	293	1448.0	1470.6	22.6	-	44.6	-	I
148	CCC(C)(I)CC	0.0	319	1393.3	1433.9	40.6	-	43.9	-	I
149	CCCC(C)(C)I	0.0	332	1376.8	1396.9	20.1	-	43.5	-	I
150	ClCBr	1.0	298	1924.9	1899.6	-25.2	-	31.5	-	Mix
151	ClCBr	1.0	304	-	1886.3	-	33.5	31.3	-2.2	Mix
152	FCCl	1.0	260	1282.1	1258.8	-23.4	21.9	22.4	0.5	Mix
153	BrCI	1.0	290	2926.0	2862.5	-63.5	-	40.6	-	Mix
154	ClCI	1.0	293	2422.0	2387.3	-34.7	-	36.5	-	Mix
155	FC(F)Br	1.0	298	1775.5	2003.4	228.0	-	26.1	-	Mix
156	FC(F)Br	1.0	244	-	2179.5	-	24.0	28.5	4.5	Mix
157	FC(F)Cl	1.0	233	1408.0	1482.2	74.2	20.2	21.6	1.4	Mix
158	FC(F)Cl	10.8	298	1193.0	1281.6	88.6	-	18.7	-	Mix
159	FC(Cl)Cl	1.8	298	1367.0	1411.4	44.5	-	24.9	-	Mix
160	FC(Cl)Cl	1.0	267	-	1480.5	-	26.1	26.2	0.1	Mix
161	FC(I)I	1.0	295	3196.9	3251.6	54.7	-	45.9	-	Mix
162	FC(I)I	1.0	314	-	3192.7	-	32.9	44.9	12.0	Mix
163	FC(F)I	1.0	272	-	2632.1	-	26.0	33.9	7.9	Mix
164	FC(Br)Br	1.0	293	2421.0	2542.9	121.9	-	36.6	-	Mix
165	ClC(Cl)Br	1.0	298	1983.5	1993.0	9.5	-	36.3	-	Mix
166	ClC(Br)Br	1.0	293	2451.0	2463.3	12.3	-	41.7	-	Mix
167	ClC(Cl)(Cl)Br	1.0	298	2002.1	2038.0	35.9	-	39.9	-	Mix
168	ClC(Cl)(Cl)Br	0.1	298	-	2038.1	-	36.1	39.9	3.7	Mix
169	ClC(Cl)(Br)Br	1.0	298	2420.0	2437.1	17.1	-	45.2	-	Mix

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
170	ClC(Br)(Br)Br	1.0	288	2710.0	2831.2	121.2	-	51.0	-	Mix
171	FC(F)(F)Br	1.0	215	1989.9	2525.6	535.7	17.5	25.6	8.1	Mix
172	FC(F)(F)Br	16.6	298	1536.1	1909.9	373.8	-	19.6	-	Mix
173	FC(Br)(Br)Br	1.0	330	-	2761.1	-	34.4	42.1	7.7	Mix
174	FC(F)(Br)Br	1.0	298	2251.2	2445.4	194.2	25.0	31.8	6.9	Mix
175	FC(F)(F)Cl	1.0	190	1527.8	1898.6	370.8	15.4	19.1	3.7	Mix
176	FC(F)(F)Cl	36.7	298	840.9	1175.2	334.3	-	12.4	-	Mix
177	FC(F)(Cl)Cl	1.0	243	1488.0	1515.8	27.8	20.1	21.8	1.7	Mix
178	FC(F)(Cl)Cl	6.7	298	1307.0	1366.8	59.8	-	19.6	-	Mix
179	FC(Cl)(Cl)Cl	1.1	298	1477.0	1512.0	35.0	24.9	27.0	2.2	Mix
180	FC(F)(F)I	20.0	298	2046.8	2420.9	374.1	-	26.6	-	Mix
181	FC(F)(F)I	1.0	281	-	2594.4	-	22.5	28.4	5.9	Mix
182	FC(Cl)Br	1.0	273	1977.1	2058.3	81.2	-	32.1	-	Mix
183	FC(F)(Cl)Br	1.0	269	1899.6	2004.0	104.4	23.1	27.0	3.9	Mix
184	FC(F)(Cl)Br	2.6	298	1810.0	1921.1	111.1	-	25.8	-	Mix
185	FC(Cl)(Cl)Br	1.0	295	1950.0	1990.5	40.5	-	32.8	-	Mix
186	FC(Cl)(Cl)Br	0.4	298	-	1985.4	-	29.1	32.7	3.6	Mix
187	FC(Cl)(Br)Br	1.0	295	2317.3	2433.9	116.6	-	38.3	-	Mix
188	CC(Cl)Br	1.0	305	-	1627.4	-	33.1	34.0	0.9	Mix
189	CC(F)Cl	1.4	298	-	1047.1	-	23.7	24.8	1.1	Mix
190	FCCCl	1.0	303	-	1144.3	-	32.1	28.1	-4.0	Mix
191	CC(F)(F)Cl	1.0	263	-	1166.4	-	22.7	22.9	0.2	Mix
192	FCC(F)Cl	0.8	298	-	1297.4	-	26.6	28.5	2.0	Mix
193	FC(F)CCl	1.0	288	1312.0	1321.5	9.5	-	30.7	-	Mix
194	FC(F)CCl	0.7	298	-	1302.9	-	26.6	30.2	3.6	Mix
195	CC(F)(Cl)Cl	0.8	298	-	1229.3	-	26.0	27.5	1.5	Mix
196	FC(Cl)CCl	0.1	298	-	1374.8	-	32.8	35.2	2.4	Mix
197	ClC(Cl)(Br)CBr	1.0	273	2298.0	2321.8	23.8	-	55.5	-	Mix
198	ClC(Cl)(Br)CBr	1.0	369	-	2152.3	-	45.9	49.6	3.7	Mix
199	ClC(Br)C(Cl)Br	1.0	293	2135.0	2313.7	178.7	-	55.3	-	Mix
200	ClC(Br)C(Cl)Br	1.0	335	-	2238.0	-	45.9	52.6	6.7	Mix
201	FC(F)(Cl)CCl	0.4	298	-	1412.6	-	28.3	32.2	3.9	Mix
202	FC(Cl)C(F)Cl	0.4	298	1405.4	1488.8	83.4	-	33.6	-	Mix
203	FC(F)(F)CBr	1.0	293	1788.1	1763.3	-24.8	-	29.8	-	Mix
204	FC(F)(F)CCl	1.9	298	-	1288.1	-	22.3	25.7	3.4	Mix
205	FC(Cl)(Cl)CCl	0.1	298	-	1502.6	-	34.7	38.8	4.1	Mix
206	FCC(Cl)(Cl)Cl	0.1	298	1575.0	1527.5	-47.5	-	38.9	-	Mix
207	FC(Cl)C(Cl)Cl	0.0	298	-	1536.5	-	36.9	38.7	1.8	Mix
208	ClCCCBr	1.0	341	-	1515.2	-	42.0	41.0	-1.0	Mix
209	CC(C)(F)Cl	0.1	298	-	964.5	-	31.5	27.1	-4.4	Mix
210	CC(F)(F)CCl	0.4	298	1191.6	1144.8	-46.8	-	30.7	-	Mix
211	FC(F)(F)CCCl	0.5	298	1290.1	1217.5	-72.5	-	27.2	-	Mix
212	FC(F)(F)CCCl	1.0	306	-	1200.8	-	29.9	26.8	-3.1	Mix
213	FCCCCCl	0.0	298	1062.7	1062.6	-0.1	-	40.1	-	Mix
214	CC(Cl)C(F)(F)F	1.0	313	-	1815.5	-	30.4	40.4	10.0	Mix
215	CC(I)CC(F)(F)F	1.0	312	-	1774.2	-	32.4	39.3	6.9	Mix
216	CCC(C)CBr	1.0	321	-	1186.2	-	37.9	38.3	0.4	Br
217	CC(C)CCBr	0.0	298	-	1208.9	-	39.7	39.8	0.1	Br
218	CC(Br)C(C)(C)Br	1.0	298	1663.0	1687.1	24.1	-	50.7	-	Br
219	CC(Br)C(C)(C)Br	0.0	335	-	1637.1	-	-	48.6	-	Br
220	CC(C)C(C)(Br)Br	0.0	337	1622.0	1624.2	2.2	-	46.4	-	Br
221	CC(C)(CBr)CBr	1.0	293	1693.4	1719.1	25.7	-	52.3	-	Br
222	CC(C)(CBr)CBr	0.0	345	-	1651.4	-	-	49.3	-	Br
223	CCC(C)(Br)CBr	1.0	294	1663.8	1694.7	30.9	-	49.3	-	Br
224	CCC(C)(Br)CBr	0.0	337	-	1638.3	-	-	47.0	-	Br
225	CCC(Br)(Br)CC	0.0	332	1610.0	1621.5	11.6	-	46.7	-	Br
226	CC(C)(Br)CCBr	1.0	273	1696.0	1711.5	15.5	-	52.8	-	Br
227	CC(C)(Br)CCBr	0.0	337	-	1626.8	-	-	49.4	-	Br
228	CCCC(C)(Br)Br	1.0	289	1645.2	1664.2	19.0	-	49.6	-	Br
229	CCCC(C)(Br)Br	0.0	335	-	1602.5	-	-	47.3	-	Br
230	CC(Br)C(C)CBr	0.0	337	1751.0	1635.9	-115.1	-	49.9	-	Br
231	CCC(C)C(Br)Br	0.0	337	1602.8	1614.0	11.3	-	47.8	-	Br
232	CC(C)C(Br)CBr	1.0	293	1677.0	1689.5	12.5	-	51.0	-	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
233	CC(C)C(Br)CBr	0.0	337	-	1629.1	-	-	48.7	-	Br
234	CCC(Br)C(C)Br	1.0	293	1673.0	1675.2	2.2	-	51.8	-	Br
235	CCC(Br)C(C)Br	0.0	341	-	1610.6	-	-	48.9	-	Br
236	CC(C)CC(Br)Br	0.0	337	1602.8	1597.9	-4.8	-	48.0	-	Br
237	CC(Br)CC(C)Br	1.0	293	1665.9	1659.7	-6.2	-	50.8	-	Br
238	CC(Br)CC(C)Br	0.0	344	-	1589.6	-	-	48.0	-	Br
239	CC(CBr)CCBr	1.0	293	1711.5	1702.7	-8.8	-	55.6	-	Br
240	CC(CBr)CCBr	0.0	337	-	1643.8	-	-	53.0	-	Br
241	CCC(Br)CCBr	1.0	293	1665.3	1683.1	17.8	-	53.0	-	Br
242	CCC(Br)CCBr	0.0	351	-	1605.6	-	-	49.8	-	Br
243	CCCC(Br)CBr	1.0	293	1670.8	1680.1	9.3	49.0	52.4	3.4	Br
244	CC(Br)CCCBr	1.0	293	1683.0	1681.9	-1.1	-	54.8	-	Br
245	CC(Br)CCCBr	1.0	392	-	1547.4	-	51.8	49.0	-2.8	Br
246	CCCCC(Br)Br	0.0	343	1588.3	1590.6	2.3	-	48.8	-	Br
247	CCCCC(Br)Br	1.0	375	-	1545.0	-	48.8	47.0	-1.8	Br
248	BrCCCCCBr	1.0	298	1694.0	1691.5	-2.5	-	57.1	-	Br
249	BrCCCCCBr	1.0	411	-	1539.0	-	54.4	50.3	-4.1	Br
250	CC(Br)C(C)(Br)CBr	1.0	293	2082.1	2095.9	13.8	-	63.8	-	Br
251	CC(CBr)(CBr)CBr	1.0	293	2091.7	2120.8	29.1	-	66.0	-	Br
252	CCCCC(Br)(Br)Br	1.0	293	1988.2	2013.5	25.3	-	60.9	-	Br
253	CCCCC(Br)(Br)Br	0.1	427	-	1812.9	-	-	52.9	-	Br
254	BrCCC(Br)CCBr	1.0	292	2065.0	2069.1	4.1	-	68.3	-	Br
255	BrCCCC(Br)CBr	1.0	295	2073.0	2065.1	-7.9	-	68.8	-	Br
256	CCC(C)(C)CBr	0.0	311	1150.8	1181.5	30.7	-	41.9	-	Br
257	CC(C)(C)CCBr	1.0	293	1155.6	1187.8	32.2	-	43.6	-	Br
258	CC(C)(C)CCBr	0.0	308	-	1171.6	-	-	42.9	-	Br
259	CC(C)C(C)CBr	1.0	298	1190.0	1182.3	-7.7	-	42.9	-	Br
260	CC(C)C(C)CBr	0.0	311	-	1168.5	-	-	42.3	-	Br
261	CCC(C)C(C)Br	0.0	303	1163.1	1167.3	4.2	-	41.9	-	Br
262	CCC(Br)C(C)C	0.0	303	1163.1	1162.6	-0.5	-	41.8	-	Br
263	CC(C)CC(C)Br	0.0	303	1144.3	1152.7	8.4	40.9	41.8	1.0	Br
264	CCC(CC)CBr	0.0	313	1159.9	1162.7	2.8	42.7	42.8	0.1	Br
265	CCC(C)CCBr	1.0	296	1171.0	1178.9	7.9	-	44.3	-	Br
266	CCC(C)CCBr	0.0	317	-	1155.8	-	-	43.3	-	Br
267	CCCC(C)CBr	1.0	293	1177.9	1179.1	1.2	-	44.2	-	Br
268	CCCC(C)CBr	0.0	314	-	1155.2	-	-	43.0	-	Br
269	CCCC(Br)CC	0.0	312	-	1147.2	-	42.5	42.4	-0.1	Br
270	CC(C)CCCBr	1.0	293	1168.3	1174.9	6.6	-	44.6	-	Br
271	CC(C)CCCBr	0.0	316	-	1149.4	-	-	43.4	-	Br
272	CCCCC(C)Br	1.0	298	1159.7	1159.8	0.1	-	43.5	-	Br
273	CCCCC(C)Br	1.0	318	-	1137.7	-	43.8	42.5	-1.3	Br
274	CC(C)(Br)C(C)(C)Br	0.3	435	-	1467.7	-	-	47.2	-	Br
275	CC(C)C(C)(Br)CBr	0.1	400	1450.3	1499.2	48.9	-	47.4	-	Br
276	CC(C)(C)C(Br)CBr	0.1	400	1462.2	1496.8	34.6	-	51.4	-	Br
277	CCCCC(C)(Br)Br	1.0	295	1546.3	1574.2	27.9	-	53.8	-	Br
278	CCCCC(C)(Br)Br	0.1	400	-	1436.8	-	-	47.7	-	Br
279	CC(C)C(CBr)CBr	1.0	293	1605.0	1623.6	18.6	-	57.2	-	Br
280	CC(CBr)C(C)CBr	0.1	400	1465.9	1490.4	24.4	-	51.8	-	Br
281	CCC(Br)C(Br)CC	1.0	293	1602.7	1590.4	-12.3	-	53.9	-	Br
282	CCC(Br)C(Br)CC	0.1	400	-	1452.7	-	-	47.9	-	Br
283	CCCC(Br)C(C)Br	1.0	293	1581.2	1587.9	6.7	-	54.8	-	Br
284	CCCC(Br)C(C)Br	0.1	400	-	1449.1	-	-	48.3	-	Br
285	CC(Br)CCC(C)Br	1.0	293	1578.8	1581.2	2.4	-	56.9	-	Br
286	CC(Br)CCC(C)Br	0.0	365	-	1489.4	-	49.5	52.3	2.8	Br
287	CCCC(CBr)CBr	1.0	293	1577.1	1612.8	35.7	-	58.4	-	Br
288	CC(CCBr)CCBr	0.1	426	1395.4	1446.3	50.9	50.8	52.1	1.3	Br
289	CCC(Br)CCCBr	0.1	400	1443.8	1460.4	16.6	-	51.8	-	Br
290	CCCCC(Br)CBr	1.0	293	1560.4	1591.0	30.6	56.5	56.7	0.2	Br
291	CC(Br)CCCCBr	0.1	400	1415.4	1459.1	43.7	-	52.8	-	Br
292	CCCCCC(Br)Br	0.1	400	1416.2	1434.7	18.5	-	49.7	-	Br
293	CCCCCC(Br)Br	1.0	393	-	1445.6	-	51.6	50.2	-1.4	Br
294	BrCCCCCCBr	1.0	298	1602.5	1601.4	-1.1	-	61.6	-	Br
295	BrCCCCCCBr	0.0	364	-	1520.2	-	57.1	57.3	0.2	Br

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
296	CCC(CBr)(CBr)CBr	1.0	293	1912.2	2014.8	102.6	-	70.0	-	Br
297	CCCC(Br)CCC	1.0	296	1133.0	1134.7	1.7	-	47.8	-	Br
298	CCCC(Br)CCC	0.0	327	-	1101.4	-	-	46.0	-	Br
299	CCCCC(Br)CC	1.0	295	1134.1	1135.5	1.4	-	47.7	-	Br
300	CCCCCC(C)Br	0.0	320	1095.5	1106.3	10.7	46.2	46.8	0.6	Br
301	CCC(Br)(CBr)C(C)C	1.0	293	1526.1	1573.0	46.9	-	58.1	-	Br
302	CC(C)(C)CC(Br)CBr	1.0	293	1502.0	1537.1	35.1	-	57.6	-	Br
303	CCCC(Br)(CC)CBr	1.0	293	1492.9	1552.3	59.4	-	59.3	-	Br
304	CC(C)(CCBr)CCBr	1.0	293	1532.0	1567.5	35.5	-	64.7	-	Br
305	CCCC(Br)C(Br)CC	1.0	293	1516.2	1520.9	4.7	-	58.6	-	Br
306	CCCC(Br)C(Br)CC	0.1	418	-	1368.7	-	-	50.6	-	Br
307	CCCCC(Br)C(C)Br	1.0	293	1513.2	1519.5	6.3	-	58.6	-	Br
308	CCCCC(Br)C(C)Br	0.1	418	-	1364.8	-	-	50.7	-	Br
309	CCC(Br)CCCCBr	0.1	418	-	1378.4	-	-	55.0	-	Br
310	CCCCCC(Br)CBr	1.0	293	1518.0	1520.8	2.8	-	61.1	-	Br
311	CCCCCC(Br)CBr	1.0	300	-	1512.5	-	54.4	60.7	6.3	Br
312	CCCCCCC(Br)Br	1.0	294	1500.0	1505.0	5.0	-	60.7	-	Br
313	CCCCCCC(Br)Br	1.0	410	-	1365.8	-	54.4	53.2	-1.2	Br
314	BrCCCCCCCBr	0.0	385	1469.2	1428.8	-40.4	57.8	60.2	2.4	Br
315	CC(C)CCCC(C)Br	1.0	293	1091.0	1107.3	16.3	-	51.7	-	Br
316	CCCCCCC(C)Br	1.0	298	1096.8	1104.6	7.8	-	52.7	-	Br
317	CCCCCCC(C)Br	1.0	358	-	1045.8	-	48.4	49.0	0.6	Br
318	CCC(C)(C)CC(Br)CBr	1.0	293	1468.9	1492.3	23.4	-	61.9	-	Br
319	CCCC(Br)C(Br)CCC	0.1	435	-	1298.2	-	-	53.2	-	Br
320	CCCCC(Br)CCCBr	0.1	435	-	1305.9	-	-	57.2	-	Br
321	CCCC(Br)CCCCBr	0.1	435	-	1306.7	-	-	57.6	-	Br
322	CCCCCCC(Br)CBr	1.0	293	1458.0	1462.1	4.1	-	65.6	-	Br
323	CCCCCCC(Br)CBr	0.1	435	-	1300.2	-	-	56.0	-	Br
324	CCCCCCCC(Br)Br	0.1	435	-	1287.8	-	-	55.5	-	Br
325	CCCCCCCC(Br)Br	1.0	427	-	1297.5	-	57.1	56.1	-1.0	Br
326	BrCCCCCCCCBr	0.0	399	1413.1	1359.2	-53.9	59.6	63.2	3.6	Br
327	CCCCCCCC(C)Br	1.0	298	1076.0	1084.8	8.8	-	57.3	-	Br
328	CCCCCCCCCBr	1.0	298	1084.9	1092.8	7.9	-	59.4	-	Br
329	CCCCCCCCCBr	1.0	391	-	1005.4	-	53.1	53.0	-0.1	Br
330	CCCCCCCC(Br)CBr	1.0	293	1398.0	1414.1	16.1	-	70.1	-	Br
331	CCCCCCCC(Br)CBr	0.1	451	-	1241.5	-	-	58.7	-	Br
332	CCCCCCCCC(Br)Br	0.1	451	-	1230.1	-	-	58.2	-	Br
333	CCCCCCCCC(Br)Br	1.0	442	-	1241.2	-	59.5	58.8	-0.7	Br
334	BrCCCCCCCCCBr	1.0	298	1428.0	1420.2	-7.8	-	75.1	-	Br
335	BrCCCCCCCCCBr	0.0	415	-	1298.4	-	61.8	65.9	4.1	Br
336	CCCCCCCCC(C)Br	1.0	298	1047.0	1067.5	20.5	-	61.8	-	Br
337	CCCCCCCCC(C)Br	0.0	383	-	990.6	-	-	55.7	-	Br
338	CCCCCCCCCCBr	1.0	298	1062.5	1074.5	12.0	-	63.9	-	Br
339	CCCCCCCCCCBr	1.0	398	-	985.1	-	56.6	56.6	0.0	Br
340	CCCCCCCCC(Br)CBr	1.0	383	-	1280.7	-	67.0	67.6	0.6	Br
341	CCCCCCCCCC(Br)Br	1.0	457	-	1191.9	-	62.2	61.6	-0.6	Br
342	CCC(C)CCl	0.0	298	-	877.7	-	36.3	36.5	0.1	Cl
343	CC(Cl)C(C)(C)Cl	0.0	307	1080.9	1062.5	-18.4	-	40.7	-	Cl
344	CC(C)C(C)(Cl)Cl	0.0	333	1051.1	1032.2	-18.9	-	40.3	-	Cl
345	CC(C)(CCl)CCl	0.0	314	1066.8	1093.5	26.6	-	45.5	-	Cl
346	CCC(C)(Cl)CCl	0.0	306	1061.9	1074.4	12.5	35.9	41.3	5.5	Cl
347	CCC(Cl)(Cl)CC	0.0	303	1043.7	1053.7	10.0	40.3	41.2	1.0	Cl
348	CC(C)(Cl)CCCl	1.0	293	1075.8	1083.7	7.9	-	45.2	-	Cl
349	CC(C)(Cl)CCCl	0.0	314	-	1063.5	-	-	44.0	-	Cl
350	CCCC(C)(Cl)Cl	0.0	299	1034.6	1048.3	13.7	40.0	42.3	2.3	Cl
351	CC(Cl)C(C)CCl	1.0	293	1093.8	1095.2	1.4	-	46.4	-	Cl
352	CC(Cl)C(C)CCl	0.0	313	-	1075.1	-	-	45.3	-	Cl
353	CCC(C)C(Cl)Cl	0.0	302	1045.7	1062.8	17.2	-	42.6	-	Cl
354	CC(C)C(Cl)CCl	1.0	293	1080.5	1087.5	7.0	-	43.2	-	Cl
355	CC(C)C(Cl)CCl	0.0	312	-	1068.6	-	42.1	42.0	-0.1	Cl
356	CCC(Cl)C(C)Cl	1.0	298	1075.0	1075.2	0.2	-	47.1	-	Cl
357	CCC(Cl)C(C)Cl	0.0	309	-	1064.0	-	41.6	46.0	4.4	Cl
358	CC(C)CC(Cl)Cl	1.0	293	1047.3	1061.5	14.2	-	42.9	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
359	CC(C)CC(Cl)Cl	0.0	302	-	1051.6	-	40.1	42.6	2.5	Cl
360	CC(Cl)CC(C)Cl	1.0	291	1063.0	1069.1	6.1	-	45.1	-	Cl
361	CC(Cl)CC(C)Cl	0.0	317	-	1042.8	-	41.5	43.6	2.1	Cl
362	CC(CCl)CCCl	1.0	294	1103.0	1103.9	0.9	-	49.8	-	Cl
363	CC(CCl)CCCl	0.0	324	-	1074.1	-	-	47.8	-	Cl
364	CCC(Cl)CCCl	1.0	293	1083.4	1084.6	1.2	-	46.3	-	Cl
365	CCC(Cl)CCCl	0.0	322	-	1055.7	-	-	44.6	-	Cl
366	CCCC(Cl)CCl	1.0	298	1074.1	1076.3	2.2	43.9	44.4	0.5	Cl
367	CC(Cl)CCCCl	1.0	293	1073.4	1087.2	13.8	48.1	48.7	0.6	Cl
368	CCCCC(Cl)Cl	0.0	304	1041.7	1049.2	7.5	-	43.4	-	Cl
369	CCCCC(Cl)Cl	1.0	298	-	1055.8	-	44.3	43.7	-0.6	Cl
370	CC(C)(Cl)C(C)(Cl)Cl	0.0	342	1144.6	1229.3	84.7	-	53.4	-	Cl
371	CC(Cl)C(C)(Cl)CCl	0.0	343	1184.5	1223.1	38.6	-	49.9	-	Cl
372	CC(C)(Cl)C(Cl)CCl	1.0	293	1264.1	1266.4	2.3	-	53.5	-	Cl
373	CC(CCl)(CCl)CCl	0.0	338	1215.5	1258.5	42.9	-	52.9	-	Cl
374	CCCCC(Cl)(Cl)Cl	0.0	298	1183.9	1196.0	12.1	-	47.9	-	Cl
375	CCC(C)(C)CCl	0.0	298	874.6	892.6	18.0	-	39.8	-	Cl
376	CC(C)(C)CCCl	0.0	298	863.1	884.5	21.5	38.5	40.3	1.8	Cl
377	CC(C)C(C)CCl	1.0	298	881.6	883.8	2.2	-	40.0	-	Cl
378	CC(C)C(C)CCl	0.0	298	-	883.5	-	-	40.0	-	Cl
379	CCC(C)C(C)Cl	0.0	298	869.9	874.8	4.9	-	39.8	-	Cl
380	CCC(Cl)C(C)C	0.0	298	869.9	870.8	0.9	-	39.4	-	Cl
381	CC(C)CC(C)Cl	0.0	298	855.9	863.6	7.6	-	39.5	-	Cl
382	CCC(CC)CCl	0.0	300	884.2	879.7	-4.5	-	40.6	-	Cl
383	CCC(C)CCCl	1.0	300	892.0	877.1	-14.9	-	40.9	-	Cl
384	CCC(C)CCCl	0.0	303	-	875.1	-	-	40.8	-	Cl
385	CCCC(C)CCl	0.0	298	869.9	876.3	6.5	-	40.9	-	Cl
386	CCCC(Cl)CC	1.0	297	871.0	867.1	-3.9	-	40.3	-	Cl
387	CCCC(Cl)CC	0.0	298	-	866.0	-	39.9	40.2	0.3	Cl
388	CC(C)CCCCl	0.0	300	868.5	872.0	3.5	-	41.1	-	Cl
389	CCCCC(C)Cl	0.0	299	864.8	864.0	-0.8	41.2	40.6	-0.6	Cl
390	CC(C)(C)C(C)(Cl)Cl	0.0	317	-	1103.3	-	-	49.2	-	Cl
391	CC(C)(C)CC(Cl)Cl	1.0	293	1027.1	1053.0	25.9	-	46.1	-	Cl
392	CC(C)(C)CC(Cl)Cl	0.0	322	-	1025.3	-	41.8	44.4	2.7	Cl
393	CC(Cl)CC(C)(C)Cl	1.0	293	1036.0	1051.0	15.0	-	46.8	-	Cl
394	CCCCC(C)(Cl)Cl	1.0	298	1015.0	1030.6	15.6	-	46.9	-	Cl
395	CCCCC(C)(Cl)Cl	0.0	338	-	991.9	-	-	44.6	-	Cl
396	CCC(Cl)C(Cl)CC	1.0	293	1061.7	1061.6	-0.1	-	52.3	-	Cl
397	CCCC(Cl)C(C)Cl	0.0	334	1015.7	1014.4	-1.3	-	47.2	-	Cl
398	CCCC(Cl)CCCl	0.0	343	-	1010.7	-	-	47.6	-	Cl
399	CCC(Cl)CCCCl	0.0	350	-	1009.5	-	-	48.9	-	Cl
400	CCCCC(Cl)CCl	1.0	293	1080.0	1056.2	-23.8	48.2	49.0	0.8	Cl
401	CC(Cl)CCCCCl	1.0	293	1108.6	1062.9	-45.7	-	54.1	-	Cl
402	CCCCCC(Cl)Cl	0.0	335	987.4	998.1	10.7	-	46.0	-	Cl
403	CCCCCC(Cl)Cl	1.0	298	-	1034.2	-	48.7	48.2	-0.5	Cl
404	CCCCCC(Cl)(Cl)Cl	0.1	390	1033.3	1065.6	32.3	-	46.7	-	Cl
405	CC(C)(C)C(C)(C)Cl	0.0	298	864.3	961.4	97.1	-	46.9	-	Cl
406	CCC(C)(Cl)C(C)C	0.0	301	861.7	889.4	27.7	-	42.7	-	Cl
407	CCC(C)C(C)(C)Cl	0.0	301	-	883.8	-	-	42.9	-	Cl
408	CC(Cl)CC(C)(C)C	0.0	302	852.3	871.2	19.0	-	42.4	-	Cl
409	CC(C)CC(C)(C)Cl	1.0	293	862.8	869.2	6.4	-	41.9	-	Cl
410	CC(C)CC(C)(C)Cl	0.0	302	-	862.5	-	-	41.5	-	Cl
411	CCC(Cl)(CC)CC	0.0	314	865.9	871.7	5.8	-	42.0	-	Cl
412	CCCC(C)(Cl)CC	0.0	308	865.5	867.5	2.0	-	42.7	-	Cl
413	CCCCC(C)(C)Cl	1.0	293	863.5	870.6	7.1	-	43.7	-	Cl
414	CCCCC(C)(C)Cl	0.0	309	-	856.9	-	-	42.8	-	Cl
415	CC(C)CCC(C)Cl	0.0	309	848.9	853.7	4.8	-	43.3	-	Cl
416	CCCC(C)CCCl	0.0	320	851.3	858.0	6.7	-	44.2	-	Cl
417	CCCC(Cl)CCC	1.0	295	869.4	869.0	-0.4	-	45.1	-	Cl
418	CCCC(Cl)CCC	0.0	315	-	852.2	-	-	43.9	-	Cl
419	CCCCC(Cl)CC	1.0	298	857.9	866.3	8.5	-	44.7	-	Cl
420	CCCCC(Cl)CC	0.0	315	-	852.2	-	-	43.8	-	Cl
421	CCCCCC(C)Cl	1.0	295	865.1	867.4	2.3	-	45.3	-	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
422	CCCCCC(C)Cl	1.0	328	-	838.9	-	44.8	43.4	-1.4	Cl
423	CC(C)(Cl)CC(C)(C)Cl	0.0	339	986.3	1000.1	13.8	-	48.0	-	Cl
424	CCC(C)(C)CC(Cl)Cl	1.0	293	1032.1	1047.4	15.3	-	50.5	-	Cl
425	CC(C)(C)CC(Cl)CCl	1.0	293	1025.9	1047.4	21.5	-	50.1	-	Cl
426	CC(C)(C)CC(Cl)CCl	0.0	344	-	1001.7	-	45.1	47.2	2.1	Cl
427	CC(C)(CCCl)CCCl	1.0	293	1056.3	1079.3	23.0	-	59.3	-	Cl
428	CC(C)(CCCl)CCCl	0.0	339	-	1039.6	-	-	56.2	-	Cl
429	CCCC(Cl)(Cl)CCC	0.0	349	1021.9	976.1	-45.9	-	48.1	-	Cl
430	CCCCCC(C)(Cl)Cl	0.0	340	968.2	974.7	6.5	-	48.7	-	Cl
431	CCCCCC(Cl)CCl	1.0	293	1062.5	1035.7	-26.8	53.2	53.4	0.2	Cl
432	CCCCCCC(Cl)Cl	0.0	353	995.8	966.1	-29.7	-	49.2	-	Cl
433	CCCCCCC(Cl)Cl	1.0	298	-	1017.2	-	53.5	52.7	-0.8	Cl
434	ClCCCCCCCCl	1.0	298	1040.8	1048.5	7.7	61.2	60.6	-0.6	Cl
435	CCCCCCC(Cl)(Cl)Cl	1.0	298	1121.2	1134.0	12.8	-	56.9	-	Cl
436	CCCCCCC(Cl)(Cl)Cl	0.1	410	-	1021.7	-	-	49.5	-	Cl
437	ClCCCCCCC(Cl)Cl	1.0	293	1174.4	1175.3	0.9	-	67.0	-	Cl
438	CCC(C)(C)C(C)(C)Cl	1.0	298	906.5	919.6	13.1	-	47.7	-	Cl
439	CCC(C)(Cl)C(C)(C)C	1.0	293	906.6	922.0	15.4	-	47.8	-	Cl
440	CC(C)(C)CC(C)(C)Cl	1.0	293	874.1	882.2	8.1	-	45.2	-	Cl
441	CC(C)(C)CC(C)(C)Cl	0.0	332	-	850.2	-	-	43.0	-	Cl
442	CC(C)C(C)C(C)(C)Cl	1.0	293	888.0	894.8	6.8	-	46.3	-	Cl
443	CCCC(C)(Cl)C(C)C	0.0	332	834.5	861.8	27.3	-	45.6	-	Cl
444	CC(C)CCC(C)(C)Cl	0.0	332	-	836.0	-	-	44.4	-	Cl
445	CCCC(C)(Cl)CCC	0.0	332	834.8	847.5	12.7	-	45.8	-	Cl
446	CCCCC(C)(Cl)CC	0.0	328	845.6	850.3	4.7	-	45.8	-	Cl
447	CCCCCC(C)(C)Cl	1.0	298	856.8	865.7	8.9	-	47.8	-	Cl
448	CCCCCC(C)(C)Cl	0.0	328	-	840.7	-	-	45.9	-	Cl
449	CC(C)CCCC(C)Cl	0.0	328	-	838.0	-	-	46.6	-	Cl
450	CCCCC(CC)CCl	1.0	293	876.9	881.8	4.9	-	49.8	-	Cl
451	CCCCC(CC)CCl	0.0	337	-	845.1	-	47.4	47.0	-0.4	Cl
452	CCC(C)CCCCCl	0.0	336	-	844.7	-	-	47.7	-	Cl
453	CCCCCCC(C)Cl	1.0	298	861.5	864.9	3.5	-	49.7	-	Cl
454	CCCCCCC(C)Cl	1.0	345	-	825.8	-	47.8	46.7	-1.1	Cl
455	CC(C)(Cl)CCC(C)(C)Cl	0.0	363	-	957.3	-	-	50.3	-	Cl
456	CCC(C)(C)CC(Cl)CCl	1.0	293	1029.0	1042.0	13.0	-	54.4	-	Cl
457	CCCCCC(Cl)C(C)Cl	0.0	368	-	950.1	-	-	51.6	-	Cl
458	CCCCCCC(Cl)CCl	1.0	298	-	1015.8	-	57.6	57.5	-0.1	Cl
459	CCCCCCCC(Cl)Cl	0.0	370	-	939.6	-	-	52.3	-	Cl
460	CCCCCCCC(Cl)Cl	1.0	298	-	1003.5	-	57.7	57.2	-0.5	Cl
461	ClCCCCCCCCCl	1.0	298	1024.8	1030.8	6.0	65.6	64.9	-0.7	Cl
462	CCCCCCCC(Cl)(Cl)Cl	0.1	430	948.0	984.6	36.6	-	51.9	-	Cl
463	CCC(Cl)(CC)C(C)(C)C	0.0	344	-	884.4	-	-	48.3	-	Cl
464	CCCC(C)(Cl)C(C)(C)C	0.0	340	858.2	880.4	22.2	-	49.4	-	Cl
465	CCCCC(Cl)(CC)CC	0.0	351	836.3	840.4	4.1	-	48.3	-	Cl
466	CCCCC(C)(Cl)CCC	0.0	347	827.0	836.0	9.0	-	49.0	-	Cl
467	CCCCCC(C)(Cl)CC	0.0	347	826.8	835.5	8.7	-	48.9	-	Cl
468	CCCCCC(Cl)C(C)C	1.0	293	856.6	873.8	17.2	-	53.2	-	Cl
469	CCCCC(Cl)CCCC	0.0	351	815.6	824.6	9.0	-	50.2	-	Cl
470	CCCCCCC(Cl)CC	0.0	352	807.5	823.3	15.8	-	50.2	-	Cl
471	CCCCCCCC(C)Cl	1.0	293	879.0	869.3	-9.7	-	54.6	-	Cl
472	CCCCCCCCCCl	1.0	298	867.4	872.6	5.2	55.9	55.9	0.0	Cl
473	CC(C)(Cl)CCCC(C)(C)Cl	0.0	374	-	936.2	-	-	54.9	-	Cl
474	CCCCCCCC(Cl)CCl	1.0	298	-	1002.9	-	62.1	62.0	-0.1	Cl
475	CCCCCCCCCC(Cl)Cl	0.1	436	-	871.4	-	-	51.7	-	Cl
476	CCCCCCCCCC(Cl)Cl	1.0	298	-	992.5	-	62.3	61.7	-0.6	Cl
477	ClCCCCCCCCCCCl	1.0	298	1017.3	1016.2	-1.1	-	69.2	-	Cl
478	ClCCCCCCCCCCCl	0.1	453	-	885.9	-	54.6	57.0	2.4	Cl
479	CCCCCCCCC(Cl)(Cl)Cl	0.1	449	914.4	952.6	38.2	-	54.4	-	Cl
480	CCCCCCCCC(C)Cl	1.0	293	870.6	869.1	-1.5	-	59.0	-	Cl
481	CCCCCCCCCCl	1.0	298	865.8	872.6	6.8	64.0	60.5	-3.5	Cl
482	CCCCCCCCCC(Cl)Cl	0.1	456	-	847.0	-	-	54.0	-	Cl
483	CCCCCCCCCC(Cl)Cl	1.0	430	-	871.8	-	56.9	56.0	-0.9	Cl
484	ClCCCCCCCCCCCl	1.0	298	992.9	1004.0	11.1	73.1	73.5	0.4	Cl

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
485	CCCCCCCCCC(Cl)(Cl)Cl	0.1	439	917.0	951.5	34.5	52.5	58.6	6.1	Cl
486	CCC(C)CF	1.0	302	-	782.5	-	30.7	30.6	-0.1	F
487	CC(C)CCF	1.0	293	694.1	790.6	96.5	-	31.0	-	F
488	CC(C)CCF	0.4	298	-	785.0	-	-	30.8	-	F
489	CCCCCF	0.2	298	-	787.4	-	30.9	31.8	0.8	F
490	CC(F)C(C)(C)F	0.1	298	-	870.4	-	-	27.8	-	F
491	CC(C)C(C)(F)F	0.1	298	-	871.7	-	-	30.4	-	F
492	CC(C)(CF)CF	0.1	298	-	960.8	-	-	35.7	-	F
493	CCC(C)(F)CF	0.1	298	-	894.0	-	-	29.0	-	F
494	CCC(F)(F)CC	1.0	293	910.6	869.1	-41.5	-	30.4	-	F
495	CCC(F)(F)CC	1.0	277	-	887.2	-	33.8	31.2	-2.6	F
496	CC(C)(F)CCF	0.1	298	-	912.0	-	-	33.2	-	F
497	CCCC(C)(F)F	1.0	293	898.7	862.3	-36.4	-	30.9	-	F
498	CCCC(C)(F)F	1.0	277	-	882.1	-	33.7	31.8	-1.9	F
499	CC(F)C(C)CF	0.1	298	-	939.6	-	-	35.5	-	F
500	CCC(C)C(F)F	0.1	298	-	918.1	-	-	33.8	-	F
501	CC(C)C(F)CF	0.1	298	-	917.2	-	-	30.8	-	F
502	CCC(F)C(C)F	0.1	298	-	898.5	-	-	29.8	-	F
503	CC(C)CC(F)F	0.1	298	-	908.5	-	-	33.2	-	F
504	CC(F)CC(C)F	0.1	298	-	905.7	-	-	34.6	-	F
505	CC(CF)CCF	0.1	298	-	962.7	-	-	36.8	-	F
506	CCC(F)CCF	0.1	298	-	932.3	-	-	35.4	-	F
507	CCCC(F)CF	0.1	298	-	918.7	-	-	32.1	-	F
508	CC(F)CCCF	0.1	298	-	935.7	-	-	36.3	-	F
509	CCCCC(F)F	0.1	298	-	908.1	-	-	33.9	-	F
510	CCCCC(F)F	1.0	283	-	925.6	-	34.4	34.7	0.3	F
511	FCCCCCF	1.0	298	957.2	968.2	11.0	-	40.0	-	F
512	FCCCCCF	0.0	298	-	967.9	-	-	40.0	-	F
513	CC(C)CC(F)(F)F	1.0	298	978.8	940.2	-38.6	-	28.5	-	F
514	CCCCC(F)(F)F	1.0	293	970.1	946.2	-23.9	-	29.8	-	F
515	CCCCC(F)(F)F	0.3	298	-	939.4	-	-	29.5	-	F
516	CCC(C)(C)CF	0.1	298	-	809.2	-	-	34.0	-	F
517	CC(C)(C)CCF	1.0	293	780.9	811.1	30.2	-	34.5	-	F
518	CC(C)(C)CCF	0.1	298	-	806.7	-	-	34.3	-	F
519	CC(C)C(C)CF	0.1	298	-	804.6	-	-	34.2	-	F
520	CCC(C)C(C)F	0.1	298	-	786.6	-	-	33.8	-	F
521	CCC(F)C(C)C	0.1	298	-	780.5	-	-	33.8	-	F
522	CC(C)CC(C)F	0.1	298	-	776.7	-	-	33.8	-	F
523	CCC(C)CCF	0.1	298	-	802.1	-	-	35.2	-	F
524	CCCC(C)CF	0.1	298	-	798.1	-	-	35.3	-	F
525	CCCC(F)CC	0.1	298	-	779.7	-	-	34.5	-	F
526	CCCC(F)CC	1.0	296	-	781.4	-	36.8	34.7	-2.1	F
527	CC(C)CCCF	0.1	298	-	796.5	-	-	35.3	-	F
528	CCCCC(C)F	0.1	298	-	778.6	-	-	34.7	-	F
529	CCCCCCF	0.1	298	-	798.6	-	35.6	36.2	0.7	F
530	CCCCCC(F)F	0.1	310	-	890.5	-	-	37.5	-	F
531	CCCCCC(F)F	1.0	305	-	896.0	-	37.7	37.8	0.1	F
532	CCCCCC(F)(F)F	1.0	293	960.8	942.3	-18.5	-	34.1	-	F
533	CCCCCC(F)(F)F	0.1	298	-	936.1	-	-	33.8	-	F
534	CCCCCCC(F)F	1.0	293	-	905.3	-	-	43.0	-	F
535	CCCCCCC(F)F	1.0	326	-	873.0	-	41.1	40.9	-0.2	F
536	CCCCCCC(F)(F)F	0.1	317	-	910.6	-	-	37.1	-	F
537	CCCCCCCCF	1.0	322	-	793.7	-	44.1	43.9	-0.2	F
538	CCCCCCCC(F)F	0.1	365	-	834.4	-	-	42.7	-	F
539	CCCCCCCC(F)F	1.0	344	-	854.9	-	44.2	44.0	-0.2	F
540	CCCCCCCC(F)(F)F	0.1	341	-	882.9	-	-	39.6	-	F
541	CCCCCCCCCF	1.0	293	-	823.0	-	-	50.3	-	F
542	CCCCCCCCCF	1.0	348	-	779.0	-	46.8	46.7	-0.1	F
543	CCCCCCCCC(F)F	0.1	389	-	812.1	-	-	45.0	-	F
544	CCCCCCCCC(F)F	1.0	362	-	838.0	-	47.2	46.9	-0.3	F
545	CCCCCCCCC(F)(F)F	1.0	293	935.7	931.1	-4.6	-	46.8	-	F
546	CCCCCCCCC(F)(F)F	0.1	363	-	857.8	-	-	42.0	-	F
547	CCCCCCCCCCF	1.0	293	819.4	827.1	7.7	-	54.8	-	F

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	SMILES	P [bar]	T [K]	ρ^{exp} [kg m^{-3}]	ρ^{sim} [kg m^{-3}]	$\rho^{\mathrm{exp}} - \rho^{\mathrm{sim}}$ [kg m^{-3}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	$\Delta H_{\mathrm{vap}}^{\mathrm{exp}} - \Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ [kJ mol^{-1}]	class
548	CCCCCCCCCCF	1.0	357	-	777.5	-	50.4	50.2	-0.2	F
549	CCCCCCCCCC(F)F	0.1	412	-	793.0	-	-	47.4	-	F
550	CCCCCCCCCC(F)F	1.0	379	-	823.5	-	50.2	49.8	-0.4	F
551	CCCCCCCCCC(F)(F)F	0.1	385	-	836.3	-	-	44.1	-	F
552	CCC(C)CI	0.0	310	1496.8	1501.4	4.6	43.1	42.2	-0.9	I
553	CC(I)C(C)(C)I	0.0	378	-	2057.8	-	-	52.8	-	I
554	CC(C)(CI)CI	0.0	385	-	2069.6	-	-	54.1	-	I
555	CCC(C)(I)CI	0.0	392	-	2042.5	-	-	52.4	-	I
556	CCC(I)(I)CC	0.0	386	-	2035.0	-	-	51.4	-	I
557	CC(C)(I)CCI	0.0	381	-	2038.9	-	-	54.5	-	I
558	CCCC(C)(I)I	0.0	386	-	2012.0	-	-	52.0	-	I
559	CCC(C)C(I)I	0.0	386	-	2020.6	-	-	52.3	-	I
560	CC(C)C(I)CI	0.0	378	-	2042.1	-	-	54.2	-	I
561	CCC(I)C(C)I	0.0	389	-	2013.5	-	-	52.5	-	I
562	CC(C)CC(I)I	0.0	389	-	1990.2	-	-	52.6	-	I
563	CC(I)CC(C)I	0.0	392	-	1985.0	-	-	52.4	-	I
564	CC(CI)CCI	0.0	398	-	2018.0	-	-	56.1	-	I
565	CCC(I)CCI	0.0	400	1966.0	1999.2	33.1	-	54.2	-	I
566	CCCC(I)CI	0.0	397	1961.6	1998.9	37.3	-	54.2	-	I
567	CC(I)CCCI	0.0	403	1970.4	1988.5	18.1	-	55.2	-	I
568	CCCCC(I)I	0.0	394	1962.8	1982.3	19.5	-	53.4	-	I
569	ICCCCCI	0.0	406	-	2001.5	-	59.7	57.5	-2.2	I
570	CCCCC(I)(I)I	0.0	469	-	2328.3	-	-	61.6	-	I
571	CCC(C)(C)CI	0.0	319	1393.3	1445.1	51.8	-	45.0	-	I
572	CC(C)(C)CCI	0.0	324	1387.2	1420.0	32.8	-	45.6	-	I
573	CC(C)C(C)CI	0.0	326	1385.2	1421.3	36.2	-	45.2	-	I
574	CCC(C)C(C)I	0.0	332	1376.8	1404.5	27.8	-	44.1	-	I
575	CCC(I)C(C)C	0.0	319	1393.3	1416.4	23.0	-	44.2	-	I
576	CC(C)CC(C)I	0.0	319	1393.3	1401.6	8.3	-	44.5	-	I
577	CCC(CC)CI	1.0	296	1440.0	1453.8	13.8	-	47.2	-	I
578	CCC(C)CCI	0.0	333	1349.7	1402.4	52.7	-	45.9	-	I
579	CCCC(C)CI	0.0	328	-	1405.5	-	-	45.7	-	I
580	CCCC(I)CC	0.0	328	1382.1	1396.7	14.7	-	44.9	-	I
581	CC(C)CCCI	1.0	293	1428.3	1444.7	16.4	-	48.2	-	I
582	CC(C)CCCI	0.0	332	-	1395.7	-	-	46.1	-	I
583	CCCCC(C)I	0.0	329	-	1390.3	-	-	45.3	-	I
584	CCCCCC(I)I	0.0	410	-	1845.2	-	-	56.4	-	I
585	ICCCCCCI	0.0	402	-	1891.0	-	-	61.8	-	I
586	CCCC(I)CCC	0.1	387	-	1270.9	-	-	46.0	-	I
587	CCCCC(I)CC	1.0	295	1365.6	1381.5	15.9	-	51.2	-	I
588	CCCCC(I)CC	0.0	349	-	1317.3	-	-	48.1	-	I
589	CCCCCC(C)I	0.0	349	1285.9	1312.5	26.6	-	48.5	-	I
590	CCCCCCC(I)I	0.1	491	-	1633.4	-	-	55.2	-	I
591	CCCCCCC(C)I	1.0	299	1316.4	1326.4	10.0	-	56.1	-	I
592	CCCCCCC(C)I	0.1	406	-	1205.6	-	-	49.5	-	I
593	CCCCCCCC(I)I	0.0	442	-	1633.1	-	-	62.2	-	I
594	ICCCCCCCCI	0.0	453	-	1645.9	-	-	66.0	-	I
595	CCCCCCCCCI	1.0	298	1283.6	1296.5	12.9	64.5	63.0	-1.5	I
596	CCCCCCCCC(C)I	1.0	298	1241.2	1257.5	16.3	-	65.3	-	I
597	CCCCCCCCCCI	1.0	293	1256.7	1268.8	12.1	69.8	68.0	-1.8	I
598	FCCCCCCl	0.0	325	1006.0	1009.4	3.5	-	43.9	-	Mix
599	FCCCCCCCl	0.0	353	962.2	963.0	0.8	-	46.5	-	Mix
600	FCCCCCCCCl	0.1	379	923.4	924.8	1.4	-	49.1	-	Mix
601	FCCCCCCCCCCl	0.1	426	870.8	864.8	-6.0	-	53.6	-	Mix
602	FCCCCCCCCCCCl	0.1	447	851.5	840.1	-11.4	-	55.5	-	Mix

S6.3 Validation crashes

Table S20: Molecules from the validation set, for which the simulations crashed due to implosion. The indices match with Tables S15-S19. Also indicated is the pressure (bar), temperature (K), density ρ ($kg\cdot$ m^{-3}), heat of vaporization ΔH_{vap} (in kJ mol^{-1}), and the melting and boiling point (in K).

index	code	SMILES	p	T	ρ^{sim}	ΔH_{vap}	m.p.	b.p.	series
165	F3301a	CC(F)(F)CF	0.42	262.40	1144.04	27.31	-	262.62	CG_EEMG
142	F1301c	FC(F)F	1.00	298.15	666.7	-	117.97	190.99	AT_EEMG
152	F2302a	FCC(F)F	1.00	314.02	1175.5	-	189.15	276.85	AT_EEMG
153	F2302b	FCC(F)F	1.01	278.00	-	23.18	189.15	276.85	AT_EEMG
154	F2302c	FCC(F)F	2.04	296.43	-	20.57	189.15	276.85	AT_EEMG
165	F3301a	CC(F)(F)CF	0.42	262.40	1144.04	27.31	-	262.62	AT_EEMG
252	X2407b	FC(F)(F)Cl	36.66	298.15	840.94	-	91.95	191.74	AT_EEMG
141	F1301b	FC(F)F	47.10	298.15	636.67	-	117.97	190.99	SHF_EEMG
142	F1301c	FC(F)F	1.00	298.15	666.7	-	117.97	190.99	SHF_EEMG
165	F3301a	CC(F)(F)CF	0.42	262.40	1144.04	27.31	-	262.62	SHF_EEMG
187	I1201a	ICI	1.00	298.15	3307.85	49.0	279.15	455.15	SHF_EEMG
141	F1301b	FC(F)F	47.10	298.15	636.67	-	117.97	190.99	SHF_EEMA
165	F3301a	CC(F)(F)CF	0.42	262.40	1144.04	27.31	-	262.62	SHF_EEMA
187	I1201a	ICI	1.00	298.15	3307.85	49.0	279.15	455.15	SHF_EEMA
252	X2407b	FC(F)(F)Cl	36.66	298.15	840.94	-	91.95	191.74	SHF_EEMA
352	B5217a	CCCC(Br)CBr	1.00	293.15	1670.8	49.0	-	457.15	SHF_EEMA