Force Field Benchmark of Organic Liquids: Density, Enthalpy of Vaporization, Heat Capacities, Surface Tension, Compressibility, Expansion Coefficient and Dielectric Constant

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1 Derivation of equations of the two-phase thermodynamics method

Here we derive the equations needed to implement the two-phase thermodynamic (2PT) model introduced by the Goddard group [1, 2, 3, 4]. This model treats a liquid as something in between a solid and an ideal gas, the rationale for this being that there is existing analytical theory for treating the thermodynamic properties of ideal gases and solids, but no such theory exists for liquids. The reason to summarize the equations here rather than to refer to the original publications, is first and foremost that in the three papers mentioned [1, 2, 3] there is no single complete derivation of the method, and second that the equations below serve as a blueprint for a new GROMACS [5] analysis tool, g_dos, that computes properties based on the density of states using the 2PT method. It is important to give credit to one of the first papers in this field by Berens *et al.* [6], that attempted to treat a fluid just like a solid, and which derived most of the equations that the 2PT method is based upon. Another contributing theory is the Carnahan-Starling model of fluids of rigid spheres [7]. Since the equations published by Berens are internally consistent and can be derived from statistical mechanics textbooks (e.g. McQuarrie [8]) we use this as the foundation for deriving the equations below, however, we note as far as possible from which source the equations below were taken. We derive equations in the context of molecular dynamics simulations, i.e. using finite sampling and simulation lengths.

We start from the mass-weighted velocity autocorrelation function:

$$C(t) \;=\; \sum_{j=1}^{N} m_j \sum_{k=1}^{3} \left\langle v_j^k(t) v_j^k(t+\tau) \right\rangle_\tau \tag{S1}$$

where $v_j^k(t)$ is the velocity of atom j in the k direction at time t, N is the number of atoms, m_j are the atomic masses and $\langle\rangle_\tau$ indicates averaging over time origins τ; C(t) has the units of energy. The Fourier transform of $C(t)$ yields the density of states as a function of frequency ν (Equation 7, reference [1]):

$$DoS(\nu) \;=\; \frac{2}{k_\mathrm{B}T} \lim_{\tau\to\infty} \int_{-\tau}^{+\tau} C(t) e^{-i2\pi\nu t} \mathrm{d}t \;\approx\; \frac{4}{k_\mathrm{B}T} \sum_{k=0}^{K-1} C(k\Delta t) e^{-i2\pi\nu kt/K} \tag{S2}$$

where Δt is the time between saving velocities in the MD trajectory (4 fs in our simulations), k_B is Boltzmann's constant and K is the number of data points, and the extra factor two in the summation comes from the lower limit being 0 instead of -∞ in the integral (cf. Equation 22 in reference [1]). Note that the Density of States (DoS) in this definition is a dimensionless quantity. The density of states at zero frequency, $DoS(0)$, is associated with the diffusion constant D through (Equation 3.16, reference [6]):

$$D \;=\; \frac{DoS(0) k_\mathrm{B} T}{12 M m} \tag{S3}$$

where M is the number of equivalent particles and m is their mass.

The 2PT method approximates

$$DoS_{\text{liquid}}(\nu) \;=\; DoS_{\text{gas}}(\nu) + DoS_{\text{solid}}(\nu) \tag{S4}$$

and if we would have an analytical expression for $DoS_{\text{gas}}(\nu)$ – note that Pascal *et al.* [3] use the subscript "diff" rather than "gas" as we do for consistency here – we could subtract this from the $DoS(\nu)$ obtained from the simulation (Eq. S2). Indeed, the gaseous (diffusive) component of the density of states $DoS(\nu)_{\text{gas}}$, described as a gas of hard spheres (Equation 24, reference [1]) can be written as:

$$DoS_{\text{gas}}(\nu) \;=\; DoS(0)\left(1+\left[\frac{DoS(0)\pi\nu}{6fN}\right]^2\right)^{-1} \tag{S5}$$

where f is the fluidicity, the fraction of the 3N degrees of freedom that corresponds to the diffusional parts of the system, or in other words

$$\int_0^\infty DoS_{\text{gas}}(\nu)\mathrm{d}\nu = 3fN, \tag{S6}$$

independent of $DoS(0)$. A derivation of the equation needed to solve for f can be found in reference [1], the final result being (Equation 12, reference [2]):

$$2(f^5/\Delta^3)^{3/2} - 6(f^5/\Delta^3) - (f^7/\Delta^3)^{1/2} + 6(f^5/\Delta^3)^{1/2} + 2f = 2 \tag{S7}$$

where Δ is the dimensionless diffusion constant defined by (Equation 13, reference [2]):

$$\Delta = \frac{2DoS(0)}{9N}\left(\frac{\pi k_{\text{B}}TN}{M}\right)^{1/2}\left(\frac{N}{V}\right)^{1/3}\left(\frac{6}{\pi}\right)^{2/3} \tag{S8}$$

with V is the volume of the system. Eq. S7 is monotonous between 0 and 1 (cf. Figure 2 in reference [1]) and hence a bisection algorithm can be used to solve for f given Δ.

Now we will try to comprehend the solid component of the density of states, $DoS_{\text{solid}}(\nu)$. Here, each mode is considered to be harmonic and we use the partition function for a quantum harmonic oscillator as given by McQuarrie [8]:

$$q^q_{\text{HO}}(\nu) = \frac{e^{-\beta h\nu/2}}{1-e^{-\beta h\nu}} \tag{S9}$$

where h is Planck's constant, $\beta = 1/k_{\text{B}}T$. Since the canonical partion function Q of a system is given by the product of the components (Equations 3.18-3.20, reference [6]):

$$Q \;=\; \prod_{i=1}^{N} q_i \tag{S10}$$

and therefore

$$\ln Q \;=\; \sum_{i=1}^{N} \ln q_i \tag{S11}$$

we can write for a system of quantum harmonic oscillators, assuming the frequencies are continuous, that:

$$\ln Q \;=\; \int_0^\infty DoS_{\mathrm{solid}}(\nu)\ln q^q_{\mathrm{HO}}(\nu)\mathrm{d}\nu. \tag{S12}$$

This equation is used for deriving the thermodynamic properties from the solid. We use the notation of Pascal *et al.* [3], but with corrections based on Berens *et al.* [6]:

$$\begin{aligned} c^Q_{\mathrm{V}} &= 2k_{\mathrm{B}}T\Big(\frac{\partial \ln Q}{\partial T}\Big)_{N,V} + k_{\mathrm{B}}T\Big(\frac{\partial^2 \ln Q}{\partial T^2}\Big)_{N,V} \\ &= k_{\mathrm{B}}\int_0^\infty DoS_{\mathrm{solid}}(\nu)W^{c_{\mathrm{V}}}_{\mathrm{solid}}(\nu)\mathrm{d}\nu \end{aligned} \tag{S13}$$

where the weighting function is defined as:

$$\begin{aligned} W^{c_{\mathrm{V}}}_{\mathrm{solid}}(\nu) &= T\Big(\frac{\partial W^S_{\mathrm{solid}}(\nu)}{\partial T}\Big) = T\left(2\frac{\partial \ln q^q_{\mathrm{HO}}(\nu)}{\partial T} + T\frac{\partial^2 \ln q^q_{\mathrm{HO}}(\nu)}{\partial T^2}\right) \\ &= \frac{(\beta h\nu)^2\, e^{\beta h\nu}}{(1-e^{\beta h\nu})^2} \end{aligned} \tag{S14}$$

Now, finally, we can estimate the heat capacity of the liquids using:

$$c_{\mathrm{V}} \;=\; k_{\mathrm{B}}\int_0^\infty \Big[DoS_{\mathrm{gas}}(\nu)W^{c_{\mathrm{V}}}_{\mathrm{gas}}(\nu) + DoS_{\mathrm{solid}}(\nu)W^{c_{\mathrm{V}}}_{\mathrm{solid}}(\nu)\Big]\,\mathrm{d}\nu \tag{S15}$$

where the weighting factor for the diffusive part is:

$$W^{c_{\mathrm{V}}}_{\mathrm{gas}} \;=\; \frac{1}{2}. \tag{S16}$$

Similar equations have been presented by the Goddard group for the Helmholtz energy, the entropy and the internal energy [1, 2, 3].

Finally, we can compare the heat capacity at constant volume c_{V} to the one at constant presssure c_{P} because they are related according to:

$$c_{\mathrm{P}} \;=\; c_{\mathrm{V}} + VT\frac{\alpha^2_{\mathrm{P}}}{\kappa_{\mathrm{T}}} \tag{S17}$$

where α_{P} is the volumetric thermal expansion coefficient and κ_{T} the isothermal compressibility (see main text).

2 Liquidity Test

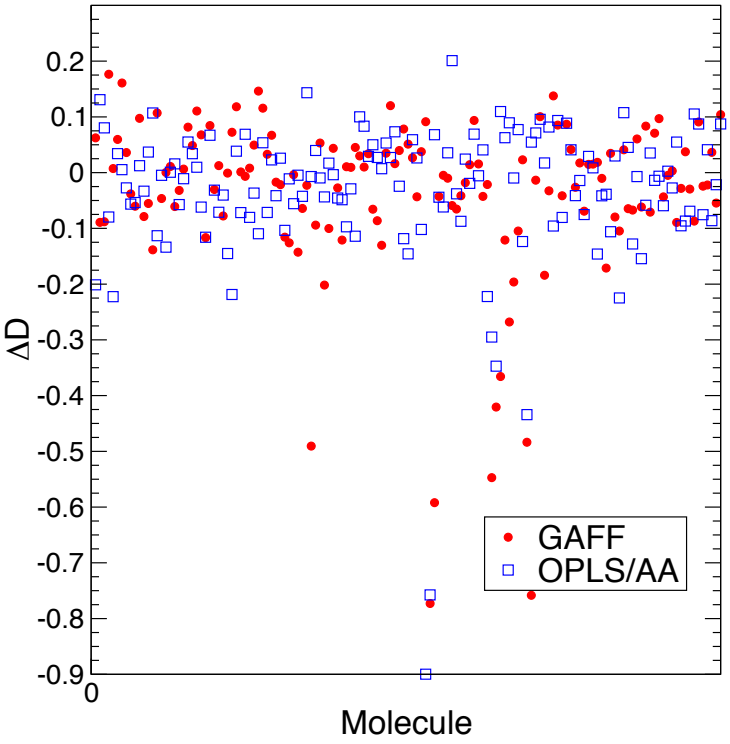

Figure S1: Liquidity test. The change in MSD, ΔD as defined in the main text. On the x-axis all the simulated molecules are listed in alphabetic order. For all simulations with $|\Delta D| \geq 0.5$ the trajectories and MSD for the entire simulation was further investigated to ensure that the system was liquid during the whole simulation.

3 Simulation Results per Property

Table S1: Name, formula, molecular weight (g/cm^3), CAS number and ChemSpider ID for all molecules in the test set.

Name	Formula	MW	CAS	CSID
1. chloroform	$CHCl_3$	119.378	67-66-3	5977
2. dichloro(fluoro)methane	$CHCl_2F$	102.923	75-43-4	6130
3. dibromomethane	CH_2Br_2	173.835	74-95-3	2916
4. dichloromethane	CH_2Cl_2	84.9325	75-09-2	6104
5. methanal	CH_2O	30.0259	50-00-0	692
6. methanoic acid	CH_2O_2	46.0253	64-18-6	278
7. bromomethane	CH_3Br	94.9384	74-83-9	6083
8. methanamide	CH_3NO	45.0405	75-12-7	693
9. nitromethane	CH_3NO_2	61.0399	75-52-5	6135
10. methanol	CH_4O	32.0417	67-56-1	864
11. 1,1,1,2,2-pentachloroethane	C_2HCl_5	202.294	76-01-7	6179
12. 1,1,2,2-tetrachloroethane	$C_2H_2Cl_4$	167.849	79-34-5	6342
13. 1,1-dichloroethene	$C_2H_2Cl_2$	96.9432	75-35-4	13835316
14. 1,1,2-trichloroethane	$C_2H_3Cl_3$	133.404	79-00-5	6326
15. acetonitrile	C_2H_3N	41.0518	75-05-8	6102
16. 1,2-dibromoethane	$C_2H_4Br_2$	187.861	106-93-4	7551
17. 1,1-dichloroethane	$C_2H_4Cl_2$	98.959	75-34-3	6125
18. 1,2-dichloroethane	$C_2H_4Cl_2$	98.959	107-06-2	13837650
19. methyl formate	$C_2H_4O_2$	60.0518	107-31-3	7577
20. bromoethane	C_2H_5Br	108.965	74-96-4	6092
21. chloroethane	C_2H_5Cl	64.5139	75-00-3	6097
22. 2-chloroethanol	C_2H_5ClO	80.5133	107-07-3	21106015
23. ethanamide	C_2H_5NO	59.067	60-35-5	173
24. N-methylformamide	C_2H_5NO	59.067	123-39-7	28994
25. nitroethane	$C_2H_5NO_2$	75.0664	79-24-3	6338
26. methoxymethane	C_2H_6O	46.0682	115-10-6	7956
27. ethanol	C_2H_6O	46.0682	64-17-5	682
28. 1,2-ethanedithiol	$C_2H_6S_2$	94.1988	540-63-6	13865015
29. methyldisulfanylmethane	$C_2H_6S_2$	94.1988	624-92-0	11731
30. methylsulfinylmethane	C_2H_6OS	78.1332	67-68-5	659
31. methylsulfanylmethane	C_2H_6S	62.1338	75-18-3	1039
32. 2-aminoethanol	C_2H_7NO	61.0828	141-43-5	13835336
33. ethane-1,2-diamine	$C_2H_8N_2$	60.098	107-15-3	13835550
34. prop-2-enenitrile	C_3H_3N	53.0625	107-13-1	7567

Table S1: Name, formula, molecular weight, CAS number, ChemSpider ID - continued.

Name	Formula	MW	CAS	CSID
35. 1,3-dioxolan-2-one	$C_3H_4O_3$	88.0619	96-49-1	7030
36. propanenitrile	C_3H_5N	55.0783	107-12-0	7566
37. 1,2-dibromopropane	$C_3H_6Br_2$	201.888	78-75-1	6305
38. 1,3-dichloropropane	$C_3H_6Cl_2$	112.985	142-28-9	8543
39. (2R)-2-methyloxirane	C_3H_6O	58.0789	15448-47-2	129014
40. propan-2-one	C_3H_6O	58.0789	67-64-1	175
41. methyl acetate	$C_3H_6O_2$	74.0783	79-20-9	6335
42. 1,3-dioxolane	$C_3H_6O_2$	74.0783	646-06-0	12066
43. 2-iodopropane	C_3H_7I	169.992	75-30-9	6122
44. 1-bromopropane	C_3H_7Br	122.991	106-94-5	7552
45. N,N-dimethylformamide	C_3H_7NO	73.0935	68-12-2	5993
46. N-methylacetamide	C_3H_7NO	73.0935	79-16-3	6334
47. 1-nitropropane	$C_3H_7NO_2$	89.0929	108-03-2	7615
48. 2-nitropropane	$C_3H_7NO_2$	89.0929	79-46-9	387
49. dimethoxymethane	$C_3H_8O_2$	76.0941	109-87-5	13837190
50. propane-1,2,3-triol	$C_3H_8O_3$	92.0935	56-81-5	733
51. propan-1-amine	C_3H_9N	59.1099	107-10-8	7564
52. propan-2-amine	C_3H_9N	59.1099	75-31-0	6123
53. 2-methylpropane	C_4H_{10}	58.1218	75-28-5	6120
54. ethylsulfanylethane	$C_4H_{10}S$	90.1868	352-93-2	9233
55. butane-1-thiol	$C_4H_{10}S$	90.1868	109-79-5	7721
56. butan-1-ol	$C_4H_{10}O$	74.1212	71-36-3	258
57. 2-methylpropan-2-ol	$C_4H_{10}O$	74.1212	75-65-0	6146
58. butane-1,4-diol	$C_4H_{10}O_2$	90.1206	110-63-4	13835209
59. (2-hydroxyethoxy)ethan-2-ol	$C_4H_{10}O_3$	106.12	111-46-6	13835180
60. N-ethylethanamine	$C_4H_{11}N$	73.1364	109-89-7	7730
61. butan-1-amine	$C_4H_{11}N$	73.1364	109-73-9	7716
62. 2-methylpropan-2-amine	$C_4H_{11}N$	73.1364	75-64-9	6145
63. 2-(2-hydroxyethylamino)ethanol	$C_4H_{11}NO_2$	105.135	111-42-2	13835604
64. pyrimidine	$C_4H_4N_2$	80.0878	289-95-2	8903
65. furan	C_4H_4O	68.0738	110-00-9	7738
66. thiophene	C_4H_4S	84.1394	110-02-1	7739
67. 1H-pyrrole	C_4H_5N	67.089	109-97-7	7736
68. ethenyl acetate	$C_4H_6O_2$	86.089	108-05-4	7616

Table S1: Name, formula, molecular weight, CAS number, ChemSpider ID - continued.

Name	Formula	MW	CAS	CSID
69. oxolan-2-one	$C_4H_6O_2$	86.089	96-48-0	7029
70. acetyl acetate	$C_4H_6O_3$	102.088	108-24-7	7630
71. 1,4-dichlorobutane	$C_4H_8Cl_2$	127.012	110-56-5	21106032
72. oxolane	C_4H_8O	72.1054	109-99-9	7737
73. ethoxyethene	C_4H_8O	72.1054	109-92-2	7732
74. ethyl acetate	$C_4H_8O_2$	88.1048	141-78-6	8525
75. tetrahydrothiophene 1,1-dioxide	$C_4H_8O_2S$	120.17	126-33-0	29080
76. thiolane	C_4H_8S	88.171	110-01-0	1095
77. 1-bromobutane	C_4H_9Br	137.018	109-65-9	7711
78. 1-chlorobutane	C_4H_9Cl	92.5669	109-69-3	7714
79. pyrrolidine	C_4H_9N	71.1206	123-75-1	29008
80. N,N-dimethylacetamide	C_4H_9NO	87.12	127-19-5	29107
81. morpholine	C_4H_9NO	87.12	110-91-8	13837537
82. pyridine	C_5H_5N	79.0997	110-86-1	1020
83. cyclopentanone	C_5H_8O	84.1161	120-92-3	8141
84. 1-cyclopropylethanone	C_5H_8O	84.1161	765-43-5	12463
85. pentane-2,4-dione	$C_5H_8O_2$	100.115	123-54-6	29001
86. methyl 2-methylprop-2-enoate	$C_5H_8O_2$	100.115	80-62-6	6406
87. pentanenitrile	C_5H_9N	83.1313	110-59-8	7770
88. ethyl propanoate	$C_5H_{10}O_2$	102.131	105-37-3	7463
89. diethyl carbonate	$C_5H_{10}O_3$	118.131	105-58-8	7478
90. pentan-1-ol	$C_5H_{12}O$	88.1477	71-41-0	6040
91. pentan-3-ol	$C_5H_{12}O$	88.1477	584-02-1	10947
92. 2-methylbutan-2-ol	$C_5H_{12}O$	88.1477	75-85-4	6165
93. pentane-1,5-diol	$C_5H_{12}O_2$	104.147	111-29-5	13839441
94. pentan-3-amine	$C_5H_{13}N$	87.1629	616-24-0	11524
95. 1,2,3,4-tetrafluorobenzene	$C_6H_2F_4$	150.074	551-62-2	21106162
96. 1,2,3,5-tetrafluorobenzene	$C_6H_2F_4$	150.074	2367-82-0	21159625
97. 1,3-difluorobenzene	$C_6H_4F_2$	114.093	372-18-9	9358
98. 1,2-difluorobenzene	$C_6H_4F_2$	114.093	367-11-3	9325
99. fluorobenzene	C_6H_5F	96.1021	462-06-6	9614
100. nitrobenzene	$C_6H_5NO_2$	123.109	98-95-3	7138
101. 2-chloroaniline	C_6H_6ClN	127.571	95-51-2	13854248
102. phenol	C_6H_6O	94.111	108-95-2	971

Table S1: Name, formula, molecular weight, CAS number, ChemSpider ID - continued.

Name	Formula	MW	CAS	CSID
103. benzenethiol	C_6H_6S	110.177	108-98-5	7681
104. 2-methylpyridine	C_6H_7N	93.1262	109-06-8	13839199
105. 3-methylpyridine	C_6H_7N	93.1262	108-99-6	21106520
106. 4-methylpyridine	C_6H_7N	93.1262	108-89-4	13874733
107. cyclohexanone	$C_6H_{10}O$	98.1426	108-94-1	7679
108. (E)-hex-2-ene	C_6H_{12}	84.159	4050-45-7	555073
109. hexan-2-one	$C_6H_{12}O$	100.158	591-78-6	11095
110. 2,4,6-trimethyl-1,3,5-trioxane	$C_6H_{12}O_3$	132.157	123-63-7	21106173
111. cyclohexanamine	$C_6H_{13}N$	99.1736	108-91-8	7677
112. 2-propan-2-yloxypropane	$C_6H_{14}O$	102.174	108-20-3	7626
113. 1-methoxy-2-(2-methoxyethoxy)ethane	$C_6H_{14}O_3$	134.173	111-96-6	13839575
114. triethyl phosphate	$C_6H_{15}O_4P$	182.154	78-40-0	6287
115. N,N-diethylethanamine	$C_6H_{15}N$	101.189	121-44-8	8158
116. N-propan-2-ylpropan-2-amine	$C_6H_{15}N$	101.189	108-18-9	7624
117. trifluoromethylbenzene	$C_7H_5F_3$	146.11	98-08-8	7090
118. benzonitrile	C_7H_5N	103.121	100-47-0	7224
119. benzaldehyde	C_7H_6O	106.122	100-52-7	235
120. toluene	C_7H_8	92.1381	108-88-3	1108
121. methoxybenzene	C_7H_8O	108.138	100-66-3	7238
122. phenylmethanol	C_7H_8O	108.137	100-51-6	13860335
123. 2-methylphenol	C_7H_8O	108.137	95-48-7	13835772
124. 3-methylphenol	C_7H_8O	108.137	108-39-4	21105871
125. 4-methylphenol	C_7H_8O	108.137	106-44-5	13839082
126. diethyl propanedioate	$C_7H_{12}O_4$	160.167	105-53-3	13863636
127. 2,4-dimethylpentan-3-one	$C_7H_{14}O$	114.185	565-80-0	10797
128. heptan-2-one	$C_7H_{14}O$	114.185	110-43-0	7760
129. ethenylbenzene	C_8H_8	104.149	100-42-5	7220
130. 1-phenylethanone	C_8H_8O	120.148	98-86-2	7132
131. methyl benzoate	$C_8H_8O_2$	136.148	93-58-3	6883
132. methyl 2-hydroxybenzoate	$C_8H_8O_3$	152.147	119-36-8	13848808
133. ethylbenzene	C_8H_{10}	106.165	100-41-4	7219
134. 1,2-dimethylbenzene	C_8H_{10}	106.165	95-47-6	6967
135. 1,2-dimethoxybenzene	$C_8H_{10}O_2$	138.163	91-16-7	13861009
136. 2,4,6-trimethylpyridine	$C_8H_{11}N$	121.179	108-75-8	21106174

Table S1: Name, formula, molecular weight, CAS number, ChemSpider ID - continued.

Name	Formula	MW	CAS	CSID
137. octan-1-ol	$C_8H_{18}O$	130.227	111-87-5	932
138. 1-butoxybutane	$C_8H_{18}O$	130.227	142-96-1	8569
139. N-butylbutan-1-amine	$C_8H_{19}N$	129.242	111-92-2	7856
140. isoquinoline	C_9H_7N	129.158	119-65-3	8098
141. quinoline	C_9H_7N	129.158	91-22-5	6780
142. (1-methylethyl)benzene	C_9H_{12}	120.191	98-82-8	7128
143. 1,2,4-trimethylbenzene	C_9H_{12}	120.191	95-63-6	6977
144. 2,6-dimethylheptan-4-one	$C_9H_{18}O$	142.238	108-83-8	7670
145. 1-chloronaphthalene	$C_{10}H_7Cl$	162.615	90-13-1	6737
146. phenoxybenzene	$C_{12}H_{10}O$	170.207	101-84-8	7302

Table S2: Liquid density ρ (g/l) calculated and experimental. Blue font indicates that the calculated value differs more than 5% from the experimental ones, a red font indicates that it differs by more than 10%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ρ	Ref.	ρ	ρ	ρ
1. chloroform	298.15	1479.30	[9]	1375.0 ± 0.3	1373.2 ± 0.3	
2. dichloro(fluoro)methane	282.05	1399.17	[10]	1308.0 ± 1.0	1314.0 ± 0.8	
3. dibromomethane	293.15	2496.90	[11]	**1958.1 ± 0.6**	2490.1 ± 0.8	
...	298.15	2490.70	[9]	**1946.1 ± 0.3**	2475.3 ± 1.5	
4. dichloromethane	293.15	1326.60	[11]	1268.5 ± 0.5	1207.1 ± 0.5	
...	298.15	1394.30	[9]	1258.1 ± 0.5	**1200.4 ± 1.5**	
5. methanal	253.15	815.00	[11]	838.0 ± 0.2	773.7 ± 0.1	
...	253.65	810.53	[12]	835.7 ± 0.3	773.0 ± 0.1	
6. methanoic acid	293.15	1220.00	[11]	**1397.1 ± 0.4**	1142.6 ± 0.1	
...	298.15	1214.50	[9]	**1371.0 ± 0.2**	1136.8 ± 0.1	
7. bromomethane	276.65	1721.95	[10]	**1400.7 ± 1.2**	1803.5 ± 0.4	
8. methanamide	298.15	1128.80	[9]	1218.5 ± 0.1	1122.1 ± 0.1	1187.2
9. nitromethane	293.15	1137.10	[11]	1231.8 ± 0.1	1110.5 ± 0.1	
...	298.15	1130.40	[9]	1226.9 ± 0.1	1103.4 ± 0.1	
10. methanol	293.15	791.40	[11]	813.0 ± 0.2	782.9 ± 0.0	
...	298.15	787.20	[9]	807.5 ± 0.2	776.8 ± 0.1	782.5
11. 1,1,1,2,2-pentachloroethane	293.15	1679.60	[11]	1669.2 ± 0.2	1681.7 ± 0.2	
12. 1,1,2,2-tetrachloroethane	293.15	1595.30	[11]	1546.2 ± 0.2	1559.6 ± 0.3	
...	298.15	1586.50	[9]	1538.1 ± 0.6	1550.6 ± 0.3	
13. 1,1-dichloroethene	293.15	1212.90	[10]	**1067.8 ± 0.5**	1186.6 ± 0.2	
...	298.15	1214.90	[10]	**1053.8 ± 0.4**	1176.6 ± 0.3	
14. 1,1,2-trichloroethane	293.15	1439.70	[11]	1417.4 ± 0.3	1432.8 ± 0.4	
...	298.15	1431.40	[9]	1408.8 ± 0.5	1424.9 ± 0.3	
15. acetonitrile	293.15	785.70	[11]	731.6 ± 0.2	762.2 ± 0.3	
...	298.15	776.00	[9]	729.6 ± 0.1	755.1 ± 0.2	774.6
16. 1,2-dibromoethane	298.15	2169.30	[9]	**1807.5 ± 0.9**	2336.3 ± 0.5	
17. 1,1-dichloroethane	293.15	1175.70	[11]	1172.8 ± 0.6	1175.5 ± 0.2	1182.2
...	298.15	1168.40	[9]	1163.9 ± 0.3	1166.6 ± 0.2	
18. 1,2-dichloroethane	298.15	1246.30	[9]	1235.3 ± 0.2	1236.8 ± 0.3	
19. methyl formate	293.15	971.30	[11]	1051.7 ± 0.1	959.1 ± 0.1	
...	298.15	967.00	[9]	1045.2 ± 0.1	952.0 ± 0.1	

Table S2: Liquid density - continued

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ρ	Ref.	ρ	ρ	ρ
20. bromoethane	293.15	1460.40	[11]	**1287.9 ± 0.6**	1539.7 ± 0.3	1495.4
...	298.15	1449.30	[13]	**1277.5 ± 0.4**	1528.5 ± 0.5	
21. chloroethane	273.15	923.90	[11]	898.5 ± 0.3	915.3 ± 0.2	915.6
...	285.45	908.44	[13]	878.1 ± 0.2	893.2 ± 0.2	
22. 2-chloroethanol	293.15	1201.90	[11]	1230.1 ± 0.2	1195.7 ± 0.2	
23. ethanamide	358.15	998.60	[11]	1030.8 ± 0.2	1018.7 ± 0.1	
24. N-methylformamide	292.15	1011.00	[11]	1052.0 ± 0.1	985.6 ± 0.1	
...	298.15	999.50	[9]	1046.9 ± 0.2	979.9 ± 0.1	
25. nitroethane	298.15	1044.10	[9]	1096.3 ± 0.0	1032.6 ± 0.1	
26. methoxymethane	240.00	742.08	[13]	773.0 ± 0.2	741.4 ± 0.1	
27. ethanol	293.15	789.30	[11]	802.4 ± 0.1	801.9 ± 0.1	
...	298.15	784.80	[9]	797.3 ± 0.1	796.3 ± 0.0	796.9
28. 1,2-ethanedithiol	293.15	1234.00	[11]	1173.1 ± 0.1	1161.4 ± 0.2	
...	298.15	1118.87	[13]	1166.5 ± 0.2	1156.2 ± 0.1	
29. methyldisulfanylmethane	293.15	1062.50	[11]	1023.3 ± 0.4	1036.9 ± 0.0	
...	298.15	1057.32	[13]	1014.7 ± 0.2	1030.0 ± 0.2	1042.8
30. methylsulfinylmethane	298.15	1095.80	[9]	1136.2 ± 0.1	1101.3 ± 0.1	1118.5
31. methylsulfanylmethane	293.15	848.30	[11]	811.3 ± 0.3	843.7 ± 0.1	
...	298.15	841.90	[9]	801.9 ± 0.2	837.1 ± 0.1	
32. 2-aminoethanol	293.15	1018.00	[11]	**1132.7 ± 0.5**	1027.4 ± 0.1	
...	320.00	995.57	[13]	**1111.2 ± 0.3**	998.5 ± 0.3	
33. ethane-1,2-diamine	293.15	897.90	[11]	**1040.6 ± 0.2**	**987.8 ± 0.2**	
...	298.15	889.10	[9]	**1035.1 ± 0.2**	**981.0 ± 0.1**	
34. prop-2-enenitrile	298.15	801.10	[9]	775.3 ± 0.2	771.2 ± 0.0	
...	350.45	738.79	[13]	707.1 ± 0.2	712.3 ± 0.1	
35. 1,3-dioxolan-2-one	312.15	1321.40	[11]	1360.1 ± 0.1	1320.7 ± 0.2	
36. propanenitrile	293.15	781.80	[11]	750.1 ± 0.1	760.1 ± 0.1	
...	298.15	776.40	[9]	744.8 ± 0.1	753.6 ± 0.1	
37. 1,2-dibromopropane	293.15	1932.40	[11]	**1710.5 ± 0.2**	2106.6 ± 0.3	
...	298.15	1924.95	[10]	**1701.6 ± 0.5**	2096.8 ± 0.3	
38. 1,3-dichloropropane	298.15	1178.50	[11]	1164.5 ± 0.1	1169.2 ± 0.2	
39. (2R)-2-methyloxirane	298.15	830.00	[11]	803.1 ± 0.2	774.7 ± 0.1	

Table S2: Liquid density - continued

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ρ	Ref.	ρ	ρ	ρ
40. propan-2-one	298.15	784.90	[9]	785.6 ± 0.1	800.3 ± 0.2	777.8
41. methyl acetate	293.15	934.20	[11]	971.4 ± 0.1	951.6 ± 0.1	
...	298.15	928.30	[9]	967.6 ± 0.1	945.6 ± 0.1	904.5
42. 1,3-dioxolane	293.15	1060.00	[11]	1122.3 ± 0.1	1053.4 ± 0.3	
...	298.15	1064.40	[9]	1116.5 ± 0.2	1046.3 ± 0.3	1025.1
43. 2-iodopropane	293.15	1704.20	[11]	1607.3 ± 0.3	1848.2 ± 0.2	
...	298.15	1737.25	[10]	1599.4 ± 0.4	1836.4 ± 0.4	
44. 1-bromopropane	293.15	1353.70	[11]	1239.3 ± 0.3	1418.4 ± 0.3	
...	298.15	1345.38	[10]	1229.9 ± 0.2	1408.6 ± 0.1	
45. N,N-dimethylformamide	298.15	943.30	[9]	984.2 ± 0.1	922.2 ± 0.1	
46. N-methylacetamide	320.00	920.52	[12]	968.4 ± 0.1	952.0 ± 0.1	
47. 1-nitropropane	298.15	995.40	[9]	1042.2 ± 0.0	989.7 ± 0.0	
48. 2-nitropropane	298.15	983.30	[9]	1034.2 ± 0.1	995.6 ± 0.0	
49. dimethoxymethane	293.15	859.30	[11]	911.5 ± 0.1	881.4 ± 0.1	
...	298.15	853.56	[10]	905.0 ± 0.1	874.6 ± 0.1	
50. propane-1,2,3-triol	293.15	1261.30	[11]	1310.2 ± 0.7	1259.7 ± 0.7	
...	320.00	1243.57	[10]	1289.5 ± 0.1	1232.3 ± 0.5	
51. propan-1-amine	293.15	717.30	[11]	762.9 ± 0.1	733.4 ± 0.3	
...	298.15	711.47	[10]	757.3 ± 0.1	726.3 ± 0.1	
52. propan-2-amine	293.15	689.10	[11]	**773.9 ± 0.2**	738.7 ± 0.1	
...	298.15	683.08	[10]	**768.3 ± 0.1**	731.6 ± 0.2	
53. 2-methylpropane	243.65	613.53	[10]	631.3 ± 0.2	643.5 ± 0.1	626.7
54. ethylsulfanylethane	293.15	836.20	[11]	814.4 ± 0.2	842.5 ± 0.1	
...	298.15	831.20	[9]	808.1 ± 0.1	836.9 ± 0.1	
55. butane-1-thiol	293.15	841.60	[11]	856.0 ± 0.2	865.5 ± 0.1	
...	298.15	837.00	[12]	850.4 ± 0.1	860.3 ± 0.2	
56. butan-1-ol	293.15	809.50	[11]	819.1 ± 0.1	810.5 ± 0.1	
...	298.15	805.70	[9]	815.0 ± 0.2	805.3 ± 0.1	
57. 2-methylpropan-2-ol	320.00	757.94	[10]	803.3 ± 0.4	800.7 ± 0.1	
58. butane-1,4-diol	293.15	1017.10	[11]	1048.5 ± 0.2	1023.9 ± 0.1	
...	298.15	1012.60	[9]	1046.7 ± 0.4	1019.0 ± 0.4	
...	320.00	1000.72	[13]	1030.0 ± 0.4	1001.1 ± 0.2	

Table S2: Liquid density - continued

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ρ	Ref.	ρ	ρ	ρ
59. (2-hydroxyethoxy)ethan-2-ol	288.15	1119.70	[11]	1202.3 ± 0.2	1107.7 ± 0.3	
60. N-ethylethanamine	293.15	705.60	[11]	737.7 ± 0.1	723.8 ± 0.1	
...	298.15	701.90	[9]	731.4 ± 0.2	717.0 ± 0.1	
61. butan-1-amine	293.15	741.40	[11]	779.1 ± 0.1	753.4 ± 0.2	
...	298.15	736.60	[9]	773.8 ± 0.1	747.2 ± 0.1	
62. 2-methylpropan-2-amine	293.15	695.80	[11]	**781.9 ± 0.1**	**767.6 ± 0.2**	
...	298.15	690.07	[10]	**776.6 ± 0.1**	**761.2 ± 0.2**	
63. 2-(2-hydroxyethylamino)ethanol	320.00	1079.23	[12]	1157.0 ± 0.7	1080.4 ± 0.5	
64. pyrimidine	298.15	1016.40	[9]	1116.0 ± 0.2	1094.5 ± 0.1	1030.9
65. furan	293.15	951.40	[11]	971.7 ± 0.3	964.4 ± 0.3	
...	298.15	931.30	[9]	966.0 ± 0.1	958.2 ± 0.6	862.9
66. thiophene	293.15	1064.90	[11]	1057.8 ± 0.3	1093.2 ± 0.2	
...	298.15	1059.01	[12]	1050.0 ± 0.1	1087.6 ± 0.3	1074.7
67. 1H-pyrrole	293.15	969.80	[11]	1020.1 ± 0.2	990.5 ± 0.2	
...	298.15	965.30	[9]	1015.1 ± 0.3	985.6 ± 0.1	952.2
68. ethenyl acetate	298.15	925.60	[11]	979.0 ± 0.0	970.2 ± 0.1	
69. oxolan-2-one	293.15	1129.60	[11]	1142.7 ± 0.0	1105.9 ± 0.2	
70. acetyl acetate	293.15	1082.00	[11]	1131.1 ± 0.1	1122.7 ± 0.1	
71. 1,4-dichlorobutane	298.15	1133.10	[11]	1125.3 ± 0.1	1128.1 ± 0.1	
72. oxolane	298.15	883.70	[9]	893.8 ± 0.2	858.8 ± 0.1	
73. ethoxyethene	293.15	758.90	[11]	766.7 ± 0.2	775.4 ± 0.1	
74. ethyl acetate	293.15	900.30	[11]	936.7 ± 0.1	927.0 ± 0.1	
...	298.15	894.50	[9]	931.8 ± 0.2	921.4 ± 0.1	886.7
75. tetrahydrothiophene 1,1-dioxide	320.00	1248.99	[12]	1299.3 ± 0.2	1260.0 ± 0.2	
76. thiolane	293.15	998.70	[11]	981.3 ± 0.2	986.8 ± 0.1	
...	298.15	994.00	[9]	975.9 ± 0.2	981.4 ± 0.1	
77. 1-bromobutane	293.15	1275.80	[11]	1187.6 ± 0.2	1325.8 ± 0.2	
...	298.15	1268.70	[9]	1180.5 ± 0.3	1317.9 ± 0.2	
78. 1-chlorobutane	293.15	885.70	[11]	876.8 ± 0.1	884.2 ± 0.0	
...	298.15	880.80	[9]	871.1 ± 0.1	877.7 ± 0.2	
79. pyrrolidine	293.15	858.60	[11]	886.5 ± 0.1	860.9 ± 0.1	
...	298.15	853.80	[9]	881.3 ± 0.1	855.0 ± 0.3	874.8

Table S2: Liquid density - continued

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ρ	Ref.	ρ	ρ	ρ
80. N,N-dimethylacetamide	298.15	936.80	[9]	945.8 ± 0.0	927.1 ± 0.1	
81. morpholine	293.15	1000.50	[11]	1088.0 ± 0.2	1045.6 ± 0.3	
82. pyridine	293.15	981.90	[11]	988.1 ± 0.3	980.6 ± 0.2	
...	298.15	977.80	[9]	982.2 ± 0.4	975.3 ± 0.2	987.6
83. cyclopentanone	293.15	948.70	[11]	940.2 ± 0.1	948.1 ± 0.1	
...	298.15	945.20	[9]	936.6 ± 0.2	942.8 ± 0.1	
84. 1-cyclopropylethanone	293.15	898.40	[11]	906.2 ± 0.1	880.3 ± 0.1	
...	298.15	894.48	[14]	901.1 ± 0.1	875.2 ± 0.1	
85. pentane-2,4-dione	298.15	972.00	[9]	985.7 ± 0.1	1015.9 ± 0.1	
86. methyl 2-methylprop-2-enoate	298.15	937.70	[11]	960.7 ± 0.0	984.3 ± 0.1	
87. pentanenitrile	293.15	800.80	[11]	779.8 ± 0.1	788.9 ± 0.1	
...	298.15	794.40	[9]	775.1 ± 0.1	783.3 ± 0.0	
88. ethyl propanoate	298.15	884.20	[9]	908.2 ± 0.1	908.3 ± 0.1	
89. diethyl carbonate	298.15	969.10	[9]	1020.9 ± 0.1	998.6 ± 0.1	
90. pentan-1-ol	293.15	814.40	[11]	823.7 ± 0.1	816.4 ± 0.1	
...	298.15	812.40	[9]	819.6 ± 0.2	811.7 ± 0.1	
...	320.00	794.74	[10]	802.2 ± 0.1	791.1 ± 0.1	
91. pentan-3-ol	293.15	820.30	[11]	821.0 ± 0.1	825.0 ± 0.1	
...	298.15	815.99	[10]	816.4 ± 0.2	819.3 ± 0.1	
92. 2-methylbutan-2-ol	293.15	809.60	[11]	839.2 ± 0.2	835.6 ± 0.1	
...	298.15	805.00	[9]	834.7 ± 0.2	829.4 ± 0.1	
...	320.00	784.30	[10]	814.1 ± 0.2	804.8 ± 0.2	
93. pentane-1,5-diol	293.15	991.40	[11]	1018.8 ± 0.6	993.6 ± 0.3	
...	298.15	986.20	[9]	1016.2 ± 0.5	990.8 ± 0.5	
94. pentan-3-amine	293.15	748.70	[11]	784.5 ± 0.1	772.4 ± 0.1	
...	298.15	743.67	[12]	779.6 ± 0.1	766.7 ± 0.1	
95. 1,2,3,4-tetrafluorobenzene	298.15	1416.10	[15]	**1247.8 ± 0.2**	1348.3 ± 0.4	
96. 1,2,3,5-tetrafluorobenzene	298.15	1393.00	[16]	**1231.9 ± 0.5**	1342.8 ± 0.3	
97. 1,3-difluorobenzene	293.15	1157.20	[11]	1068.5 ± 0.2	1115.6 ± 0.2	
...	298.15	1162.02	[12]	1090.6 ± 0.2	1107.1 ± 0.6	1206.7
98. 1,2-difluorobenzene	293.15	1157.07	[12]	1078.2 ± 0.2	1127.6 ± 0.2	
...	298.15	1150.01	[12]	1099.3 ± 0.4	1119.3 ± 0.4	

Table S2: Liquid density - continued

Name	Experiment			GAFF	OPLS/AA	CGenFF
	T	ρ	Ref.	ρ	ρ	ρ
99. fluorobenzene	293.15	1022.50	[11]	977.3 ± 0.5	1021.4 ± 0.1	
...	298.15	1019.10	[9]	989.6 ± 0.3	1015.0 ± 0.1	1029.6
100. nitrobenzene	293.15	1203.70	[11]	1238.0 ± 0.2	1179.4 ± 0.2	
...	298.15	1198.70	[9]	1233.1 ± 0.2	1174.4 ± 0.2	1155.0
101. 2-chloroaniline	293.15	1210.00	[11]	1239.2 ± 0.2	1228.8 ± 0.1	
102. phenol	318.15	1054.50	[11]	1051.5 ± 0.2	1057.0 ± 0.2	
103. benzenethiol	293.15	1077.50	[11]	1067.7 ± 0.3	1056.8 ± 0.3	
...	298.15	1073.01	[12]	1061.4 ± 0.2	1051.1 ± 0.2	
104. 2-methylpyridine	293.15	944.30	[11]	946.5 ± 0.2	952.9 ± 0.1	
...	298.15	939.80	[9]	941.5 ± 0.2	948.0 ± 0.2	
105. 3-methylpyridine	293.15	956.60	[11]	949.2 ± 0.1	957.0 ± 0.1	
...	298.15	953.30	[9]	944.2 ± 0.2	952.1 ± 0.1	942.9
106. 4-methylpyridine	293.15	954.80	[11]	951.3 ± 0.1	952.9 ± 0.2	
...	298.15	950.30	[9]	950.3 ± 0.2	948.4 ± 0.1	954.6
107. cyclohexanone	293.15	947.80	[11]	941.4 ± 0.1	953.1 ± 0.2	
...	298.15	941.90	[9]	936.8 ± 0.1	947.9 ± 0.2	
108. (E)-hex-2-ene	293.15	678.50	[11]	660.3 ± 0.1	682.0 ± 0.1	668.7
109. hexan-2-one	298.15	807.00	[10]	803.4 ± 0.0	821.5 ± 0.1	
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15	994.30	[11]	**1095.7 ± 0.3**	**1094.8 ± 0.7**	
111. cyclohexanamine	298.15	863.00	[12]	921.1 ± 0.5	898.0 ± 0.2	
112. 2-propan-2-yloxypropane	298.15	718.10	[9]	762.7 ± 0.1	748.2 ± 0.1	
113. 1-methoxy-2-(2-methoxyethoxy)ethane	293.15	943.40	[11]	1014.4 ± 0.1	960.3 ± 0.1	
...	298.15	938.30	[9]	1009.1 ± 0.2	954.5 ± 0.1	
114. triethyl phosphate	293.15	1069.50	[11]	1125.2 ± 0.3	1087.1 ± 0.1	
...	298.15	1069.60	[9]	1120.6 ± 0.1	1082.1 ± 0.3	
...	320.00	1057.30	[12]	1099.0 ± 0.2	1058.3 ± 0.1	
115. N,N-diethylethanamine	293.15	727.50	[11]	758.0 ± 0.1	749.5 ± 0.1	
...	298.15	722.80	[9]	753.1 ± 0.1	744.1 ± 0.1	
116. N-propan-2-ylpropan-2-amine	293.15	715.30	[11]	767.2 ± 0.1	756.4 ± 0.1	
...	298.15	712.27	[10]	762.3 ± 0.1	751.0 ± 0.1	
117. trifluoromethylbenzene	293.15	1188.40	[11]	1179.4 ± 0.1	1198.3 ± 0.2	
...	298.15	1177.98	[12]	1171.9 ± 0.3	1191.0 ± 0.1	

Table S2: Liquid density - continued

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ρ	Ref.	ρ	ρ	ρ
118. benzonitrile	288.15	1009.30	[11]	989.3 ± 0.2	1014.1 ± 0.0	
119. benzaldehyde	298.15	1043.60	[9]	1036.9 ± 0.2	1031.4 ± 0.1	1018.6
120. toluene	298.15	861.90	[9]	851.2 ± 0.1	872.0 ± 0.1	845.3
121. methoxybenzene	293.15	994.00	[11]	994.1 ± 0.1	986.0 ± 0.1	
...	298.15	989.40	[9]	991.9 ± 0.1	980.7 ± 0.1	945.1
122. phenylmethanol	297.15	1041.90	[11]	1045.2 ± 0.1	1041.5 ± 0.2	
123. 2-methylphenol	308.15	1032.70	[11]	1040.4 ± 0.1	1039.4 ± 0.2	
124. 3-methylphenol	320.00	1012.38	[10]	1020.4 ± 0.2	1022.2 ± 0.1	
125. 4-methylphenol	313.15	1018.50	[11]	1005.4 ± 0.2	1027.1 ± 0.0	986.6
...	320.00	1012.87	[10]	998.9 ± 0.1	1021.3 ± 0.1	
126. diethyl propanedioate	293.15	1055.10	[11]	1097.8 ± 0.2	1086.4 ± 0.1	
127. 2,4-dimethylpentan-3-one	293.15	810.80	[11]	819.2 ± 0.1	832.8 ± 0.1	
...	298.15	799.93	[10]	816.6 ± 0.0	828.1 ± 0.1	
128. heptan-2-one	293.15	811.10	[11]	813.1 ± 0.1	830.3 ± 0.1	
...	298.15	811.00	[9]	809.4 ± 0.1	825.5 ± 0.1	
129. ethenylbenzene	298.15	901.00	[9]	892.2 ± 0.1	912.1 ± 0.1	
130. 1-phenylethanone	293.15	1028.10	[11]	1026.5 ± 0.1	1030.6 ± 0.1	
...	298.15	1023.40	[9]	1021.5 ± 0.1	1026.0 ± 0.1	
131. methyl benzoate	298.15	1084.00	[9]	1111.3 ± 0.1	1096.8 ± 0.1	
132. methyl 2-hydroxybenzoate	298.15	1181.00	[11]	1222.1 ± 0.4	1200.2 ± 0.2	
...	320.00	1155.59	[12]	1192.7 ± 0.2	1179.5 ± 0.1	
133. ethylbenzene	298.15	862.50	[9]	853.1 ± 0.1	870.0 ± 0.0	847.6
134. 1,2-dimethylbenzene	293.15	879.95	[10]	862.2 ± 0.1	889.0 ± 0.1	860.0
...	298.15	876.00	[9]	857.1 ± 0.1	884.4 ± 0.1	
135. 1,2-dimethoxybenzene	298.15	1082.00	[9]	1075.0 ± 0.0	1057.0 ± 0.1	
136. 2,4,6-trimethylpyridine	295.15	916.60	[11]	908.1 ± 0.1	929.5 ± 0.1	
...	298.15	910.40	[9]	910.2 ± 0.2	926.7 ± 0.1	
137. octan-1-ol	298.15	822.20	[9]	834.2 ± 0.2	888.3 ± 0.1	
...	320.00	806.39	[10]	816.2 ± 0.2	865.3 ± 1.0	
138. 1-butoxybutane	293.15	768.40	[11]	776.5 ± 0.1	773.0 ± 0.1	
...	298.15	764.30	[9]	772.0 ± 0.1	767.8 ± 0.1	
139. N-butylbutan-1-amine	293.15	767.00	[11]	775.3 ± 0.1	774.6 ± 0.1	
...	298.15	757.60	[9]	771.1 ± 0.0	769.6 ± 0.1	

Table S2: Liquid density - continued

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ρ	Ref.	ρ	ρ	ρ
140. isoquinoline	303.15	1091.00	[11]	1105.0 ± 0.2	1124.4 ± 0.2	
...	320.00	1078.37	[12]	1071.8 ± 0.2	1099.9 ± 0.5	
141. quinoline	288.15	1097.70	[11]	1097.2 ± 0.1	1086.4 ± 0.2	
...	298.15	1090.00	[9]	1088.5 ± 0.2	1077.7 ± 0.2	1072.4
142. (1-methylethyl)benzene	298.15	857.30	[9]	856.2 ± 0.1	873.9 ± 0.1	845.7
143. 1,2,4-trimethylbenzene	293.15	875.91	[12]	859.2 ± 0.2	888.8 ± 0.1	864.0
...	298.15	872.00	[12]	854.6 ± 0.1	884.4 ± 0.1	
144. 2,6-dimethylheptan-4-one	293.15	806.20	[11]	823.6 ± 0.1	840.7 ± 0.1	
...	298.15	802.43	[10]	819.3 ± 0.0	836.1 ± 0.1	
145. 1-chloronaphthalene	298.15	1188.00	[11]	1191.0 ± 0.1	1171.7 ± 0.1	
146. phenoxybenzene	303.15	1066.10	[11]	1073.0 ± 0.1	1082.1 ± 0.2	

Table S3: Heat of vaporization ΔH_{vap} (kJ/mol) calculated and experimental. Blue font indicates that the calculated value differs more than 10% from the experimental ones, a red font indicates that it differs by more than 25%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ΔH_{vap}	Ref.	ΔH_{vap}	ΔH_{vap}	ΔH_{vap}
1. chloroform	298.15	31.28	[9]	28.42 ± 0.01	29.20 ± 0.01	
2. dichloro(fluoro)methane	282.05	24.95	[13]	23.86 ± 0.02	21.92 ± 0.01	
3. dibromomethane	293.15	37.67	[13]	29.05 ± 0.02	34.41 ± 0.03	
...	298.15	37.45	[9]	28.55 ± 0.01	34.17 ± 0.02	
4. dichloromethane	293.15	29.50	[13]	27.02 ± 0.03	23.84 ± 0.02	
...	298.15	28.82	[9]	26.48 ± 0.01	23.36 ± 0.03	
5. methanal	253.15	23.10	[13]	24.85 ± 0.02	24.11 ± 0.01	
...	253.65	23.08	[13]	24.79 ± 0.01	24.08 ± 0.01	
6. methanoic acid	293.15	19.82	[13]	**68.74 ± 0.05**	**42.79 ± 0.02**	
...	298.15	19.90	[9]	**65.46 ± 0.02**	**42.48 ± 0.01**	
8. methanamide	298.15	60.57	[9]	62.15 ± 0.01	59.76 ± 0.01	
9. nitromethane	293.15	38.39	[13]	**55.62 ± 0.03**	43.06 ± 0.06	
...	298.15	38.62	[9]	**55.31 ± 0.01**	38.07 ± 0.01	
10. methanol	293.15	37.94	[13]	39.92 ± 0.03	36.89 ± 0.02	
...	298.15	37.43	[9]	39.62 ± 0.02	36.44 ± 0.01	36.86
11. 1,1,1,2,2-pentachloroethane	293.15	46.29	[13]	46.74 ± 0.02	47.53 ± 0.02	
12. 1,1,2,2-tetrachloroethane	293.15	44.84	[13]	41.77 ± 0.05	43.31 ± 0.06	
...	298.15	45.71	[9]	41.62 ± 0.05	42.94 ± 0.04	
13. 1,1-dichloroethene	293.15	26.75	[13]	23.13 ± 0.03	27.05 ± 0.03	
...	298.15	26.48	[13]	22.87 ± 0.02	26.85 ± 0.01	
14. 1,1,2-trichloroethane	293.15	39.52	[13]	39.61 ± 0.05	39.81 ± 0.21	
...	298.15	40.28	[9]	39.22 ± 0.05	39.64 ± 0.09	
15. acetonitrile	293.15	33.28	[13]	32.76 ± 0.03	30.65 ± 0.03	
...	298.15	33.23	[9]	32.60 ± 0.01	30.42 ± 0.02	
16. 1,2-dibromoethane	298.15	41.73	[9]	34.71 ± 0.04	48.83 ± 0.08	
17. 1,1-dichloroethane	293.15	31.09	[13]	32.00 ± 0.02	28.53 ± 0.03	
...	298.15	30.62	[9]	31.73 ± 0.03	28.29 ± 0.01	30.59
18. 1,2-dichloroethane	298.15	35.16	[9]	36.99 ± 0.02	35.08 ± 0.05	
19. methyl formate	293.15	28.85	[13]	**38.68 ± 0.02**	29.67 ± 0.03	
...	298.15	30.59	[9]	**38.29 ± 0.01**	29.36 ± 0.02	

Table S3: Heat of vaporization - continued

Name	Experiment T	Experiment ΔH_{vap}	Experiment Ref.	GAFF ΔH_{vap}	OPLS/AA ΔH_{vap}	CGenFF ΔH_{vap}
20. bromoethane	293.15	27.87	[13]	25.36 ± 0.03	29.85 ± 0.03	
...	298.15	27.62	[13]	25.15 ± 0.02	29.65 ± 0.01	
21. chloroethane	273.15	25.39	[13]	24.86 ± 0.02	24.27 ± 0.01	
...	285.45	24.85	[13]	24.28 ± 0.01	23.67 ± 0.02	
22. 2-chloroethanol	293.15	46.02	[13]	55.03 ± 0.04	48.65 ± 0.11	
23. ethanamide	358.15	62.06	[13]	65.11 ± 0.02	64.67 ± 0.02	
24. N-methylformamide	292.15	57.79	[13]	57.25 ± 0.03	50.52 ± 0.02	
...	298.15	56.25	[9]	56.76 ± 0.02	49.85 ± 0.02	
25. nitroethane	298.15	40.24	[9]	**55.23 ± 0.01**	41.08 ± 0.01	
26. methoxymethane	240.00	21.72	[13]	24.12 ± 0.02	**30.87 ± 0.03**	
27. ethanol	293.15	42.85	[13]	46.03 ± 0.04	42.79 ± 0.03	
...	298.15	42.32	[9]	44.62 ± 0.02	42.32 ± 0.02	42.59
28. 1,2-ethanedithiol	293.15	44.37	[13]	41.95 ± 0.02	47.04 ± 0.04	
...	298.15	44.15	[13]	41.66 ± 0.04	46.75 ± 0.01	
29. methyldisulfanylmethane	293.15	38.56	[13]	33.08 ± 0.03	37.87 ± 0.04	
...	298.15	38.32	[13]	32.75 ± 0.02	37.52 ± 0.02	35.35
30. methylsulfinylmethane	298.15	52.89	[9]	57.50 ± 0.02	55.62 ± 0.02	
31. methylsulfanylmethane	293.15	28.06	[13]	26.03 ± 0.04	30.59 ± 0.03	
...	298.15	27.65	[9]	23.88 ± 0.02	29.65 ± 0.02	
32. 2-aminoethanol	293.15	64.03	[13]	**82.46 ± 0.05**	55.17 ± 0.12	
...	320.00	61.71	[13]	**79.96 ± 0.05**	53.17 ± 0.19	
33. ethane-1,2-diamine	293.15	45.46	[13]	**58.51 ± 0.09**	50.58 ± 0.40	
...	298.15	46.60	[9]	57.95 ± 0.08	49.79 ± 0.22	
34. prop-2-enenitrile	298.15	33.26	[9]	33.33 ± 0.01	31.47 ± 0.02	
...	350.45	31.71	[13]	30.64 ± 0.01	29.03 ± 0.02	
35. 1,3-dioxolan-2-one	312.15	60.96	[13]	75.55 ± 0.02	64.90 ± 0.02	
36. propanenitrile	293.15	36.31	[13]	36.64 ± 0.04	33.89 ± 0.02	
...	298.15	36.03	[9]	36.29 ± 0.02	33.57 ± 0.03	
37. 1,2-dibromopropane	293.15	48.36	[12]	40.51 ± 0.15	51.03 ± 0.16	
...	298.15	42.20	[17]	40.24 ± 0.04	50.99 ± 0.12	
38. 1,3-dichloropropane	298.15	40.05	[13]	41.97 ± 0.05	40.08 ± 0.06	
39. (2R)-2-methyloxirane	298.15	27.90	[17]	27.87 ± 0.02	26.93 ± 0.01	

Table S3: Heat of vaporization - continued

Name	Experiment T	Experiment ΔH_{vap}	Experiment Ref.	GAFF ΔH_{vap}	OPLS/AA ΔH_{vap}	CGenFF ΔH_{vap}
40. propan-2-one	298.15	30.99	[9]	34.47 ± 0.02	30.76 ± 0.02	30.63
41. methyl acetate	293.15	32.67	[13]	**41.57 ± 0.06**	38.05 ± 0.04	
...	298.15	32.29	[9]	**41.20 ± 0.02**	36.34 ± 0.01	32.38
42. 1,3-dioxolane	293.15	35.80	[17]	43.45 ± 0.01	36.49 ± 0.02	
...	298.15	35.60	[9]	43.18 ± 0.03	36.22 ± 0.04	
43. 2-iodopropane	293.15	34.40	[13]	34.08 ± 0.03	34.26 ± 0.03	
...	298.15	34.20	[13]	33.71 ± 0.02	33.85 ± 0.02	
44. 1-bromopropane	293.15	32.49	[13]	31.98 ± 0.05	35.35 ± 0.04	
...	298.15	32.20	[13]	31.41 ± 0.02	34.83 ± 0.02	
45. N,N-dimethylformamide	298.15	47.57	[9]	52.57 ± 0.02	46.08 ± 0.02	
46. N-methylacetamide	320.00	58.32	[13]	59.68 ± 0.07	55.12 ± 0.08	
47. 1-nitropropane	298.15	43.39	[9]	**59.32 ± 0.04**	44.97 ± 0.01	
48. 2-nitropropane	298.15	41.34	[9]	**56.44 ± 0.02**	43.74 ± 0.01	
49. dimethoxymethane	293.15	29.87	[13]	34.92 ± 0.07	32.63 ± 0.07	
...	298.15	29.54	[13]	34.47 ± 0.02	32.23 ± 0.04	
50. propane-1,2,3-triol	293.15	90.21	[13]	99.60 ± 0.06	95.44 ± 0.29	
51. propan-1-amine	293.15	31.29	[13]	39.07 ± 0.05	33.83 ± 0.12	
...	298.15	30.98	[13]	38.36 ± 0.03	33.08 ± 0.04	
52. propan-2-amine	293.15	28.92	[13]	**41.27 ± 0.08**	34.23 ± 0.06	
...	298.15	28.56	[13]	**40.67 ± 0.03**	32.70 ± 0.02	
53. 2-methylpropane	243.65	22.35	[13]	25.03 ± 0.02	24.61 ± 0.01	
54. ethylsulfanylethane	293.15	35.89	[13]	35.03 ± 0.07	39.54 ± 0.06	
...	298.15	35.77	[9]	34.55 ± 0.02	39.05 ± 0.03	
55. butane-1-thiol	293.15	37.40	[12]	38.50 ± 0.06	40.94 ± 0.06	
...	298.15	37.14	[12]	38.01 ± 0.04	38.81 ± 0.06	
56. butan-1-ol	293.15	54.04	[13]	60.52 ± 0.11	52.12 ± 0.03	
...	298.15	52.35	[9]	60.08 ± 0.08	51.39 ± 0.05	
57. 2-methylpropan-2-ol	320.00	44.01	[13]	**57.28 ± 0.08**	47.20 ± 0.07	
58. butane-1,4-diol	293.15	76.71	[13]	90.32 ± 0.22	81.48 ± 0.42	
...	298.15	76.60	[9]	87.23 ± 0.31	81.43 ± 0.24	
...	320.00	75.32	[13]	92.18 ± 1.57	78.62 ± 0.14	
59. (2-hydroxyethoxy)ethan-2-ol	288.15	83.13	[13]	103.66 ± 0.06	78.15 ± 0.19	

Table S3: Heat of vaporization - continued

Name	Experiment T	Experiment ΔH_{vap}	Experiment Ref.	GAFF ΔH_{vap}	OPLS/AA ΔH_{vap}	CGenFF ΔH_{vap}
60. N-ethylethanamine	293.15	31.54	[13]	37.64 ± 0.12	34.12 ± 0.10	
...	298.15	31.32	[9]	36.96 ± 0.05	33.34 ± 0.07	
61. butan-1-amine	293.15	35.89	[13]	**46.59 ± 0.06**	39.15 ± 0.08	
...	298.15	35.74	[9]	**45.83 ± 0.09**	38.53 ± 0.08	
62. 2-methylpropan-2-amine	293.15	29.09	[13]	**46.33 ± 0.04**	**37.24 ± 0.06**	
...	298.15	28.80	[13]	**45.68 ± 0.03**	**36.68 ± 0.03**	
63. 2-(2-hydroxyethylamino)ethanol	320.00	83.64	[13]	**110.71 ± 0.14**	88.94 ± 0.30	
64. pyrimidine	298.15	49.81	[9]	50.47 ± 0.02	49.33 ± 0.02	51.09
65. furan	293.15	27.83	[13]	30.65 ± 0.04	30.12 ± 0.04	
...	298.15	27.46	[9]	30.33 ± 0.02	29.81 ± 0.02	23.60
66. thiophene	293.15	34.89	[13]	34.26 ± 0.04	39.51 ± 0.04	
...	298.15	34.65	[13]	32.72 ± 0.01	39.15 ± 0.02	35.40
67. 1H-pyrrole	293.15	45.70	[13]	52.93 ± 0.04	44.54 ± 0.04	
...	298.15	45.15	[9]	52.51 ± 0.03	44.14 ± 0.02	
68. ethenyl acetate	298.15	34.58	[13]	**43.40 ± 0.01**	**44.07 ± 0.02**	
69. oxolan-2-one	293.15	52.84	[12]	64.60 ± 0.02	53.12 ± 0.03	
70. acetyl acetate	293.15	47.32	[13]	**68.65 ± 0.04**	**61.27 ± 0.03**	
71. 1,4-dichlorobutane	298.15	46.00	[13]	48.84 ± 0.14	46.92 ± 0.04	
72. oxolane	298.15	31.80	[9]	37.14 ± 0.02	32.14 ± 0.02	
73. ethoxyethene	293.15	27.84	[13]	31.93 ± 0.02	31.51 ± 0.03	
74. ethyl acetate	293.15	35.96	[13]	**46.32 ± 0.05**	42.40 ± 0.06	
...	298.15	35.59	[9]	**45.81 ± 0.04**	41.91 ± 0.02	35.10
75. tetrahydrothiophene 1,1-dioxide	320.00	66.59	[13]	**86.42 ± 0.07**	72.33 ± 0.06	
76. thiolane	293.15	39.74	[13]	39.05 ± 0.05	42.93 ± 0.08	
...	298.15	38.62	[9]	38.85 ± 0.02	41.12 ± 0.02	
77. 1-bromobutane	293.15	37.12	[13]	39.92 ± 0.06	40.51 ± 0.05	
...	298.15	36.60	[9]	36.91 ± 0.03	40.05 ± 0.03	
78. 1-chlorobutane	293.15	34.23	[12]	37.73 ± 0.03	37.41 ± 0.05	
...	298.15	33.52	[9]	35.63 ± 0.03	33.77 ± 0.05	
79. pyrrolidine	293.15	37.58	[13]	42.68 ± 0.05	40.94 ± 0.04	
...	298.15	37.57	[9]	42.13 ± 0.02	38.28 ± 0.06	
80. N,N-dimethylacetamide	298.15	50.23	[9]	53.55 ± 0.02	51.82 ± 0.02	

Table S3: Heat of vaporization - continued

Name	Experiment T	Experiment ΔH_{vap}	Experiment Ref.	GAFF ΔH_{vap}	OPLS/AA ΔH_{vap}	CGenFF ΔH_{vap}
81. morpholine	293.15	45.32	[13]	**59.56 ± 0.39**	54.13 ± 0.36	
82. pyridine	293.15	40.34	[13]	41.70 ± 0.06	41.72 ± 0.07	
...	298.15	40.15	[9]	41.27 ± 0.03	41.34 ± 0.03	41.97
83. cyclopentanone	293.15	42.38	[13]	48.54 ± 0.07	43.45 ± 0.04	
...	298.15	42.63	[9]	48.17 ± 0.02	42.89 ± 0.02	
84. 1-cyclopropylethanone	293.15			46.09 ± 0.03	44.37 ± 0.04	
...	298.15	39.40	[17]	45.66 ± 0.02	44.04 ± 0.02	
85. pentane-2,4-dione	298.15	41.80	[9]	**60.19 ± 0.02**	**56.39 ± 0.02**	
86. methyl 2-methylprop-2-enoate	298.15	39.13	[13]	46.34 ± 0.02	**54.73 ± 0.16**	
87. pentanenitrile	293.15	44.33	[13]	46.82 ± 0.04	43.13 ± 0.06	
...	298.15	44.08	[9]	46.25 ± 0.03	42.65 ± 0.05	
88. ethyl propanoate	298.15	39.25	[9]	**49.58 ± 0.04**	46.45 ± 0.03	
89. diethyl carbonate	298.15	41.10	[9]	**60.79 ± 0.08**	**52.66 ± 0.04**	
90. pentan-1-ol	293.15	57.64	[13]	65.96 ± 0.12	57.47 ± 0.08	
...	298.15	57.02	[9]	65.43 ± 0.11	56.79 ± 0.08	
...	320.00	54.67	[13]	63.52 ± 0.09	54.33 ± 0.08	
91. pentan-3-ol	293.15	52.82	[13]	58.83 ± 0.14	63.78 ± 0.10	
...	298.15	52.37	[13]	57.79 ± 0.12	53.65 ± 0.16	
92. 2-methylbutan-2-ol	293.15	50.19	[13]	**67.55 ± 0.07**	51.39 ± 0.27	
...	298.15	50.20	[9]	**66.93 ± 0.04**	50.64 ± 0.19	
...	320.00	47.17	[13]	**64.86 ± 0.08**	47.75 ± 0.17	
93. pentane-1,5-diol	293.15	76.36	[13]	**101.55 ± 0.22**	90.02 ± 0.08	
...	298.15	82.40	[9]	101.08 ± 0.31	89.14 ± 0.14	
94. pentan-3-amine	293.15	39.97	[12]	47.54 ± 0.12	41.05 ± 0.24	
...	298.15	39.64	[12]	46.96 ± 0.10	40.45 ± 0.22	
95. 1,2,3,4-tetrafluorobenzene	298.15	36.61	[18]	35.45 ± 0.02	36.85 ± 0.03	
96. 1,2,3,5-tetrafluorobenzene	298.15	35.40	[18]	33.81 ± 0.02	37.10 ± 0.04	
97. 1,3-difluorobenzene	293.15	36.85	[12]	33.31 ± 0.03	34.84 ± 0.04	
...	298.15	36.58	[12]	33.78 ± 0.02	34.03 ± 0.03	42.76
98. 1,2-difluorobenzene	293.15	36.37	[12]	34.05 ± 0.03	35.27 ± 0.03	
...	298.15	36.11	[12]	35.24 ± 0.03	35.59 ± 0.03	
99. fluorobenzene	293.15	34.79	[13]	33.46 ± 0.08	34.45 ± 0.03	
...	298.15	34.58	[9]	33.87 ± 0.02	34.37 ± 0.01	37.03

Table S3: Heat of vaporization - continued

Name	Experiment T	Experiment ΔH_{vap}	Experiment Ref.	GAFF ΔH_{vap}	OPLS/AA ΔH_{vap}	CGenFF ΔH_{vap}
100. nitrobenzene	293.15	55.25	[13]	**70.34 ± 0.04**	55.09 ± 0.06	
...	298.15	55.01	[9]	**70.79 ± 0.03**	55.40 ± 0.02	54.73
101. 2-chloroaniline	293.15	57.60	[13]	56.13 ± 0.03	57.28 ± 0.02	
102. phenol	318.15	56.32	[13]	53.16 ± 0.03	61.26 ± 0.05	
103. benzenethiol	293.15	48.75	[13]	43.85 ± 0.05	41.43 ± 0.05	
...	298.15	48.47	[13]	43.75 ± 0.02	41.11 ± 0.02	
104. 2-methylpyridine	293.15	42.62	[13]	45.34 ± 0.03	46.07 ± 0.05	
...	298.15	42.92	[9]	44.87 ± 0.02	45.90 ± 0.02	
105. 3-methylpyridine	293.15	44.47	[13]	45.70 ± 0.02	47.37 ± 0.05	
...	298.15	45.23	[9]	45.59 ± 0.03	47.14 ± 0.01	42.80
106. 4-methylpyridine	293.15	44.61	[13]	46.42 ± 0.04	46.70 ± 0.07	
...	298.15	44.81	[9]	46.06 ± 0.02	46.40 ± 0.02	44.60
107. cyclohexanone	293.15	45.42	[13]	52.48 ± 0.10	54.76 ± 0.41	
...	298.15	45.13	[9]	52.10 ± 0.04	47.61 ± 0.03	
108. (E)-hex-2-ene	293.15	32.20	[11]	32.14 ± 0.04	33.62 ± 0.07	31.88
109. hexan-2-one	298.15	42.90	[13]	48.63 ± 0.04	46.44 ± 0.04	
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15	44.96	[13]	**76.61 ± 0.04**	**74.17 ± 0.14**	
111. cyclohexanamine	298.15	43.23	[13]	**61.77 ± 0.08**	50.02 ± 0.03	
112. 2-propan-2-yloxypropane	298.15	32.60	[9]	**42.90 ± 0.05**	36.69 ± 0.03	
113. 1-methoxy-2-(2-methoxyethoxy)ethane	293.15	52.61	[13]	**73.12 ± 0.05**	63.02 ± 0.09	
...	298.15	43.15	[9]	**72.34 ± 0.11**	**62.23 ± 0.05**	
114. triethyl phosphate	293.15	57.56	[13]	**86.80 ± 0.07**	**78.29 ± 0.08**	
...	298.15	57.30	[9]	**86.07 ± 0.06**	**77.69 ± 0.08**	
...	320.00	56.27	[13]	**83.39 ± 0.08**	**75.07 ± 0.07**	
115. N,N-diethylethanamine	293.15	34.87	[13]	**44.09 ± 0.23**	38.47 ± 0.33	
...	298.15	34.88	[9]	42.25 ± 0.05	38.16 ± 0.29	
116. N-propan-2-ylpropan-2-amine	293.15	34.98	[13]	**45.03 ± 0.06**	39.86 ± 0.05	
...	298.15	34.65	[13]	**44.51 ± 0.02**	39.44 ± 0.06	
117. trifluoromethylbenzene	293.15	38.02	[13]	41.51 ± 0.04	38.61 ± 0.07	
...	298.15	37.73	[13]	41.92 ± 0.02	38.88 ± 0.01	
118. benzonitrile	288.15	52.14	[13]	53.52 ± 0.03	54.09 ± 0.02	
119. benzaldehyde	298.15	39.60	[9]	**52.83 ± 0.02**	**54.47 ± 0.02**	47.03

Table S3: Heat of vaporization - continued

Name	Experiment T	Experiment ΔH_{vap}	Experiment Ref.	GAFF ΔH_{vap}	OPLS/AA ΔH_{vap}	CGenFF ΔH_{vap}
120. toluene	298.15	37.99	[9]	37.39 ± 0.02	40.02 ± 0.02	36.19
121. methoxybenzene	293.15	46.86	[13]	48.86 ± 0.03	47.52 ± 0.04	
...	298.15	45.00	[9]	48.89 ± 0.02	47.53 ± 0.02	41.63
122. phenylmethanol	297.15	65.59	[13]	62.62 ± 0.02	62.16 ± 0.05	
123. 2-methylphenol	308.15	56.90	[13]	63.66 ± 0.04	63.93 ± 0.03	
124. 3-methylphenol	320.00	60.91	[13]	65.20 ± 0.05	66.28 ± 0.07	
125. 4-methylphenol	313.15	63.23	[13]	57.23 ± 0.03	67.37 ± 0.04	
...	320.00	62.67	[13]	56.17 ± 0.04	66.15 ± 0.04	
126. diethyl propanedioate	293.15	57.26	[13]	**83.55 ± 0.09**	**75.40 ± 0.03**	
127. 2,4-dimethylpentan-3-one	293.15	40.71	[13]	**56.17 ± 0.10**	50.04 ± 0.06	
...	298.15	40.50	[13]	**56.03 ± 0.07**	49.73 ± 0.03	
128. heptan-2-one	293.15	47.37	[13]	55.11 ± 0.09	52.16 ± 0.08	
...	298.15	47.24	[9]	54.72 ± 0.10	51.74 ± 0.05	
129. ethenylbenzene	298.15	43.93	[9]	42.43 ± 0.01	45.02 ± 0.03	
130. 1-phenylethanone	293.15	54.54	[13]	58.76 ± 0.04	61.68 ± 0.08	
...	298.15	53.40	[9]	59.11 ± 0.02	61.62 ± 0.02	
131. methyl benzoate	298.15	55.57	[9]	64.21 ± 0.02	62.22 ± 0.02	
132. methyl 2-hydroxybenzoate	298.15	61.04	[13]	71.92 ± 0.07	71.44 ± 0.27	
133. ethylbenzene	298.15	42.25	[9]	42.36 ± 0.02	44.48 ± 0.02	37.49
134. 1,2-dimethylbenzene	293.15	43.73	[13]	42.40 ± 0.06	46.08 ± 0.06	
...	298.15	43.43	[9]	42.77 ± 0.02	46.45 ± 0.02	41.00
135. 1,2-dimethoxybenzene	298.15	48.38	[9]	**64.77 ± 0.01**	**63.53 ± 0.02**	
136. 2,4,6-trimethylpyridine	295.15	49.31	[13]	55.78 ± 0.03	56.74 ± 0.07	
...	298.15	50.34	[9]	54.66 ± 0.03	56.80 ± 0.02	
137. octan-1-ol	298.15	72.00	[9]	85.16 ± 0.11	86.24 ± 0.09	
...	320.00	69.53	[13]	82.02 ± 0.13	82.58 ± 0.25	
138. 1-butoxybutane	293.15	45.48	[13]	53.93 ± 0.08	50.87 ± 0.10	
...	298.15	44.40	[9]	53.39 ± 0.07	50.20 ± 0.04	
139. N-butylbutan-1-amine	293.15	49.81	[13]	58.97 ± 0.12	55.64 ± 0.12	
...	298.15	49.44	[9]	58.56 ± 0.20	55.05 ± 0.12	
140. isoquinoline	303.15	59.43	[13]	62.63 ± 0.03	**74.94 ± 0.05**	
...	320.00	58.61	[13]	59.23 ± 0.04	70.91 ± 0.10	

Table S3: Heat of vaporization - continued

	Experiment			GAFF	OPLS/AA	CGenFF
Name	T	ΔH_{vap}	Ref.	ΔH_{vap}	ΔH_{vap}	ΔH_{vap}
141. quinoline	288.15	59.51	[13]	61.13 ± 0.06	60.40 ± 0.05	
...	298.15	64.10	[9]	61.37 ± 0.03	61.05 ± 0.03	57.57
142. (1-methylethyl)benzene	298.15	45.14	[9]	46.90 ± 0.02	48.71 ± 0.02	41.80
143. 1,2,4-trimethylbenzene	293.15	47.81	[13]	47.39 ± 0.03	51.84 ± 0.05	
...	298.15	47.57	[13]	47.04 ± 0.03	51.45 ± 0.04	45.19
144. 2,6-dimethylheptan-4-one	293.15	50.83	[13]	58.68 ± 0.15	59.85 ± 0.16	
...	298.15	50.51	[13]	58.14 ± 0.08	59.43 ± 0.12	
145. 1-chloronaphthalene	298.15	64.66	[13]	61.67 ± 0.02	61.67 ± 0.03	
146. phenoxybenzene	303.15	58.42	[13]	69.65 ± 0.03	72.70 ± 0.04	

Table S4: Surface tension γ (10^{-3}Nm^{-1}) calculated and experimental. Blue font indicates that the calculated value differs more than 10% from the experimental ones, a red font indicates that it differs by more than 25%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA
Name	T	γ	Ref.	γ	γ
1. chloroform	298.15	26.67	[11]	**11.7 ± 0.5**	**11.8 ± 0.3**
2. dichloro(fluoro)methane	282.05	20.09	[12]	**11.8 ± 0.3**	**7.9 ± 0.2**
...	300.00	17.60	[14]	**9.8 ± 0.6**	**7.2 ± 0.3**
3. dibromomethane	298.15	39.05	[11]	**13.3 ± 0.5**	**25.1 ± 0.4**
4. dichloromethane	298.15	27.20	[11]	**15.7 ± 0.4**	**10.5 ± 0.4**
5. methanal	253.15	26.01	[12]	23.0 ± 0.2	22.5 ± 0.2
...	253.65	25.91	[12]	23.0 ± 0.2	22.6 ± 0.4
6. methanoic acid	298.15	37.13	[11]	**66.9 ± 4.4**	32.0 ± 0.4
7. bromomethane	276.65	27.18	[12]	**8.7 ± 0.5**	21.1 ± 0.1
8. methanamide	298.15	57.03	[11]	58.4 ± 2.3	53.1 ± 1.1
9. nitromethane	298.15	36.53	[11]	**55.2 ± 0.6**	29.2 ± 0.4
10. methanol	298.15	22.07	[11]	20.6 ± 0.7	20.1 ± 0.4
12. 1,1,2,2-tetrachloroethane	298.15	35.58	[11]	**22.1 ± 0.8**	**24.5 ± 0.7**
13. 1,1-dichloroethene	298.15	21.66	[12]	**9.8 ± 0.4**	**15.7 ± 0.5**
14. 1,1,2-trichloroethane	298.15	34.02	[11]	**23.1 ± 0.6**	**25.0 ± 0.4**
15. acetonitrile	298.15	28.66	[11]	21.6 ± 0.3	**16.6 ± 0.3**
16. 1,2-dibromoethane	298.15	39.55	[11]	**17.9 ± 0.3**	38.0 ± 0.7
17. 1,1-dichloroethane	298.15	24.07	[11]	**17.1 ± 0.4**	**15.1 ± 0.4**
18. 1,2-dichloroethane	298.15	31.86	[11]	24.4 ± 0.6	**23.2 ± 0.5**
19. methyl formate	298.15	24.36	[11]	**32.3 ± 0.5**	20.8 ± 0.3
20. bromoethane	293.15	24.15	[12]	**11.7 ± 0.3**	18.9 ± 0.6
...	298.15	23.62	[11]	**11.0 ± 0.4**	18.2 ± 0.6
21. chloroethane	273.15	21.87	[12]	**13.6 ± 0.4**	**13.8 ± 0.3**
...	285.45	20.13	[12]	**12.0 ± 0.4**	**11.9 ± 0.4**
23. ethanamide	358.15	38.96	[14]	34.1 ± 1.4	36.2 ± 1.6
24. N-methylformamide	292.15	39.35	[12]	39.7 ± 0.5	38.6 ± 0.2
...	298.15	38.52	[12]	38.2 ± 0.5	36.9 ± 0.2
25. nitroethane	298.15	32.13	[11]	39.1 ± 0.6	26.4 ± 0.4
26. methoxymethane	240.00	20.41	[14]	17.7 ± 0.3	**15.1 ± 0.2**
...	298.08	11.80	[14]	**8.3 ± 0.2**	**6.0 ± 0.3**

Table S4: Surface tension - continued

	Experiment			GAFF	OPLS/AA
Name	T	γ	Ref.	γ	γ
27. ethanol	298.15	21.97	[11]	18.6 ± 0.2	18.7 ± 0.3
28. 1,2-ethanedithiol	298.15			28.2 ± 0.3	35.9 ± 0.4
29. methyldisulfanylmethane	298.15	33.39	[11]	**16.9 ± 0.5**	**20.7 ± 0.5**
30. methylsulfinylmethane	298.15	42.92	[11]	41.6 ± 0.9	42.4 ± 0.9
31. methylsulfanylmethane	298.15	24.06	[11]	**10.6 ± 0.3**	**17.6 ± 0.4**
32. 2-aminoethanol	293.15	49.17	[12]	56.1 ± 2.4	40.5 ± 1.4
...	298.15	48.32	[11]	57.4 ± 9.7	39.4 ± 0.9
33. ethane-1,2-diamine	298.15	41.12	[12]	45.2 ± 2.2	32.5 ± 0.7
34. prop-2-enenitrile	298.15	26.63	[14]	**19.4 ± 0.4**	20.4 ± 0.3
...	350.45	20.45	[12]	**12.4 ± 0.3**	**13.3 ± 0.3**
35. 1,3-dioxolan-2-one	312.15	63.28	[12]	65.2 ± 2.3	54.7 ± 1.0
...	313.15	50.60	[14]	**63.5 ± 2.5**	54.4 ± 1.4
36. propanenitrile	298.15	26.75	[11]	21.1 ± 0.4	**16.2 ± 0.2**
37. 1,2-dibromopropane	298.15	34.50	[12]	**20.1 ± 0.6**	33.9 ± 0.8
38. 1,3-dichloropropane	298.15	33.93	[12]	**25.1 ± 0.6**	**23.6 ± 0.5**
39. (2R)-2-methyloxirane	298.15			14.7 ± 0.4	13.0 ± 0.4
40. propan-2-one	298.15	22.72	[11]	19.2 ± 0.4	17.2 ± 0.2
41. methyl acetate	298.15	24.73	[11]	26.1 ± 0.3	23.2 ± 0.4
42. 1,3-dioxolane	293.15			38.2 ± 0.7	26.6 ± 1.2
...	298.15	32.61	[14]	37.6 ± 0.2	26.0 ± 0.6
43. 2-iodopropane	298.15	26.62	[12]	**15.8 ± 0.5**	**19.1 ± 0.6**
44. 1-bromopropane	298.15	25.26	[11]	**14.5 ± 0.4**	19.4 ± 0.2
45. N,N-dimethylformamide	298.15	35.74	[11]	36.1 ± 0.5	31.5 ± 0.8
46. N-methylacetamide	320.00	31.26	[12]	31.1 ± 0.3	33.0 ± 0.4
47. 1-nitropropane	298.15	29.85	[12]	34.9 ± 0.7	24.0 ± 0.5
48. 2-nitropropane	298.15	29.29	[11]	33.6 ± 0.5	24.9 ± 0.8
49. dimethoxymethane	298.04	20.36	[14]	20.3 ± 0.4	17.1 ± 0.3
...	298.15	18.75	[12]	20.3 ± 0.4	17.1 ± 0.3
50. propane-1,2,3-triol	293.15	77.25	[12]	74.9 ± 17.0	63.1 ± 15.0
...	298.15	63.00	[14]	70.5 ± 17.0	51.8 ± 7.5
51. propan-1-amine	298.15	21.75	[11]	17.2 ± 1.0	**12.6 ± 0.6**
52. propan-2-amine	298.15	17.36	[12]	17.9 ± 0.2	13.0 ± 0.3

Table S4: Surface tension - continued

	Experiment			GAFF	OPLS/AA
Name	T	γ	Ref.	γ	γ
53. 2-methylpropane	243.65	16.42	[12]	13.0 ± 0.2	12.6 ± 0.3
54. ethylsulfanylethane	298.15	24.57	[11]	**14.5 ± 0.2**	18.7 ± 0.5
55. butane-1-thiol	298.15	25.22	[12]	**17.6 ± 0.3**	19.9 ± 0.3
56. butan-1-ol	298.15	24.93	[11]	19.5 ± 1.0	**18.6 ± 0.8**
57. 2-methylpropan-2-ol	320.00			17.3 ± 1.9	15.8 ± 0.4
58. butane-1,4-diol	298.15	45.47	[14]	48.4 ± 14.0	45.6 ± 3.4
...	320.00	44.23	[12]	35.4 ± 3.4	39.6 ± 3.2
59. (2-hydroxyethoxy)ethan-2-ol	288.15	56.61	[12]	65.6 ± 5.6	**41.7 ± 8.2**
60. N-ethylethanamine	298.15	19.85	[11]	15.8 ± 0.3	**12.6 ± 0.2**
61. butan-1-amine	298.15	23.44	[11]	17.6 ± 0.7	**14.5 ± 0.1**
62. 2-methylpropan-2-amine	298.15	16.87	[11]	17.1 ± 0.8	15.3 ± 0.2
63. 2-(2-hydroxyethylamino)ethanol	320.00	50.60	[12]	49.4 ± 9.1	45.7 ± 7.3
64. pyrimidine	298.15	30.33	[11]	**41.1 ± 1.1**	**41.7 ± 1.2**
65. furan	298.15	22.65	[12]	18.7 ± 0.6	19.6 ± 0.4
66. thiophene	298.15	30.68	[11]	**19.5 ± 0.6**	29.4 ± 0.5
67. 1H-pyrrole	298.15	36.95	[12]	29.9 ± 0.8	28.9 ± 0.9
68. ethenyl acetate	298.15	22.03	[12]	24.0 ± 0.3	27.4 ± 0.6
71. 1,4-dichlorobutane	298.15	35.42	[12]	**26.3 ± 0.7**	**25.4 ± 0.7**
72. oxolane	298.15	26.65	[12]	24.4 ± 0.6	**17.7 ± 0.5**
74. ethyl acetate	298.15	23.39	[11]	24.1 ± 0.5	23.2 ± 0.6
75. tetrahydrothiophene 1,1-dioxide	320.00	53.33	[12]	55.9 ± 5.6	46.2 ± 1.6
76. thiolane	298.15	33.82	[12]	**23.7 ± 0.8**	26.9 ± 0.6
77. 1-bromobutane	298.15	25.90	[11]	**16.5 ± 0.7**	20.3 ± 0.6
78. 1-chlorobutane	298.15	23.18	[11]	**15.8 ± 0.7**	**15.1 ± 0.3**
79. pyrrolidine	298.15	37.06	[11]	**25.7 ± 1.1**	**19.0 ± 0.8**
80. N,N-dimethylacetamide	298.15	33.09	[12]	31.3 ± 0.6	32.1 ± 0.6
81. morpholine	293.15	39.50	[12]	43.7 ± 2.0	33.6 ± 3.2
...	298.15	37.68	[14]	44.4 ± 1.9	32.7 ± 1.2
82. pyridine	298.15	36.56	[11]	27.6 ± 0.5	29.1 ± 0.8
83. cyclopentanone	298.15	32.80	[11]	30.3 ± 0.5	26.2 ± 0.8
84. 1-cyclopropylethanone	298.15			22.9 ± 1.1	24.8 ± 0.7
85. pentane-2,4-dione	298.15	30.90	[14]	33.8 ± 0.6	32.9 ± 0.9

Table S4: Surface tension - continued

Name	Experiment T	Experiment γ	Ref.	GAFF γ	OPLS/AA γ
86. methyl 2-methylprop-2-enoate	298.15	24.24	[12]	23.4 ± 0.5	29.4 ± 0.7
87. pentanenitrile	297.75	27.09	[14]	21.3 ± 0.9	**17.8 ± 0.7**
...	298.15	26.97	[12]	21.5 ± 1.0	**17.5 ± 0.8**
88. ethyl propanoate	298.15	23.80	[11]	22.8 ± 0.4	22.3 ± 0.5
89. diethyl carbonate	298.15	25.92	[14]	29.2 ± 1.4	25.0 ± 0.8
90. pentan-1-ol	298.15	25.36	[11]	19.4 ± 1.1	19.0 ± 1.0
91. pentan-3-ol	298.15	23.65	[12]	19.7 ± 1.2	18.8 ± 0.7
92. 2-methylbutan-2-ol	298.15			19.2 ± 2.5	18.4 ± 0.9
93. pentane-1,5-diol	298.15	46.32	[12]	51.4 ± 6.9	46.8 ± 5.3
94. pentan-3-amine	298.15	22.26	[12]	18.1 ± 0.5	**15.8 ± 0.3**
95. 1,2,3,4-tetrafluorobenzene	298.15			11.2 ± 0.4	14.2 ± 0.4
96. 1,2,3,5-tetrafluorobenzene	298.15			9.4 ± 0.2	13.1 ± 0.8
97. 1,3-difluorobenzene	298.15	25.95	[12]	**15.0 ± 0.3**	**14.1 ± 0.5**
98. 1,2-difluorobenzene	298.15	26.07	[12]	**16.1 ± 0.3**	**16.1 ± 0.3**
99. fluorobenzene	298.15	26.66	[11]	**16.7 ± 0.2**	**18.3 ± 0.7**
100. nitrobenzene	298.15	43.23	[12]	45.3 ± 1.7	33.6 ± 1.0
...	364.15	34.20	[14]	36.0 ± 0.6	**25.0 ± 0.7**
101. 2-chloroaniline	293.15	40.73	[14]	30.9 ± 0.7	33.1 ± 0.8
102. phenol	318.15	38.72	[12]	**27.6 ± 0.6**	30.1 ± 2.0
103. benzenethiol	298.15	38.70	[14]	**23.9 ± 0.6**	**21.6 ± 0.3**
104. 2-methylpyridine	298.15	33.00	[11]	25.7 ± 0.5	27.6 ± 0.2
105. 3-methylpyridine	293.15	36.63	[14]	**26.1 ± 0.5**	29.3 ± 0.5
...	298.15	35.04	[12]	26.6 ± 0.5	29.0 ± 0.5
106. 4-methylpyridine	298.15	35.43	[12]	26.8 ± 0.8	27.9 ± 0.3
107. cyclohexanone	298.15	34.57	[11]	30.0 ± 0.9	27.3 ± 1.1
108. (E)-hex-2-ene	293.15			10.8 ± 0.2	12.8 ± 0.3
109. hexan-2-one	298.15	25.45	[11]	20.2 ± 0.7	19.3 ± 0.6
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15	26.16	[14]	**36.9 ± 1.9**	30.1 ± 2.9
...	373.15	17.66	[11]	**24.9 ± 0.5**	20.9 ± 0.9
111. cyclohexanamine	298.15	31.22	[11]	29.1 ± 2.6	24.0 ± 1.1
112. 2-propan-2-yloxypropane	298.15	17.27	[11]	16.6 ± 0.2	13.2 ± 0.2
113. 1-methoxy-2-(2-methoxyethoxy)ethane	298.15	29.30	[12]	33.5 ± 1.5	24.9 ± 1.1

Table S4: Surface tension - continued

Name	Experiment T	Experiment γ	Ref.	GAFF γ	OPLS/AA γ
114. triethyl phosphate	298.15	29.61	[12]	31.2 ± 2.7	28.8 ± 1.1
...	311.65	28.30	[14]	29.4 ± 2.3	26.8 ± 1.1
115. N,N-diethylethanamine	298.15	20.22	[11]	16.8 ± 0.3	**13.9 ± 0.3**
116. N-propan-2-ylpropan-2-amine	298.15	19.14	[11]	18.0 ± 0.7	15.0 ± 0.3
117. trifluoromethylbenzene	298.15	23.21	[12]	**16.7 ± 0.7**	**16.0 ± 0.5**
118. benzonitrile	288.15	39.95	[12]	**28.6 ± 0.3**	35.0 ± 0.6
...	293.15	38.59	[14]	**28.0 ± 0.3**	33.9 ± 1.1
119. benzaldehyde	298.15	38.00	[11]	31.0 ± 0.4	32.5 ± 0.5
120. toluene	298.15	27.73	[11]	**17.0 ± 0.3**	20.9 ± 0.5
121. methoxybenzene	298.15	35.10	[11]	**25.9 ± 0.5**	**25.0 ± 0.7**
122. phenylmethanol	297.15	36.98	[12]	30.0 ± 1.4	31.9 ± 0.8
...	298.15	35.97	[14]	29.1 ± 0.9	30.9 ± 1.9
123. 2-methylphenol	308.15	36.11	[12]	**27.1 ± 0.7**	29.7 ± 1.5
125. 4-methylphenol	313.15	34.88	[14]	**24.6 ± 0.6**	29.0 ± 1.5
127. 2,4-dimethylpentan-3-one	298.15	24.78	[12]	21.4 ± 0.7	20.5 ± 0.5
128. heptan-2-one	298.15	26.12	[11]	21.1 ± 0.5	19.9 ± 0.2
129. ethenylbenzene	298.15	32.00	[12]	**18.5 ± 0.5**	**23.0 ± 0.5**
130. 1-phenylethanone	298.15	39.04	[11]	**29.1 ± 0.7**	33.4 ± 1.2
...	298.25	39.02	[14]	30.0 ± 1.0	33.8 ± 1.1
131. methyl benzoate	298.15	37.17	[11]	34.8 ± 1.3	33.6 ± 0.3
132. methyl 2-hydroxybenzoate	298.15	39.22	[11]	33.9 ± 2.1	36.5 ± 1.4
133. ethylbenzene	298.15	28.75	[11]	**18.3 ± 0.8**	**20.7 ± 0.6**
134. 1,2-dimethylbenzene	298.15	29.76	[11]	**18.4 ± 0.3**	22.8 ± 0.2
135. 1,2-dimethoxybenzene	298.15	32.80	[14]	31.2 ± 0.6	30.4 ± 1.2
136. 2,4,6-trimethylpyridine	295.15	33.64	[12]	**23.4 ± 0.6**	26.7 ± 0.7
...	298.15	33.30	[12]	**24.2 ± 1.1**	26.4 ± 0.4
137. octan-1-ol	298.15	27.10	[11]	23.1 ± 1.6	**15.6 ± 6.0**
138. 1-butoxybutane	298.15	22.44	[14]	18.2 ± 0.2	**16.5 ± 0.8**
139. N-butylbutan-1-amine	298.15	24.12	[11]	19.1 ± 0.7	**16.7 ± 0.6**
140. isoquinoline	303.15	45.94	[14]	34.6 ± 1.1	38.3 ± 1.9
141. quinoline	288.15	43.55	[12]	33.6 ± 1.3	35.0 ± 0.7
...	298.15	42.59	[11]	32.1 ± 0.4	33.7 ± 0.9

Table S4: Surface tension - continued

	Experiment			GAFF	OPLS/AA
Name	T	γ	Ref.	γ	γ
142. (1-methylethyl)benzene	298.15	27.69	[11]	**19.8 ± 0.3**	21.4 ± 0.4
143. 1,2,4-trimethylbenzene	293.15	29.72	[12]	**19.5 ± 0.5**	24.5 ± 0.7
...	298.15	29.19	[12]	**18.8 ± 0.6**	24.0 ± 0.4
144. 2,6-dimethylheptan-4-one	298.15	25.80	[12]	20.2 ± 0.7	20.2 ± 0.4
145. 1-chloronaphthalene	298.15	39.23	[12]	**28.9 ± 0.8**	**28.4 ± 0.7**
146. phenoxybenzene	303.15	38.24	[12]	28.8 ± 0.7	32.6 ± 1.2

Table S5: Dielectric constant $\varepsilon(0)$ calculated and experimental. Missing simulated $\varepsilon(0)$ due to simulations not having converged, see main text. Blue font indicates that the calculated value differs more than 25% from the experimental ones, a red font indicates that it differs by more than 50%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA
Name	T	$\varepsilon(0)$	Ref.	$\varepsilon(0)$	$\varepsilon(0)$
1. chloroform	298.15	4.71	[11]		3.3 ± 0.0
2. dichloro(fluoro)methane	282.05			5.6 ± 0.1	2.4 ± 0.0
3. dibromomethane	293.15	7.41	[11]	5.9 ± 0.1	5.2 ± 0.1
...	298.15	7.23	[11]		5.1 ± 0.1
4. dichloromethane	293.15	9.00	[11]	10.1 ± 0.1	**4.4 ± 0.0**
...	298.15	8.82	[11]	9.8 ± 0.1	**4.2 ± 0.1**
5. methanal	253.15			37.9 ± 0.2	37.1 ± 0.3
...	253.65			37.2 ± 0.4	37.2 ± 0.6
6. methanoic acid	293.15	53.33	[11]		**8.1 ± 0.2**
...	298.15	51.10	[11]		**7.8 ± 0.1**
7. bromomethane	276.65			7.2 ± 0.1	14.3 ± 0.1
8. methanamide	298.15	108.94	[11]	**41.1 ± 1.6**	
9. nitromethane	293.15	37.27	[11]	32.7 ± 0.5	26.5 ± 0.4
...	298.15	36.56	[11]	30.8 ± 1.1	25.8 ± 0.2
10. methanol	293.15	33.00	[11]	25.5 ± 0.9	26.5 ± 0.7
...	298.15	31.92		25.5 ± 1.0	24.7 ± 0.7
11. 1,1,1,2,2-pentachloroethane	293.15	3.79		2.5 ± 0.0	2.1 ± 0.0
12. 1,1,2,2-tetrachloroethane	293.15	8.50	[11]	**3.1 ± 0.1**	**3.8 ± 0.1**
...	298.15	7.91		**2.9 ± 0.1**	**3.6 ± 0.1**
13. 1,1-dichloroethene	293.15	4.60	[11]	4.2 ± 0.0	
...	298.15			4.1 ± 0.0	3.7 ± 0.0
14. 1,1,2-trichloroethane	293.15	7.36	[11]	6.5 ± 0.1	
...	298.15	7.19	[11]	6.4 ± 0.2	6.1 ± 0.1
15. acetonitrile	293.15	36.64	[11]	24.3 ± 0.3	20.6 ± 0.3
...	298.15	35.69	[11]	23.7 ± 0.3	20.4 ± 0.3
16. 1,2-dibromoethane	298.15	4.93	[11]	5.7 ± 0.1	**20.8 ± 0.6**
17. 1,1-dichloroethane	293.15	10.36	[11]		**3.3 ± 0.0**
...	298.15	10.10	[11]	10.0 ± 0.3	**3.2 ± 0.0**
18. 1,2-dichloroethane	298.15	10.13	[11]	**19.8 ± 0.4**	13.4 ± 0.2
19. methyl formate	293.15	9.02	[11]	6.6 ± 0.2	5.6 ± 0.1
...	298.15	8.84	[11]		5.4 ± 0.1

Table S5: Dielectric constant - continued

Name	Experiment T	Experiment $\varepsilon(0)$	Experiment Ref.	GAFF $\varepsilon(0)$	OPLS/AA $\varepsilon(0)$
20. bromoethane	293.15	9.25	[11]	8.3 ± 0.1	9.4 ± 0.2
...	298.15	9.01	[11]	8.0 ± 0.1	9.4 ± 0.1
21. chloroethane	273.15	10.41	[11]	10.8 ± 0.1	8.1 ± 0.1
...	285.45	9.80	[11]	10.1 ± 0.2	7.4 ± 0.1
22. 2-chloroethanol	293.15	25.80	[11]	23.2 ± 1.4	18.7 ± 0.9
23. ethanamide	358.15	67.87			**32.8 ± 1.6**
24. N-methylformamide	292.15			13.6 ± 0.6	18.8 ± 0.6
...	298.15	189.00	[13]	**13.3 ± 0.3**	**19.2 ± 0.7**
25. nitroethane	298.15	28.29	[11]	20.8 ± 0.7	18.9 ± 0.3
26. methoxymethane	240.00	6.88	[11]	7.8 ± 0.1	8.8 ± 0.1
27. ethanol	293.15	25.30	[11]	16.0 ± 0.9	21.7 ± 1.3
...	298.15	24.85	[11]	14.2 ± 0.6	
28. 1,2-ethanedithiol	293.15	7.26	[11]	**11.1 ± 0.1**	7.4 ± 0.1
...	298.15	7.20	[11]	**10.8 ± 0.2**	6.9 ± 0.0
29. methyldisulfanylmethane	293.15	9.81		9.1 ± 0.1	
...	298.15	9.60	[11]	8.6 ± 0.1	**18.3 ± 0.3**
30. methylsulfinylmethane	298.15	46.83	[11]	59.6 ± 2.5	43.6 ± 2.1
31. methylsulfanylmethane	293.15	6.58		7.0 ± 0.0	**10.3 ± 0.1**
...	298.15	6.45		6.8 ± 0.1	**9.8 ± 0.1**
32. 2-aminoethanol	293.15	32.10			**48.9 ± 3.3**
...	320.00			22.3 ± 1.9	37.5 ± 1.9
33. ethane-1,2-diamine	293.15	13.82	[11]	14.8 ± 0.6	**22.1 ± 1.0**
...	298.15	13.52	[11]	14.2 ± 0.4	**22.8 ± 0.5**
34. prop-2-enenitrile	298.15	32.36	[11]	22.3 ± 0.5	**11.1 ± 0.2**
...	350.45	24.94	[11]	17.8 ± 0.2	**8.8 ± 0.1**
35. 1,3-dioxolan-2-one	312.15	89.91		85.8 ± 6.6	
36. propanenitrile	293.15	29.70	[11]	18.3 ± 0.4	15.4 ± 0.1
...	298.15	29.32	[11]	17.7 ± 0.5	15.0 ± 0.2
37. 1,2-dibromopropane	293.15	4.57	[11]	5.4 ± 0.1	**15.0 ± 0.5**
...	298.15	4.55	[11]	5.2 ± 0.1	
38. 1,3-dichloropropane	298.15	10.18		8.3 ± 0.1	6.7 ± 0.1
39. (2R)-2-methyloxirane	298.15				14.7 ± 0.2

Table S5: Dielectric constant - continued

Name	Experiment T	Experiment $\varepsilon(0)$	Experiment Ref.	GAFF $\varepsilon(0)$	OPLS/AA $\varepsilon(0)$
40. propan-2-one	298.15	20.49	[11]	12.0 ± 0.2	15.4 ± 0.2
41. methyl acetate	293.15	6.97	[11]	5.0 ± 0.1	
...	298.15	6.86	[11]	5.0 ± 0.1	4.6 ± 0.0
42. 1,3-dioxolane	293.15	7.11		**3.4 ± 0.0**	**3.1 ± 0.0**
...	298.15	6.98		**3.3 ± 0.0**	**3.0 ± 0.0**
43. 2-iodopropane	293.15			8.4 ± 0.3	
...	298.15	8.19	[11]	8.3 ± 0.2	**2.7 ± 0.0**
44. 1-bromopropane	293.15	8.09	[11]	7.3 ± 0.1	8.0 ± 0.2
...	298.15	8.05	[11]	7.2 ± 0.1	7.8 ± 0.1
45. N,N-dimethylformamide	298.15			24.5 ± 0.8	14.9 ± 0.5
46. N-methylacetamide	320.00			10.4 ± 0.4	14.2 ± 0.4
47. 1-nitropropane	298.15	23.73	[11]	14.5 ± 0.7	12.2 ± 0.2
48. 2-nitropropane	298.15	25.65	[11]	15.6 ± 0.3	15.0 ± 0.4
49. dimethoxymethane	293.15	2.64	[11]		**4.5 ± 0.0**
...	298.15	2.65		3.9 ± 0.0	**4.4 ± 0.0**
50. propane-1,2,3-triol	320.00	41.69	[11]	24.5 ± 1.1	25.6 ± 0.9
51. propan-1-amine	293.15	5.12	[11]		6.1 ± 0.1
...	298.15	5.11	[19]	5.9 ± 0.2	5.7 ± 0.1
52. propan-2-amine	293.15	5.63	[11]	5.7 ± 0.1	5.4 ± 0.1
...	298.15	5.47	[19]	5.5 ± 0.1	
53. 2-methylpropane	243.65	1.85	[11]	1.1 ± 0.0	1.0 ± 0.0
54. ethylsulfanylethane	293.15	5.83		5.6 ± 0.1	7.7 ± 0.2
...	298.15	5.72	[11]	5.5 ± 0.1	7.7 ± 0.2
55. butane-1-thiol	293.15	5.11	[11]	6.1 ± 0.2	4.4 ± 0.1
...	298.15	5.01	[11]	6.0 ± 0.1	4.2 ± 0.1
56. butan-1-ol	293.15	17.84	[11]	**8.4 ± 0.2**	14.1 ± 0.9
...	298.15	17.33	[11]	9.8 ± 0.2	12.8 ± 0.7
58. butane-1,4-diol	293.15	32.86	[11]		18.0 ± 0.9
...	320.00	27.87	[11]	19.0 ± 0.3	20.5 ± 2.0
59. (2-hydroxyethoxy)ethan-2-ol	288.15	32.81	[11]		**16.3 ± 0.7**
60. N-ethylethanamine	293.15	3.68	[11]	4.4 ± 0.1	
...	298.15	3.58	[11]	4.5 ± 0.1	4.6 ± 0.1

Table S5: Dielectric constant - continued

Name	Experiment T	Experiment $\varepsilon(0)$	Experiment Ref.	GAFF $\varepsilon(0)$	OPLS/AA $\varepsilon(0)$
61. butan-1-amine	293.15	4.71	[11]	5.4 ± 0.2	4.9 ± 0.1
...	298.15	4.62	[11]	5.2 ± 0.2	4.7 ± 0.0
62. 2-methylpropan-2-amine	293.15	4.40		3.5 ± 0.1	
...	298.15	4.01		3.4 ± 0.1	3.8 ± 0.1
64. pyrimidine	298.15			8.6 ± 0.3	8.8 ± 0.3
65. furan	293.15	2.97		1.5 ± 0.0	1.6 ± 0.0
...	298.15	2.94		1.5 ± 0.0	1.5 ± 0.0
66. thiophene	293.15	2.74	[11]	1.4 ± 0.0	2.7 ± 0.0
...	298.15	2.73			2.6 ± 0.0
67. 1H-pyrrole	293.15	8.01	[11]	4.0 ± 0.1	**4.0 ± 0.1**
...	298.15	7.92	[11]	4.2 ± 0.1	4.0 ± 0.1
68. ethenyl acetate	298.15			3.3 ± 0.1	4.1 ± 0.1
69. oxolan-2-one	293.15	39.00	[11]		30.2 ± 0.9
70. acetyl acetate	293.15	22.45	[11]	12.5 ± 0.5	**8.9 ± 0.2**
71. 1,4-dichlorobutane	298.15	9.51	[19]	8.6 ± 0.2	8.4 ± 0.2
72. oxolane	298.15	8.04	[19]		5.7 ± 0.1
73. ethoxyethene	293.15				4.4 ± 0.0
74. ethyl acetate	293.15	6.08	[11]	3.9 ± 0.1	4.2 ± 0.1
...	298.15	5.99	[11]	3.9 ± 0.1	4.0 ± 0.1
75. tetrahydrothiophene 1,1-dioxide	320.00	41.24		25.1 ± 2.5	**15.5 ± 0.5**
76. thiolane	293.15			6.3 ± 0.1	7.2 ± 0.2
...	298.15			6.1 ± 0.1	7.1 ± 0.1
77. 1-bromobutane	293.15	7.02	[11]	5.4 ± 0.1	6.5 ± 0.1
...	298.15	6.89	[11]	5.6 ± 0.1	6.3 ± 0.1
78. 1-chlorobutane	298.15	7.09	[11]	6.2 ± 0.1	4.9 ± 0.1
79. pyrrolidine	293.15	8.28	[11]		5.5 ± 0.2
...	298.15	8.04	[11]	4.8 ± 0.1	5.2 ± 0.1
80. N,N-dimethylacetamide	298.15	38.90	[13]	**19.4 ± 0.5**	**14.3 ± 0.2**
81. morpholine	293.15	7.46	[19]	5.8 ± 0.2	4.2 ± 0.3
82. pyridine	293.15	13.26	[11]	6.8 ± 0.1	6.9 ± 0.2
...	298.15	12.98	[11]		6.7 ± 0.1
83. cyclopentanone	293.15	13.76	[11]	8.3 ± 0.2	9.6 ± 0.2
...	298.15	13.58	[11]	8.3 ± 0.2	9.5 ± 0.2

Table S5: Dielectric constant - continued

Name	Experiment T	Experiment $\varepsilon(0)$	Experiment Ref.	GAFF $\varepsilon(0)$	OPLS/AA $\varepsilon(0)$
84. 1-cyclopropylethanone	293.15			14.8 ± 0.6	14.6 ± 0.4
...	298.15			13.8 ± 0.5	13.9 ± 0.3
85. pentane-2,4-dione	298.15	26.28		28.9 ± 1.0	**5.1 ± 0.1**
86. methyl 2-methylprop-2-enoate	298.15	6.53	[19]	4.0 ± 0.1	**25.0 ± 1.0**
87. pentanenitrile	293.15	20.04	[11]	12.9 ± 0.5	10.9 ± 0.3
...	298.15	19.89	[11]		10.7 ± 0.3
88. ethyl propanoate	298.15	5.76	[13]	3.0 ± 0.1	3.7 ± 0.0
89. diethyl carbonate	298.15	2.84	[19]	**1.3 ± 0.0**	
90. pentan-1-ol	293.15	15.26	[11]	9.1 ± 0.4	10.2 ± 0.6
...	298.15	15.13	[11]	9.5 ± 0.1	10.6 ± 0.6
...	320.00	12.38	[11]	10.9 ± 0.4	7.2 ± 0.3
91. pentan-3-ol	293.15	14.07	[11]	7.7 ± 0.4	7.6 ± 0.5
...	298.15	13.35	[11]	8.4 ± 0.2	8.5 ± 0.6
92. 2-methylbutan-2-ol	293.15	5.97	[11]		5.3 ± 0.2
...	320.00			2.0 ± 0.1	
94. pentan-3-amine	293.15			3.5 ± 0.1	
94. pentan-3-amine	298.15				3.4 ± 0.1
95. 1,2,3,4-tetrafluorobenzene	298.15			7.2 ± 0.1	5.3 ± 0.1
97. 1,3-difluorobenzene	293.15	5.14	[11]	3.1 ± 0.0	3.9 ± 0.1
...	298.15	5.06	[11]		3.8 ± 0.1
98. 1,2-difluorobenzene	293.15	13.94	[11]	8.8 ± 0.2	
...	298.15	13.59	[11]		11.3 ± 0.2
99. fluorobenzene	293.15	5.46	[11]	3.3 ± 0.0	4.4 ± 0.1
...	298.15	5.34	[19]	3.3 ± 0.0	
100. nitrobenzene	293.15	35.65	[11]	25.6 ± 1.7	**8.4 ± 0.3**
...	298.15	34.81	[11]	25.2 ± 1.6	**8.0 ± 0.3**
101. 2-chloroaniline	293.15	13.40	[11]	**4.7 ± 0.1**	8.0 ± 0.3
102. phenol	318.15	11.15	[11]		5.8 ± 0.3
103. benzenethiol	293.15	4.29		3.0 ± 0.0	2.5 ± 0.0
...	298.15	4.27		2.9 ± 0.0	2.4 ± 0.0
104. 2-methylpyridine	293.15	10.18	[11]	5.4 ± 0.1	5.4 ± 0.1
...	298.15	9.95	[11]		5.2 ± 0.1

Table S5: Dielectric constant - continued

Name	Experiment T	Experiment $\varepsilon(0)$	Experiment Ref.	GAFF $\varepsilon(0)$	OPLS/AA $\varepsilon(0)$
105. 3-methylpyridine	293.15	11.97		**5.9 ± 0.1**	6.9 ± 0.1
...	298.15	11.64		**5.6 ± 0.1**	7.1 ± 0.2
106. 4-methylpyridine	293.15	12.18	[11]	6.1 ± 0.2	7.3 ± 0.2
...	298.15	11.96	[11]	6.6 ± 0.2	
107. cyclohexanone	293.15	15.92	[11]	9.1 ± 0.3	**7.6 ± 0.1**
...	298.15	15.62	[11]	8.5 ± 0.3	**7.6 ± 0.2**
108. (E)-hex-2-ene	293.15			1.0 ± 0.0	1.0 ± 0.0
109. hexan-2-one	298.15	14.60	[13]		10.1 ± 0.2
111. cyclohexanamine	298.15	4.55	[13]	4.0 ± 0.2	4.3 ± 0.1
112. 2-propan-2-yloxypropane	298.15	3.97	[19]	**13.9 ± 0.6**	2.6 ± 0.0
113. 1-methoxy-2-(2-methoxyethoxy)ethane	293.15			8.4 ± 0.5	6.1 ± 0.1
...	298.15	7.23	[11]	7.8 ± 0.3	6.0 ± 0.2
114. triethyl phosphate	293.15				20.0 ± 1.1
...	298.15	13.20	[11]	**3.4 ± 0.1**	**28.2 ± 0.3**
...	320.00	12.01	[11]	**3.9 ± 0.1**	**24.7 ± 0.7**
115. N,N-diethylethanamine	293.15	2.42	[11]	1.4 ± 0.0	2.8 ± 0.0
...	298.15	2.38	[11]	1.4 ± 0.0	2.7 ± 0.1
116. N-propan-2-ylpropan-2-amine	293.15			5.9 ± 0.1	2.6 ± 0.0
116. N-propan-2-ylpropan-2-amine	298.15				2.5 ± 0.0
117. trifluoromethylbenzene	293.15			6.6 ± 0.2	6.5 ± 0.2
...	298.15	9.22	[11]	6.5 ± 0.2	
118. benzonitrile	288.15	26.41	[11]	16.9 ± 0.8	**6.6 ± 0.3**
119. benzaldehyde	298.15	17.40	[19]	10.9 ± 0.6	
120. toluene	298.15	2.37	[11]	**1.1 ± 0.0**	1.2 ± 0.0
121. methoxybenzene	293.15	4.41	[19]	2.6 ± 0.0	2.4 ± 0.0
...	298.15	4.22	[11]	2.6 ± 0.0	2.4 ± 0.0
122. phenylmethanol	297.15	13.09		**5.8 ± 0.1**	7.9 ± 0.5
123. 2-methylphenol	308.15	6.44	[11]	4.2 ± 0.3	4.2 ± 0.2
124. 3-methylphenol	320.00	10.43	[11]	**5.2 ± 0.3**	6.9 ± 0.4
125. 4-methylphenol	313.15	11.21	[11]	**3.9 ± 0.1**	7.1 ± 0.5
...	320.00	10.62	[11]	**3.5 ± 0.1**	7.8 ± 0.3
126. diethyl propanedioate	293.15	8.10		4.1 ± 0.2	4.6 ± 0.2

Table S5: Dielectric constant - continued

Name	Experiment T	Experiment $\varepsilon(0)$	Experiment Ref.	GAFF $\varepsilon(0)$	OPLS/AA $\varepsilon(0)$
127. 2,4-dimethylpentan-3-one	293.15			38.7 ± 2.1	13.4 ± 0.7
...	298.15			60.8 ± 2.7	12.9 ± 0.6
128. heptan-2-one	293.15	11.95	[11]	6.6 ± 0.2	9.5 ± 0.3
...	298.15	11.66	[11]	6.7 ± 0.1	9.1 ± 0.3
129. ethenylbenzene	298.15	2.46	[11]	**1.1 ± 0.0**	**1.0 ± 0.0**
130. 1-phenylethanone	293.15	17.73	[19]		**7.5 ± 0.2**
...	298.15	17.44	[11]	11.0 ± 0.7	**6.9 ± 0.3**
131. methyl benzoate	298.15	6.64	[13]	3.9 ± 0.2	3.4 ± 0.1
132. methyl 2-hydroxybenzoate	298.15	9.47	[11]	6.0 ± 0.2	
...	320.00	8.71	[11]	6.8 ± 0.4	7.1 ± 0.2
133. ethylbenzene	298.15	2.43	[11]	**1.1 ± 0.0**	**1.2 ± 0.0**
134. 1,2-dimethylbenzene	293.15	2.56	[11]	**1.2 ± 0.0**	1.5 ± 0.0
...	298.15	2.55	[11]	**1.2 ± 0.0**	1.5 ± 0.0
135. 1,2-dimethoxybenzene	298.15	4.41	[11]		4.0 ± 0.1
136. 2,4,6-trimethylpyridine	295.15	7.92		4.4 ± 0.1	4.8 ± 0.1
...	298.15	7.81	[11]	4.0 ± 0.2	4.4 ± 0.2
137. octan-1-ol	298.15	9.86	[11]		5.6 ± 0.3
...	320.00	8.29	[11]		5.8 ± 0.3
138. 1-butoxybutane	293.15	3.08	[11]	2.2 ± 0.0	2.3 ± 0.0
...	298.15	3.05	[11]		2.2 ± 0.0
139. N-butylbutan-1-amine	293.15	2.77	[11]	2.3 ± 0.1	3.1 ± 0.1
...	298.15	2.74	[11]	2.2 ± 0.1	3.1 ± 0.1
140. isoquinoline	303.15	10.60	[11]	**4.5 ± 0.3**	**2.2 ± 0.0**
...	320.00	9.56	[11]	**4.5 ± 0.1**	**2.0 ± 0.1**
141. quinoline	288.15	9.31	[11]	**4.3 ± 0.1**	**4.2 ± 0.1**
...	298.15	9.00	[11]	**4.0 ± 0.1**	**4.0 ± 0.1**
143. 1,2,4-trimethylbenzene	293.15	2.38	[11]	**1.1 ± 0.0**	1.2 ± 0.0
...	298.15	2.37	[11]	**1.1 ± 0.0**	1.2 ± 0.0
144. 2,6-dimethylheptan-4-one	293.15	9.91	[11]	**4.2 ± 0.1**	9.3 ± 0.4
...	298.15	9.70	[11]	**4.0 ± 0.1**	8.8 ± 0.4
145. 1-chloronaphthalene	298.15	5.04	[11]		3.3 ± 0.1
146. phenoxybenzene	303.15	3.65	[19]		**1.7 ± 0.0**

Table S6: Thermal expansion coefficient α_P (10^{-3} /K), calculated and experimental. Blue font indicates that the calculated value differs more than 25% from the experimental ones, a red font indicates that it differs by more than 50%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA
Name	T	α_P	Ref.	α_P	α_P
1. chloroform	298.15	1.29	[9]	1.91 ± 0.05	**2.28 ± 0.11**
2. dichloro(fluoro)methane	282.05	1.66	[20]	2.48 ± 0.11	**2.56 ± 0.09**
3. dibromomethane	293.15	1.01	[20]	**1.64 ± 0.05**	1.43 ± 0.07
...	298.15	1.02	[9]	1.48 ± 0.06	1.44 ± 0.05
4. dichloromethane	293.15	1.42	[20]	1.52 ± 0.10	1.89 ± 0.09
...	298.15	1.35	[9]	1.73 ± 0.06	**2.31 ± 0.09**
5. methanal	253.15	2.10	[20]	2.01 ± 0.07	1.82 ± 0.05
...	253.65	2.11	[20]	1.96 ± 0.07	1.88 ± 0.07
6. methanoic acid	293.15	0.99	[20]	0.88 ± 0.05	1.00 ± 0.07
...	298.15	1.02	[9]	0.58 ± 0.13	1.05 ± 0.05
7. bromomethane	276.65	1.53	[20]	**2.39 ± 0.13**	1.75 ± 0.07
8. methanamide	298.15	0.75	[9]	0.75 ± 0.07	0.80 ± 0.05
9. nitromethane	293.15	1.15	[20]	0.80 ± 0.09	1.25 ± 0.05
...	298.15	1.22	[9]	0.92 ± 0.10	1.31 ± 0.06
10. methanol	293.15	1.14	[20]	1.33 ± 0.09	1.47 ± 0.11
...	298.15	1.19	[9]	1.41 ± 0.12	1.53 ± 0.06
11. 1,1,1,2,2-pentachloroethane	293.15	0.86	[20]	1.01 ± 0.07	1.14 ± 0.02
12. 1,1,2,2-tetrachloroethane	293.15	0.95	[20]	1.08 ± 0.07	1.15 ± 0.08
...	298.15	0.97	[9]	1.05 ± 0.08	1.19 ± 0.07
13. 1,1-dichloroethene	293.15	1.43	[20]	**2.75 ± 0.10**	1.81 ± 0.11
...	298.15	1.50	[20]	**2.90 ± 0.15**	2.23 ± 0.10
14. 1,1,2-trichloroethane	293.15	1.12	[20]	1.16 ± 0.06	1.17 ± 0.06
...	298.15	1.00	[9]	1.35 ± 0.08	1.17 ± 0.08
15. acetonitrile	293.15	1.33	[20]	1.57 ± 0.11	1.89 ± 0.04
...	298.15	1.38	[9]	1.59 ± 0.07	1.92 ± 0.09
16. 1,2-dibromoethane	298.15	0.94	[9]	**1.42 ± 0.05**	1.06 ± 0.08
17. 1,1-dichloroethane	293.15	1.31	[20]	1.36 ± 0.08	1.52 ± 0.10
...	298.15	1.33	[9]	1.46 ± 0.07	1.60 ± 0.07
18. 1,2-dichloroethane	298.15	1.15	[9]	1.25 ± 0.07	1.43 ± 0.06
19. methyl formate	293.15	1.50	[20]	0.98 ± 0.13	1.44 ± 0.08
...	298.15	1.61	[9]	1.16 ± 0.10	1.32 ± 0.06

Table S6: Thermal expansion coefficient - continued

	Experiment			GAFF	OPLS/AA
Name	T	α_P	Ref.	α_P	α_P
20. bromoethane	293.15	1.41	[20]	1.75 ± 0.17	1.53 ± 0.07
...	298.15	1.40	[20]	**2.14 ± 0.13**	1.47 ± 0.07
21. chloroethane	273.15	1.30	[20]	1.79 ± 0.18	**2.07 ± 0.11**
...	285.45	1.37	[20]	1.83 ± 0.18	**2.09 ± 0.08**
22. 2-chloroethanol	293.15	0.86	[20]	0.91 ± 0.11	1.00 ± 0.09
23. ethanamide	358.15	0.90	[20]	0.87 ± 0.14	0.79 ± 0.05
...	494.30	1.21	[20]	1.20 ± 0.14	1.11 ± 0.05
24. N-methylformamide	292.15	0.83	[20]	0.80 ± 0.09	1.16 ± 0.11
...	298.15	0.88	[9]	0.85 ± 0.10	0.99 ± 0.06
25. nitroethane	298.15	1.14	[9]	1.08 ± 0.20	1.16 ± 0.06
26. methoxymethane	240.00	1.81	[20]	1.73 ± 0.18	2.36 ± 0.11
27. ethanol	293.15	1.16	[20]	1.14 ± 0.16	1.33 ± 0.08
...	298.15	1.09	[9]	1.26 ± 0.14	1.44 ± 0.12
28. 1,2-ethanedithiol	293.15			0.96 ± 0.09	0.96 ± 0.07
...	298.15			1.14 ± 0.10	1.06 ± 0.07
29. methyldisulfanylmethane	293.15	1.04	[20]	1.47 ± 0.10	1.28 ± 0.06
...	298.15	1.10	[20]	1.60 ± 0.07	1.40 ± 0.08
30. methylsulfinylmethane	298.15	0.91	[9]	0.74 ± 0.06	1.03 ± 0.05
31. methylsulfanylmethane	293.15	1.40	[20]	1.71 ± 0.13	1.65 ± 0.06
...	298.15	1.30	[9]	**2.03 ± 0.19**	1.69 ± 0.07
32. 2-aminoethanol	293.15	0.77	[20]	0.59 ± 0.15	0.96 ± 0.14
...	320.00	0.82	[20]	0.61 ± 0.11	1.17 ± 0.07
33. ethane-1,2-diamine	293.15	0.92	[20]	1.02 ± 0.13	1.28 ± 0.10
...	298.15	0.79	[9]	0.86 ± 0.13	**1.25 ± 0.13**
34. prop-2-enenitrile	298.15	1.42	[9]	1.70 ± 0.06	1.30 ± 0.12
...	350.45	1.70	[20]	2.04 ± 0.11	1.78 ± 0.07
35. 1,3-dioxolan-2-one	312.15	0.75	[20]	0.84 ± 0.08	0.72 ± 0.08
36. propanenitrile	293.15	1.22	[20]	1.55 ± 0.11	1.61 ± 0.11
...	298.15	1.33	[9]	1.71 ± 0.16	1.77 ± 0.10
37. 1,2-dibromopropane	293.15	0.78	[20]	1.13 ± 0.11	0.99 ± 0.06
...	298.15	0.80	[20]	1.11 ± 0.08	1.04 ± 0.08
38. 1,3-dichloropropane	298.15	1.00	[20]	1.12 ± 0.08	1.09 ± 0.08

Table S6: Thermal expansion coefficient - continued

Name	Experiment T	Experiment α_P	Experiment Ref.	GAFF α_P	OPLS/AA α_P
39. (2R)-2-methyloxirane	298.15			1.93 ± 0.08	2.00 ± 0.47
40. propan-2-one	298.15	1.45	[9]	1.56 ± 0.19	1.57 ± 0.06
41. methyl acetate	293.15	1.37	[20]	1.28 ± 0.04	1.18 ± 0.08
...	298.15	1.42	[9]	1.16 ± 0.11	1.34 ± 0.08
42. 1,3-dioxolane	293.15			0.97 ± 0.12	1.22 ± 0.07
...	298.15	1.18	[9]	0.95 ± 0.07	1.45 ± 0.10
43. 2-iodopropane	293.15	1.13	[20]	1.23 ± 0.16	1.27 ± 0.06
...	298.15	1.10	[20]	0.91 ± 0.13	1.13 ± 0.08
44. 1-bromopropane	293.15	1.25	[20]	1.35 ± 0.13	1.29 ± 0.09
...	298.15	1.30	[20]	1.56 ± 0.14	1.28 ± 0.07
45. N,N-dimethylformamide	298.15	1.00	[9]	0.71 ± 0.10	1.21 ± 0.13
46. N-methylacetamide	320.00	0.85	[20]	1.07 ± 0.14	0.90 ± 0.07
47. 1-nitropropane	298.15	1.01	[9]	0.93 ± 0.12	1.34 ± 0.09
48. 2-nitropropane	298.15	1.04	[9]	0.91 ± 0.11	1.07 ± 0.09
49. dimethoxymethane	293.15	1.49	[20]	1.41 ± 0.10	1.56 ± 0.08
...	298.15	1.50	[20]	1.50 ± 0.16	1.57 ± 0.11
50. propane-1,2,3-triol	293.15	0.46	[20]	**0.20 ± 0.10**	0.59 ± 0.10
...	320.00	0.49	[20]	**1.64 ± 0.08**	0.63 ± 0.10
51. propan-1-amine	293.15	1.39	[20]	1.68 ± 0.17	1.99 ± 0.08
...	298.15	1.40	[20]	1.50 ± 0.19	2.03 ± 0.07
52. propan-2-amine	293.15	1.57	[20]	1.46 ± 0.19	1.89 ± 0.15
...	298.15	1.60	[20]	1.40 ± 0.14	1.82 ± 0.11
53. 2-methylpropane	243.65	1.68	[20]	1.80 ± 0.20	2.12 ± 0.15
54. ethylsulfanylethane	293.15	1.13	[20]	1.43 ± 0.15	1.36 ± 0.13
...	298.15	1.45	[9]	1.60 ± 0.17	1.39 ± 0.12
55. butane-1-thiol	293.15	1.14	[20]	1.37 ± 0.16	1.17 ± 0.11
...	298.15	1.20	[20]	1.61 ± 0.22	1.07 ± 0.10
56. butan-1-ol	293.15	1.00	[20]	1.07 ± 0.13	1.35 ± 0.12
...	298.15	0.93	[9]	0.91 ± 0.10	1.18 ± 0.12
57. 2-methylpropan-2-ol	320.00			1.24 ± 0.17	1.52 ± 0.12
58. butane-1,4-diol	293.15	0.89	[20]	0.49 ± 0.17	0.60 ± 0.12
...	298.15	0.65	[9]	0.82 ± 0.13	0.60 ± 0.14
...	320.00	0.94	[20]	0.76 ± 0.10	0.58 ± 0.17

Table S6: Thermal expansion coefficient - continued

Name	Experiment T	Experiment α_P	Experiment Ref.	GAFF α_P	OPLS/AA α_P
59. (2-hydroxyethoxy)ethan-2-ol	288.15	0.63	[20]	**0.19 ± 0.10**	0.80 ± 0.13
60. N-ethylethanamine	293.15	1.44	[20]	1.76 ± 0.17	1.86 ± 0.09
...	298.15	1.56	[9]	1.78 ± 0.18	2.05 ± 0.09
61. butan-1-amine	293.15	1.18	[20]	1.14 ± 0.14	1.68 ± 0.15
...	298.15	1.35	[9]	1.25 ± 0.15	1.69 ± 0.08
62. 2-methylpropan-2-amine	293.15	1.36	[20]	1.26 ± 0.21	1.57 ± 0.09
...	298.15	1.40	[20]	1.56 ± 0.38	1.73 ± 0.07
63. 2-(2-hydroxyethylamino)ethanol	320.00	0.61	[20]	0.63 ± 0.11	0.76 ± 0.09
64. pyrimidine	298.15	0.89	[9]	1.14 ± 0.17	1.04 ± 0.08
65. furan	293.15	1.46	[20]	1.64 ± 0.13	1.43 ± 0.12
...	298.15	0.73	[9]	**1.51 ± 0.15**	**1.56 ± 0.09**
66. thiophene	293.15	1.10	[20]	1.42 ± 0.10	1.15 ± 0.05
...	298.15	1.10	[20]	1.40 ± 0.09	1.01 ± 0.10
67. 1H-pyrrole	293.15	0.86	[20]	0.99 ± 0.05	0.93 ± 0.11
...	298.15	0.87	[9]	0.81 ± 0.07	1.05 ± 0.09
68. ethenyl acetate	298.15	1.30	[20]	1.41 ± 0.14	1.04 ± 0.09
69. oxolan-2-one	293.15	0.74	[20]	0.80 ± 0.09	0.69 ± 0.09
70. acetyl acetate	293.15	1.15	[20]	0.83 ± 0.16	0.85 ± 0.05
71. 1,4-dichlorobutane	298.15	1.00	[20]	0.92 ± 0.10	1.10 ± 0.11
72. oxolane	298.15	1.29	[9]	1.32 ± 0.15	1.83 ± 0.15
73. ethoxyethene	293.15	1.57	[20]	1.82 ± 0.24	1.65 ± 0.08
74. ethyl acetate	293.15	1.30	[20]	0.99 ± 0.12	1.35 ± 0.11
...	298.15	1.38	[9]	1.44 ± 0.16	1.16 ± 0.04
75. tetrahydrothiophene 1,1-dioxide	320.00			0.88 ± 0.11	0.88 ± 0.08
76. thiolane	293.15	0.76	[20]	**1.48 ± 0.14**	**1.17 ± 0.07**
...	298.15	0.95	[9]	1.07 ± 0.11	1.07 ± 0.13
77. 1-bromobutane	293.15	1.11	[20]	1.47 ± 0.13	1.19 ± 0.12
...	298.15	1.14	[9]	1.30 ± 0.10	1.21 ± 0.12
78. 1-chlorobutane	293.15	1.28	[20]	1.53 ± 0.15	1.34 ± 0.10
...	298.15	0.80	[9]	**1.34 ± 0.13**	**1.56 ± 0.08**
79. pyrrolidine	293.15	1.06	[20]	1.16 ± 0.16	1.51 ± 0.16
...	298.15	1.13	[9]	1.25 ± 0.10	1.38 ± 0.13

Table S6: Thermal expansion coefficient - continued

Name	Experiment			GAFF	OPLS/AA
	T	α_P	Ref.	α_P	α_P
80. N,N-dimethylacetamide	298.15	0.98	[9]	1.21 ± 0.15	1.03 ± 0.11
81. morpholine	293.15	0.91	[20]	0.81 ± 0.11	1.01 ± 0.13
82. pyridine	293.15	1.08	[20]	1.06 ± 0.08	1.02 ± 0.08
...	298.15	1.02	[9]	1.14 ± 0.15	1.07 ± 0.11
83. cyclopentanone	293.15	1.01	[20]	1.04 ± 0.10	1.09 ± 0.08
...	298.15	1.02	[9]	0.86 ± 0.13	0.92 ± 0.08
84. 1-cyclopropylethanone	293.15			1.04 ± 0.23	1.24 ± 0.05
...	298.15			1.13 ± 0.16	1.29 ± 0.09
85. pentane-2,4-dione	298.15	1.09	[9]	0.85 ± 0.17	1.02 ± 0.07
86. methyl 2-methylprop-2-enoate	298.15	1.20	[20]	1.05 ± 0.10	1.03 ± 0.11
87. pentanenitrile	293.15	1.04	[20]	1.09 ± 0.17	1.27 ± 0.11
...	298.15	1.06	[9]	1.19 ± 0.12	1.43 ± 0.14
88. ethyl propanoate	298.15	1.25	[9]	1.39 ± 0.17	1.24 ± 0.10
89. diethyl carbonate	298.15	1.10	[9]	0.72 ± 0.16	1.10 ± 0.08
90. pentan-1-ol	293.15	0.95	[20]	0.98 ± 0.09	1.00 ± 0.15
...	298.15	0.89	[9]	0.86 ± 0.11	1.11 ± 0.11
...	320.00	1.02	[20]	1.01 ± 0.17	1.35 ± 0.14
91. pentan-3-ol	293.15	1.20	[20]	0.98 ± 0.16	1.04 ± 0.11
...	298.15	1.20	[20]	1.25 ± 0.22	1.51 ± 0.13
92. 2-methylbutan-2-ol	293.15			0.89 ± 0.18	1.51 ± 0.07
...	298.15	1.14	[9]	0.92 ± 0.11	1.23 ± 0.14
...	320.00			1.03 ± 0.12	1.65 ± 0.12
93. pentane-1,5-diol	293.15	0.88	[20]	0.64 ± 0.10	0.48 ± 0.14
...	298.15	0.61	[9]	0.56 ± 0.15	0.86 ± 0.12
94. pentan-3-amine	293.15	1.31	[20]	1.37 ± 0.19	1.36 ± 0.13
...	298.15	1.30	[20]	1.41 ± 0.13	1.62 ± 0.17
95. 1,2,3,4-tetrafluorobenzene	298.15			1.77 ± 0.05	1.52 ± 0.08
96. 1,2,3,5-tetrafluorobenzene	298.15			1.80 ± 0.14	1.77 ± 0.07
97. 1,3-difluorobenzene	293.15	1.18	[20]	1.71 ± 0.14	1.59 ± 0.05
...	298.15	1.20	[20]	1.36 ± 0.12	1.75 ± 0.09
98. 1,2-difluorobenzene	293.15	1.17	[20]	1.58 ± 0.10	1.38 ± 0.08
...	298.15	1.20	[20]	1.53 ± 0.11	1.67 ± 0.10

Table S6: Thermal expansion coefficient - continued

Name	Experiment			GAFF	OPLS/AA
	T	α_P	Ref.	α_P	α_P
99. fluorobenzene	293.15	1.12	[20]	1.53 ± 0.09	1.25 ± 0.09
...	298.15	1.18	[9]	1.60 ± 0.10	1.20 ± 0.05
100. nitrobenzene	293.15	0.81	[20]	0.65 ± 0.07	0.66 ± 0.06
...	298.15	0.85	[9]	0.77 ± 0.08	0.82 ± 0.09
101. 2-chloroaniline	293.15			0.86 ± 0.10	0.90 ± 0.07
102. phenol	318.15	0.80	[20]	1.15 ± 0.08	0.92 ± 0.11
103. benzenethiol	293.15	0.88	[20]	1.28 ± 0.09	1.18 ± 0.05
...	298.15	0.90	[20]	**1.38 ± 0.05**	1.11 ± 0.10
104. 2-methylpyridine	293.15	0.98	[20]	1.01 ± 0.17	1.10 ± 0.10
...	298.15	0.99	[9]	0.96 ± 0.13	1.14 ± 0.05
105. 3-methylpyridine	293.15	0.96	[20]	1.15 ± 0.07	1.11 ± 0.08
...	298.15	0.97	[9]	0.97 ± 0.10	0.96 ± 0.10
106. 4-methylpyridine	293.15	0.94	[20]	1.20 ± 0.11	0.99 ± 0.13
...	298.15	0.96	[9]	1.29 ± 0.16	0.95 ± 0.11
107. cyclohexanone	293.15	0.89	[20]	1.12 ± 0.14	1.02 ± 0.12
...	298.15	0.95	[9]	1.05 ± 0.13	0.99 ± 0.07
108. (E)-hex-2-ene	293.15			1.70 ± 0.10	1.53 ± 0.16
109. hexan-2-one	298.15	1.10	[20]	1.45 ± 0.18	1.28 ± 0.15
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15	1.10	[20]	0.63 ± 0.22	1.18 ± 0.09
111. cyclohexanamine	298.15	1.00	[20]	0.83 ± 0.18	1.20 ± 0.16
112. 2-propan-2-yloxypropane	298.15	1.48	[9]	1.46 ± 0.21	1.59 ± 0.12
113. 1-methoxy-2-(2-methoxyethoxy)ethane	293.15	1.05	[20]	0.84 ± 0.21	0.91 ± 0.21
...	298.15	1.07	[9]	1.10 ± 0.13	1.03 ± 0.14
114. triethyl phosphate	293.15	0.91	[20]	1.21 ± 0.19	1.01 ± 0.13
...	298.15	0.96	[9]	**0.24 ± 0.20**	1.03 ± 0.13
...	320.00	0.95	[20]	1.03 ± 0.17	0.94 ± 0.12
115. N,N-diethylethanamine	293.15	1.22	[20]	1.33 ± 0.08	1.46 ± 0.12
...	298.15	1.30	[9]	1.47 ± 0.20	1.79 ± 0.17
116. N-propan-2-ylpropan-2-amine	293.15	1.28	[20]	1.22 ± 0.24	1.49 ± 0.13
...	298.15	1.30	[20]	1.19 ± 0.16	1.35 ± 0.14
117. trifluoromethylbenzene	293.15	1.14	[20]	1.28 ± 0.06	1.23 ± 0.13
...	298.15	1.20	[20]	1.36 ± 0.08	1.35 ± 0.09

Table S6: Thermal expansion coefficient - continued

	Experiment			GAFF	OPLS/AA
Name	T	α_P	Ref.	α_P	α_P
118. benzonitrile	288.15	0.83	[20]	1.05 ± 0.13	0.89 ± 0.05
119. benzaldehyde	298.15	0.25	[9]	**1.06 ± 0.06**	**0.77 ± 0.06**
120. toluene	298.15	1.07	[9]	**1.62 ± 0.15**	1.49 ± 0.04
121. methoxybenzene	293.15	0.91	[20]	1.05 ± 0.12	1.22 ± 0.10
...	298.15	0.95	[9]	1.18 ± 0.13	1.08 ± 0.09
122. phenylmethanol	297.15	0.69	[20]	0.81 ± 0.07	0.80 ± 0.17
123. 2-methylphenol	308.15	0.79	[20]	0.96 ± 0.13	0.93 ± 0.08
124. 3-methylphenol	320.00	0.75	[20]	1.00 ± 0.12	0.98 ± 0.14
125. 4-methylphenol	313.15	0.85	[20]	0.96 ± 0.07	0.81 ± 0.07
...	320.00	0.86	[20]	0.81 ± 0.12	0.86 ± 0.14
126. diethyl propanedioate	293.15	0.99	[20]	0.93 ± 0.16	0.97 ± 0.09
127. 2,4-dimethylpentan-3-one	293.15	1.12	[20]	0.95 ± 0.14	1.15 ± 0.09
...	298.15	1.10	[20]	1.08 ± 0.17	1.10 ± 0.14
128. heptan-2-one	293.15	1.05	[20]	1.46 ± 0.17	1.17 ± 0.12
...	298.15	1.06	[9]	0.91 ± 0.17	1.01 ± 0.12
129. ethenylbenzene	298.15	0.97	[9]	1.14 ± 0.11	1.18 ± 0.11
130. 1-phenylethanone	293.15			1.01 ± 0.10	0.92 ± 0.09
...	298.15	0.84	[9]	1.00 ± 0.08	0.89 ± 0.08
131. methyl benzoate	298.15	0.88	[9]	0.72 ± 0.10	0.71 ± 0.12
132. methyl 2-hydroxybenzoate	298.15	0.70	[20]	0.99 ± 0.11	0.80 ± 0.08
...	320.00	0.78	[20]	0.94 ± 0.11	0.89 ± 0.07
133. ethylbenzene	298.15	1.02	[9]	1.35 ± 0.16	1.19 ± 0.10
134. 1,2-dimethylbenzene	293.15	0.92	[20]	1.17 ± 0.17	1.20 ± 0.13
...	298.15	0.95	[9]	1.40 ± 0.12	1.05 ± 0.09
135. 1,2-dimethoxybenzene	298.15	0.93	[9]	0.97 ± 0.10	1.00 ± 0.08
136. 2,4,6-trimethylpyridine	295.15	0.92	[20]	0.92 ± 0.39	0.89 ± 0.09
...	298.15	0.83	[9]	0.86 ± 0.54	0.99 ± 0.09
137. octan-1-ol	298.15	0.84	[9]	0.64 ± 0.18	0.70 ± 0.14
...	320.00	0.94	[20]	0.89 ± 0.15	**2.09 ± 0.16**
138. 1-butoxybutane	293.15	1.09	[20]	1.42 ± 0.25	1.51 ± 0.11
...	298.15	1.13	[9]	0.77 ± 0.18	1.52 ± 0.14
139. N-butylbutan-1-amine	293.15	1.01	[20]	1.25 ± 0.24	1.18 ± 0.08
...	298.15	1.12	[9]	1.27 ± 0.15	1.41 ± 0.16

Table S6: Thermal expansion coefficient - continued

	Experiment			GAFF	OPLS/AA
Name	T	α_P	Ref.	α_P	α_P
140. isoquinoline	303.15	0.68	[20]	0.84 ± 0.11	0.45 ± 0.14
...	320.00	0.70	[20]	0.81 ± 0.11	0.91 ± 0.12
141. quinoline	288.15	0.66	[20]	0.94 ± 0.11	0.81 ± 0.07
...	298.15	0.73	[9]	0.78 ± 0.08	0.90 ± 0.04
142. (1-methylethyl)benzene	298.15	0.98	[9]	1.43 ± 0.17	0.99 ± 0.10
143. 1,2,4-trimethylbenzene	293.15	0.89	[20]	1.15 ± 0.18	1.23 ± 0.09
...	298.15	0.90	[20]	1.05 ± 0.12	0.99 ± 0.12
144. 2,6-dimethylheptan-4-one	293.15	0.95	[20]	**1.42 ± 0.21**	1.07 ± 0.16
...	298.15	1.00	[20]	0.93 ± 0.27	1.33 ± 0.16
145. 1-chloronaphthalene	298.15	0.70	[20]	0.75 ± 0.11	0.99 ± 0.11
146. phenoxybenzene	303.15	0.65	[20]	0.74 ± 0.14	0.76 ± 0.11

Table S7: Isothermal compressibility κ_T (1/GPa), calculated and experimental Blue font indicates that the calculated value differs more than 10% from the experimental ones, a red font indicates that it differs by more than 25%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA
Name	T	κ_T	Ref.	κ_T	κ_T
1. chloroform	298.15	1.03	[9]	**1.79 ± 0.06**	**2.16 ± 0.09**
2. dichloro(fluoro)methane	282.05			2.56 ± 0.10	2.82 ± 0.12
3. dibromomethane	293.15			1.65 ± 0.05	0.86 ± 0.02
...	298.15	0.70	[9]	**1.45 ± 0.05**	**0.91 ± 0.01**
4. dichloromethane	293.15	0.99		**1.30 ± 0.03**	**1.74 ± 0.07**
...	298.15	1.03	[9]	**1.47 ± 0.04**	**2.22 ± 0.09**
5. methanal	253.15			1.18 ± 0.03	1.12 ± 0.03
...	253.65			1.15 ± 0.02	1.15 ± 0.04
6. methanoic acid	293.15			0.22 ± 0.00	0.54 ± 0.01
...	298.15	0.65	[9]	**0.24 ± 0.01**	0.54 ± 0.01
7. bromomethane	276.65			2.84 ± 0.11	1.14 ± 0.03
8. methanamide	298.15	0.40	[9]	**0.29 ± 0.01**	0.36 ± 0.01
9. nitromethane	293.15			0.30 ± 0.01	0.72 ± 0.01
...	298.15	0.72	[9]	**0.31 ± 0.01**	0.77 ± 0.01
10. methanol	293.15	1.22		1.01 ± 0.02	1.08 ± 0.03
...	298.15	1.25	[9]	1.02 ± 0.02	1.08 ± 0.02
11. 1,1,1,2,2-pentachloroethane	293.15			0.71 ± 0.01	0.77 ± 0.01
12. 1,1,2,2-tetrachloroethane	293.15	0.65		0.79 ± 0.02	0.80 ± 0.03
...	298.15	0.62	[9]	**0.83 ± 0.03**	**0.84 ± 0.02**
13. 1,1-dichloroethene	293.15			3.48 ± 0.14	1.84 ± 0.05
...	298.15			3.88 ± 0.17	2.13 ± 0.05
14. 1,1,2-trichloroethane	293.15	0.73		0.82 ± 0.02	0.80 ± 0.02
...	298.15	0.75		0.91 ± 0.02	0.80 ± 0.03
15. acetonitrile	293.15			1.15 ± 0.03	1.60 ± 0.03
...	298.15	1.07	[9]	1.18 ± 0.04	**1.62 ± 0.05**
16. 1,2-dibromoethane	298.15	0.64	[9]	**1.17 ± 0.04**	0.54 ± 0.02
17. 1,1-dichloroethane	293.15			1.22 ± 0.03	1.39 ± 0.03
...	298.15	1.15	[9]	1.26 ± 0.04	1.33 ± 0.04
18. 1,2-dichloroethane	298.15	0.82	[9]	0.86 ± 0.02	0.95 ± 0.03
19. methyl formate	293.15			0.57 ± 0.01	0.99 ± 0.04
...	298.15			0.62 ± 0.01	1.00 ± 0.02

Table S7: Isothermal compressibility - continued

	Experiment			GAFF	OPLS/AA
Name	T	κ_T	Ref.	κ_T	κ_T
20. bromoethane	293.15	1.19		**1.92 ± 0.07**	1.14 ± 0.03
...	298.15	1.25		**2.10 ± 0.08**	1.17 ± 0.03
21. chloroethane	273.15	1.02	[21]	**1.63 ± 0.06**	**1.68 ± 0.05**
...	285.45			1.91 ± 0.10	1.88 ± 0.05
22. 2-chloroethanol	293.15			0.49 ± 0.01	0.56 ± 0.02
23. ethanamide	358.15			0.48 ± 0.01	0.46 ± 0.01
...	494.30			1.20 ± 0.02	1.05 ± 0.03
24. N-methylformamide	292.15	0.58		**0.41 ± 0.01**	0.47 ± 0.01
...	298.15	0.56	[9]	**0.41 ± 0.01**	0.46 ± 0.01
25. nitroethane	298.15	0.79	[9]	**0.41 ± 0.01**	0.71 ± 0.02
26. methoxymethane	240.00			1.23 ± 0.04	1.51 ± 0.04
27. ethanol	293.15	1.10		0.91 ± 0.02	0.93 ± 0.03
...	298.15	1.15	[9]	0.98 ± 0.03	0.95 ± 0.01
28. 1,2-ethanedithiol	293.15			0.67 ± 0.02	0.51 ± 0.01
...	298.15			0.74 ± 0.01	0.50 ± 0.01
29. methyldisulfanylmethane	293.15			1.17 ± 0.04	0.99 ± 0.01
...	298.15			1.28 ± 0.02	1.01 ± 0.03
30. methylsulfinylmethane	298.15	0.52	[9]	0.41 ± 0.01	0.41 ± 0.01
31. methylsulfanylmethane	293.15			2.07 ± 0.07	1.23 ± 0.04
...	298.15			2.22 ± 0.08	1.28 ± 0.04
32. 2-aminoethanol	293.15	0.38		**0.22 ± 0.01**	0.45 ± 0.01
...	320.00	0.44		**0.25 ± 0.01**	**0.55 ± 0.01**
33. ethane-1,2-diamine	293.15			0.34 ± 0.01	0.53 ± 0.01
...	298.15	0.51	[9]	**0.33 ± 0.01**	0.53 ± 0.02
34. prop-2-enenitrile	298.15			1.33 ± 0.03	1.00 ± 0.02
...	350.45			2.36 ± 0.09	1.74 ± 0.05
35. 1,3-dioxolan-2-one	312.15			0.26 ± 0.01	0.32 ± 0.01
36. propanenitrile	293.15			1.05 ± 0.03	1.41 ± 0.04
...	298.15	1.11	[9]	1.14 ± 0.03	**1.50 ± 0.05**
37. 1,2-dibromopropane	293.15			0.89 ± 0.02	0.49 ± 0.01
...	298.15			0.96 ± 0.03	0.52 ± 0.01
38. 1,3-dichloropropane	298.15	0.76		0.83 ± 0.02	0.85 ± 0.01

Table S7: Isothermal compressibility - continued

	Experiment			GAFF	OPLS/AA
Name	T	κ_T	Ref.	κ_T	κ_T
39. (2R)-2-methyloxirane	298.15			1.47 ± 0.04	1.70 ± 0.04
40. propan-2-one	298.15	1.32	[9]	1.14 ± 0.02	1.31 ± 0.02
41. methyl acetate	293.15	1.10		**0.64 ± 0.01**	**0.76 ± 0.02**
...	298.15	1.14	[9]	**0.69 ± 0.02**	**0.83 ± 0.01**
42. 1,3-dioxolane	293.15	0.72		**0.44 ± 0.01**	0.69 ± 0.01
...	298.15	0.76		**0.47 ± 0.01**	0.77 ± 0.02
43. 2-iodopropane	293.15			1.20 ± 0.03	0.93 ± 0.02
...	298.15			1.26 ± 0.03	1.01 ± 0.03
44. 1-bromopropane	293.15	1.09		1.31 ± 0.03	0.96 ± 0.03
...	298.15	1.13		**1.47 ± 0.05**	0.99 ± 0.02
45. N,N-dimethylformamide	298.15	0.64	[9]	**0.48 ± 0.01**	0.58 ± 0.01
46. N-methylacetamide	320.00			0.55 ± 0.02	0.50 ± 0.01
47. 1-nitropropane	298.15	0.80	[9]	**0.44 ± 0.01**	0.74 ± 0.01
48. 2-nitropropane	298.15	0.89	[9]	**0.47 ± 0.01**	0.73 ± 0.02
49. dimethoxymethane	293.15			0.88 ± 0.03	1.15 ± 0.02
...	298.15			1.02 ± 0.03	1.18 ± 0.01
50. propane-1,2,3-triol	293.15	0.24		**0.15 ± 0.00**	0.22 ± 0.01
...	320.00	0.26		0.31 ± 0.01	**0.33 ± 0.02**
51. propan-1-amine	293.15	1.16		0.97 ± 0.02	**1.49 ± 0.04**
...	298.15	1.21		1.00 ± 0.03	**1.55 ± 0.03**
52. propan-2-amine	293.15			0.90 ± 0.02	1.40 ± 0.05
...	298.15			0.95 ± 0.02	1.50 ± 0.05
53. 2-methylpropane	243.65			1.45 ± 0.03	1.66 ± 0.04
54. ethylsulfanylethane	293.15			1.27 ± 0.04	0.98 ± 0.02
...	298.15			1.34 ± 0.05	1.06 ± 0.03
55. butane-1-thiol	293.15			1.06 ± 0.02	0.89 ± 0.02
...	298.15			1.10 ± 0.03	0.95 ± 0.02
56. butan-1-ol	293.15	0.91		0.73 ± 0.02	0.86 ± 0.02
...	298.15	0.94	[9]	0.77 ± 0.03	0.88 ± 0.02
57. 2-methylpropan-2-ol	320.00			1.03 ± 0.03	1.08 ± 0.02
58. butane-1,4-diol	293.15			0.30 ± 0.02	0.32 ± 0.01
...	298.15	0.44	[9]	**0.32 ± 0.02**	0.34 ± 0.01
...	320.00			0.33 ± 0.01	0.38 ± 0.01

Table S7: Isothermal compressibility - continued

Name	Experiment T	Experiment κ_T	Experiment Ref.	GAFF κ_T	OPLS/AA κ_T
59. (2-hydroxyethoxy)ethan-2-ol	288.15			0.16 ± 0.00	0.35 ± 0.02
60. N-ethylethanamine	293.15			1.15 ± 0.04	1.54 ± 0.03
...	298.15	1.51	[9]	1.18 ± 0.02	1.62 ± 0.04
61. butan-1-amine	293.15			0.85 ± 0.02	1.20 ± 0.03
...	298.15	1.14	[9]	0.90 ± 0.02	1.28 ± 0.03
62. 2-methylpropan-2-amine	293.15			0.86 ± 0.03	1.15 ± 0.02
...	298.15			0.93 ± 0.02	1.25 ± 0.03
63. 2-(2-hydroxyethylamino)ethanol	320.00			0.23 ± 0.01	0.37 ± 0.02
64. pyrimidine	298.15			0.41 ± 0.01	0.44 ± 0.02
65. furan	293.15			1.00 ± 0.03	0.99 ± 0.06
...	298.15			1.01 ± 0.04	1.04 ± 0.03
66. thiophene	293.15			0.97 ± 0.02	0.63 ± 0.03
...	298.15			0.96 ± 0.03	0.62 ± 0.03
67. 1H-pyrrole	293.15			0.52 ± 0.01	0.57 ± 0.01
...	298.15	0.65	[9]	0.51 ± 0.01	0.60 ± 0.01
68. ethenyl acetate	298.15			0.78 ± 0.02	0.67 ± 0.02
69. oxolan-2-one	293.15			0.34 ± 0.01	0.42 ± 0.01
70. acetyl acetate	293.15			0.39 ± 0.01	0.36 ± 0.01
71. 1,4-dichlorobutane	298.15	0.69		0.71 ± 0.02	0.80 ± 0.01
72. oxolane	298.15	0.95	[9]	0.76 ± 0.02	1.10 ± 0.02
73. ethoxyethene	293.15			1.50 ± 0.03	1.40 ± 0.04
74. ethyl acetate	293.15			0.71 ± 0.02	0.76 ± 0.02
...	298.15	1.21	[9]	**0.74 ± 0.02**	**0.80 ± 0.02**
75. tetrahydrothiophene 1,1-dioxide	320.00			0.26 ± 0.01	0.36 ± 0.01
76. thiolane	293.15			0.73 ± 0.02	0.65 ± 0.02
...	298.15			0.77 ± 0.02	0.67 ± 0.04
77. 1-bromobutane	293.15			1.15 ± 0.03	0.88 ± 0.03
...	298.15	1.03	[9]	1.20 ± 0.02	0.93 ± 0.03
78. 1-chlorobutane	293.15	1.07		1.24 ± 0.04	1.26 ± 0.02
...	298.15	1.21		1.23 ± 0.02	1.34 ± 0.01
79. pyrrolidine	293.15			0.64 ± 0.01	0.96 ± 0.03
...	298.15	0.81	[9]	0.66 ± 0.02	0.92 ± 0.02

Table S7: Isothermal compressibility - continued

	Experiment			GAFF	OPLS/AA
Name	T	κ_T	Ref.	κ_T	κ_T
80. N,N-dimethylacetamide	298.15	0.63	[9]	0.56 ± 0.02	0.53 ± 0.00
81. morpholine	293.15			0.32 ± 0.01	0.51 ± 0.02
82. pyridine	293.15	0.67		0.59 ± 0.02	0.60 ± 0.02
...	298.15	0.71	[9]	0.64 ± 0.02	0.64 ± 0.03
83. cyclopentanone	293.15			0.57 ± 0.01	0.66 ± 0.01
...	298.15			0.56 ± 0.02	0.69 ± 0.01
84. 1-cyclopropylethanone	293.15			0.76 ± 0.01	0.72 ± 0.02
...	298.15			0.75 ± 0.02	0.76 ± 0.03
85. pentane-2,4-dione	298.15			0.51 ± 0.01	0.50 ± 0.01
86. methyl 2-methylprop-2-enoate	298.15			0.73 ± 0.03	0.61 ± 0.01
87. pentanenitrile	293.15	0.91		0.84 ± 0.01	1.09 ± 0.03
...	298.15	0.95		0.88 ± 0.02	1.15 ± 0.03
88. ethyl propanoate	298.15	1.30	[9]	**0.77 ± 0.01**	**0.77 ± 0.01**
89. diethyl carbonate	298.15	1.00	[9]	**0.53 ± 0.01**	**0.68 ± 0.02**
90. pentan-1-ol	293.15	0.85		0.69 ± 0.03	0.80 ± 0.02
...	298.15	0.88	[9]	0.74 ± 0.02	0.82 ± 0.01
...	320.00	1.01		0.81 ± 0.02	1.02 ± 0.01
91. pentan-3-ol	293.15	0.89		0.74 ± 0.03	0.77 ± 0.01
...	298.15	0.93		0.76 ± 0.02	0.88 ± 0.02
92. 2-methylbutan-2-ol	293.15	1.03		**0.70 ± 0.02**	0.82 ± 0.02
...	298.15	1.11	[9]	**0.69 ± 0.02**	0.87 ± 0.02
...	320.00			0.91 ± 0.02	1.07 ± 0.02
93. pentane-1,5-diol	293.15	0.40		**0.29 ± 0.02**	**0.29 ± 0.01**
...	298.15	0.46	[9]	**0.30 ± 0.01**	0.41 ± 0.01
94. pentan-3-amine	293.15			0.84 ± 0.03	1.08 ± 0.03
...	298.15			0.91 ± 0.01	1.15 ± 0.03
95. 1,2,3,4-tetrafluorobenzene	298.15			1.84 ± 0.06	1.39 ± 0.03
96. 1,2,3,5-tetrafluorobenzene	298.15			1.96 ± 0.09	1.51 ± 0.04
97. 1,3-difluorobenzene	293.15			1.45 ± 0.05	1.28 ± 0.05
...	298.15			1.25 ± 0.05	1.44 ± 0.06
98. 1,2-difluorobenzene	293.15			1.43 ± 0.03	1.20 ± 0.05
...	298.15			1.26 ± 0.02	1.40 ± 0.05

Table S7: Isothermal compressibility - continued

Name	Experiment T	Experiment κ_T	Experiment Ref.	GAFF κ_T	OPLS/AA κ_T
99. fluorobenzene	293.15			1.31 ± 0.04	0.94 ± 0.01
...	298.15	0.94	[9]	**1.26 ± 0.05**	1.01 ± 0.02
100. nitrobenzene	293.15			0.33 ± 0.01	0.47 ± 0.01
...	298.15	0.51	[9]	**0.34 ± 0.00**	0.48 ± 0.01
101. 2-chloroaniline	293.15			0.51 ± 0.01	0.47 ± 0.01
102. phenol	318.15			0.61 ± 0.02	0.54 ± 0.02
103. benzenethiol	293.15			0.85 ± 0.02	0.86 ± 0.02
...	298.15			0.85 ± 0.02	0.83 ± 0.03
104. 2-methylpyridine	293.15			0.69 ± 0.02	0.62 ± 0.02
...	298.15			0.72 ± 0.01	0.63 ± 0.02
105. 3-methylpyridine	293.15			0.67 ± 0.02	0.58 ± 0.02
...	298.15			0.66 ± 0.01	0.59 ± 0.01
106. 4-methylpyridine	293.15			0.64 ± 0.02	0.60 ± 0.01
...	298.15	0.70	[9]	0.67 ± 0.02	0.60 ± 0.02
107. cyclohexanone	293.15			0.52 ± 0.01	0.60 ± 0.02
...	298.15	0.66	[9]	0.56 ± 0.02	0.65 ± 0.02
108. (E)-hex-2-ene	293.15			1.86 ± 0.08	1.55 ± 0.04
109. hexan-2-one	298.15	1.01		0.87 ± 0.02	0.93 ± 0.03
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15			0.31 ± 0.01	0.55 ± 0.01
111. cyclohexanamine	298.15			0.50 ± 0.01	0.68 ± 0.01
112. 2-propan-2-yloxypropane	298.15	1.61	[9]	**1.08 ± 0.02**	1.48 ± 0.05
113. 1-methoxy-2-(2-methoxyethoxy)ethane	293.15			0.46 ± 0.01	0.64 ± 0.02
...	298.15	0.64		**0.46 ± 0.01**	0.68 ± 0.01
114. triethyl phosphate	293.15			0.46 ± 0.01	0.54 ± 0.01
...	298.15	1.49	[9]	**0.37 ± 0.01**	**0.58 ± 0.02**
...	320.00			0.47 ± 0.01	0.66 ± 0.02
115. N,N-diethylethanamine	293.15			0.96 ± 0.02	1.28 ± 0.03
...	298.15	1.38	[9]	**1.03 ± 0.02**	1.34 ± 0.04
116. N-propan-2-ylpropan-2-amine	293.15			0.93 ± 0.01	1.19 ± 0.02
...	298.15	1.45		**0.99 ± 0.04**	1.26 ± 0.02
117. trifluoromethylbenzene	293.15			1.05 ± 0.02	1.11 ± 0.04
...	298.15			1.16 ± 0.03	1.15 ± 0.02

Table S7: Isothermal compressibility - continued

Name	Experiment T	Experiment κ_T	Experiment Ref.	GAFF κ_T	OPLS/AA κ_T
118. benzonitrile	288.15			0.68 ± 0.02	0.48 ± 0.01
119. benzaldehyde	298.15	0.23	[9]	**0.58 ± 0.01**	**0.48 ± 0.01**
120. toluene	298.15	0.92	[9]	1.06 ± 0.03	0.88 ± 0.03
121. methoxybenzene	293.15			0.66 ± 0.02	0.62 ± 0.01
...	298.15	0.69	[9]	0.65 ± 0.01	0.65 ± 0.02
122. phenylmethanol	297.15			0.51 ± 0.01	0.46 ± 0.02
123. 2-methylphenol	308.15			0.52 ± 0.02	0.50 ± 0.01
124. 3-methylphenol	320.00	0.61		0.56 ± 0.01	0.53 ± 0.01
125. 4-methylphenol	313.15			0.60 ± 0.01	0.49 ± 0.02
...	320.00			0.63 ± 0.03	0.48 ± 0.02
126. diethyl propanedioate	293.15			0.42 ± 0.01	0.49 ± 0.01
127. 2,4-dimethylpentan-3-one	293.15			0.80 ± 0.02	0.82 ± 0.02
...	298.15			0.77 ± 0.02	0.84 ± 0.02
128. heptan-2-one	293.15	0.93		0.79 ± 0.02	0.83 ± 0.02
...	298.15	0.96		0.79 ± 0.01	0.87 ± 0.02
129. ethenylbenzene	298.15			0.88 ± 0.02	0.74 ± 0.02
130. 1-phenylethanone	293.15			0.54 ± 0.01	0.44 ± 0.01
...	298.15	0.56	[9]	0.54 ± 0.01	0.48 ± 0.01
131. methyl benzoate	298.15	0.45	[9]	0.47 ± 0.01	0.47 ± 0.01
132. methyl 2-hydroxybenzoate	298.15			0.37 ± 0.01	0.39 ± 0.01
...	320.00			0.47 ± 0.02	0.47 ± 0.01
133. ethylbenzene	298.15	0.86	[9]	0.96 ± 0.02	0.83 ± 0.01
134. 1,2-dimethylbenzene	293.15	0.78		0.93 ± 0.02	0.70 ± 0.03
...	298.15	0.81	[9]	0.98 ± 0.02	0.74 ± 0.02
135. 1,2-dimethoxybenzene	298.15			0.50 ± 0.01	0.53 ± 0.01
136. 2,4,6-trimethylpyridine	295.15			0.68 ± 0.02	0.59 ± 0.02
...	298.15			0.65 ± 0.01	0.58 ± 0.01
137. octan-1-ol	298.15	0.76	[9]	0.60 ± 0.02	**0.49 ± 0.02**
...	320.00	0.89		**0.66 ± 0.02**	0.91 ± 0.02
138. 1-butoxybutane	293.15			0.91 ± 0.02	1.09 ± 0.02
...	298.15			0.96 ± 0.03	1.13 ± 0.03
139. N-butylbutan-1-amine	293.15			0.83 ± 0.03	1.02 ± 0.03
...	298.15	1.06	[9]	0.86 ± 0.03	1.06 ± 0.04

Table S7: Isothermal compressibility - continued

	Experiment			GAFF	OPLS/AA
Name	T	κ_T	Ref.	κ_T	κ_T
140. isoquinoline	303.15			0.43 ± 0.01	0.27 ± 0.01
...	320.00			0.56 ± 0.02	0.42 ± 0.02
141. quinoline	288.15			0.50 ± 0.02	0.45 ± 0.01
...	298.15	0.44	[9]	0.49 ± 0.03	0.48 ± 0.02
142. (1-methylethyl)benzene	298.15	0.98	[9]	0.90 ± 0.01	0.79 ± 0.02
143. 1,2,4-trimethylbenzene	293.15	0.79		0.85 ± 0.02	0.68 ± 0.01
...	298.15	0.84		0.90 ± 0.02	0.70 ± 0.01
144. 2,6-dimethylheptan-4-one	293.15			0.73 ± 0.02	0.76 ± 0.02
...	298.15			0.77 ± 0.02	0.77 ± 0.02
145. 1-chloronaphthalene	298.15	0.49		0.53 ± 0.01	0.55 ± 0.01
146. phenoxybenzene	303.15			0.56 ± 0.03	0.46 ± 0.01

Table S8: Heat capacity at constant pressure c_P (J/mol K) calculated (based on density of states) and experimental. Blue font indicates that the calculated value differs more than 25% from the experimental ones, a red font indicates that it differs by more than 50%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA
Name	T	c_P	Ref.	c_P	c_P
1. chloroform	298.15	117.00	[9]	94.2 ± 4.4	94.4 ± 7.7
2. dichloro(fluoro)methane	282.05	107.07	[13]	80.7 ± 5.8	78.9 ± 5.0
3. dibromomethane	298.15	104.90	[9]	83.1 ± 5.7	81.2 ± 4.4
4. dichloromethane	298.15	100.88	[13]	76.9 ± 4.0	70.4 ± 4.9
5. methanal	253.65	79.78	[22]	50.9 ± 2.5	57.1 ± 3.3
6. methanoic acid	298.15	99.00	[9]	74.8 ± 24.2	79.5 ± 5.9
7. bromomethane	276.65	78.75	[13]		59.2 ± 3.5
8. methanamide	298.15	107.60	[9]	83.0 ± 11.7	87.1 ± 7.9
9. nitromethane	298.15	105.80	[9]	101.9 ± 15.8	96.6 ± 6.8
10. methanol	298.15	81.47	[9]	73.4 ± 9.3	75.8 ± 4.8
11. 1,1,1,2,2-pentachloroethane	293.15	173.96	[22]	154.6 ± 14.8	154.8 ± 5.2
12. 1,1,2,2-tetrachloroethane	298.15	165.70	[9]	139.7 ± 16.5	135.4 ± 12.3
13. 1,1-dichloroethene	298.15	111.33	[13]	81.8 ± 6.9	86.7 ± 5.9
14. 1,1,2-trichloroethane	298.15	148.50	[9]	122.6 ± 10.3	119.7 ± 12.8
15. acetonitrile	298.15	91.40	[9]	74.7 ± 5.2	58.2 ± 4.4
16. 1,2-dibromoethane	298.15	136.00	[9]	105.1 ± 6.8	112.6 ± 12.2
17. 1,1-dichloroethane	298.15	126.20	[9]	106.9 ± 7.7	103.8 ± 7.0
18. 1,2-dichloroethane	298.15	128.90	[9]	104.4 ± 9.0	106.6 ± 7.2
19. methyl formate	298.15	119.70	[9]	100.2 ± 11.9	102.6 ± 6.7
20. bromoethane	298.15	99.73	[13]	84.4 ± 7.7	90.6 ± 6.4
21. chloroethane	273.15	101.18	[13]	82.9 ± 12.4	83.2 ± 6.5
...	285.45	102.80	[13]	83.1 ± 12.4	82.8 ± 5.0
22. 2-chloroethanol	293.15	109.03	[13]	117.6 ± 19.6	120.0 ± 16.5
23. ethanamide	358.15	148.39	[13]	133.0 ± 29.7	137.2 ± 13.8
24. N-methylformamide	298.15	123.80	[9]	115.0 ± 19.7	119.4 ± 10.8
25. nitroethane	298.15	138.50	[9]	131.7 ± 34.1	127.5 ± 9.9
27. ethanol	298.15	112.30	[9]	106.2 ± 16.5	109.0 ± 12.5
28. 1,2-ethanedithiol	298.15			133.5 ± 15.9	144.4 ± 14.5
29. methyldisulfanylmethane	298.15	145.96	[13]	126.9 ± 7.9	133.7 ± 12.3
30. methylsulfinylmethane	298.15	153.10	[9]	132.4 ± 16.7	132.0 ± 9.1

Table S8: Heat capacity at constant pressure c_P based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_P	Ref.	c_P	c_P
31. methylsulfanylmethane	298.15	118.10	[9]	96.3 ± 13.1	105.7 ± 6.8
32. 2-aminoethanol	293.15			128.0 ± 47.4	133.5 ± 28.2
33. ethane-1,2-diamine	298.15	172.50	[9]	139.6 ± 29.5	143.4 ± 20.8
34. prop-2-enenitrile	298.15	108.60	[9]	83.4 ± 4.7	81.2 ± 10.8
...	350.45	114.98	[13]	89.3 ± 7.7	82.3 ± 5.2
35. 1,3-dioxolan-2-one	312.15	133.84	[13]	135.8 ± 18.5	142.4 ± 22.0
36. propanenitrile	298.15	119.70	[9]	105.0 ± 13.9	89.3 ± 7.5
37. 1,2-dibromopropane	298.15	172.80	[22]	136.9 ± 14.3	147.0 ± 16.7
38. 1,3-dichloropropane	298.15	159.45	[13]	136.2 ± 14.1	137.1 ± 14.0
39. (2R)-2-methyloxirane	298.15			103.0 ± 6.8	111.7 ± 36.9
40. propan-2-one	298.15	124.90	[9]	111.7 ± 18.9	117.3 ± 6.6
41. methyl acetate	298.15	143.90	[9]	133.4 ± 18.4	135.9 ± 11.8
42. 1,3-dioxolane	293.15	120.32	[23]	123.7 ± 21.8	124.3 ± 10.6
43. 2-iodopropane	298.15	139.72	[13]	123.6 ± 24.7	125.7 ± 12.5
44. 1-bromopropane	298.15	133.47	[13]	116.5 ± 15.8	122.8 ± 9.5
45. N,N-dimethylformamide	298.15	148.30	[9]	142.9 ± 28.4	148.9 ± 22.2
47. 1-nitropropane	298.15	175.30	[9]	161.7 ± 31.0	159.7 ± 16.0
48. 2-nitropropane	298.15	170.20	[9]	163.6 ± 28.9	163.6 ± 20.3
49. dimethoxymethane	298.15	161.50	[13]	144.1 ± 21.8	145.7 ± 14.6
50. propane-1,2,3-triol	293.15	216.70	[22]	171.3 ± 121.9	174.1 ± 43.9
51. propan-1-amine	298.15	162.79	[13]	138.5 ± 25.8	139.0 ± 7.2
52. propan-2-amine	298.15	163.81	[13]	142.5 ± 20.7	141.9 ± 13.4
54. ethylsulfanylethane	298.15	171.40	[9]	156.3 ± 24.1	167.8 ± 21.2
55. butane-1-thiol	298.15	171.20	[11]	161.2 ± 32.0	170.5 ± 21.9
56. butan-1-ol	298.15	177.00	[9]	168.1 ± 26.7	174.0 ± 25.6
58. butane-1,4-diol	298.15	202.20	[9]	185.1 ± 44.0	195.5 ± 63.8
59. (2-hydroxyethoxy)ethan-2-ol	288.15	256.39	[22]	197.6 ± 147.8	210.7 ± 51.8
60. N-ethylethanamine	298.15	176.70	[9]	161.7 ± 22.8	164.2 ± 10.6
61. butan-1-amine	298.15	188.00	[9]	170.5 ± 29.0	172.8 ± 12.8
62. 2-methylpropan-2-amine	298.15	192.10	[13]	180.1 ± 62.5	182.0 ± 12.0
64. pyrimidine	298.15	133.70	[9]	120.9 ± 25.9	124.6 ± 14.7
65. furan	298.15	114.80	[9]	97.3 ± 13.9	99.3 ± 9.0

Table S8: Heat capacity at constant pressure c_P based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_P	Ref.	c_P	c_P
66. thiophene	298.15	123.98	[13]	104.4 ± 10.4	110.3 ± 16.9
67. 1H-pyrrole	298.15	128.20	[9]	113.9 ± 14.1	116.2 ± 14.7
68. ethenyl acetate	298.15	171.47	[13]	144.3 ± 20.3	150.9 ± 19.0
69. oxolan-2-one	293.15	139.96	[22]	140.5 ± 23.4	147.3 ± 27.2
70. acetyl acetate	293.15	189.13	[13]	172.0 ± 46.3	179.8 ± 15.1
71. 1,4-dichlorobutane	298.15	189.23	[13]	167.3 ± 25.6	169.3 ± 24.1
72. oxolane	298.15	123.90	[9]	131.6 ± 22.0	134.8 ± 16.0
73. ethoxyethene	293.15	153.58	[13]	130.4 ± 24.6	135.2 ± 10.0
74. ethyl acetate	298.15	167.70	[9]	164.6 ± 25.6	169.6 ± 10.0
76. thiolane	298.15	139.80	[9]	139.6 ± 20.7	147.2 ± 26.4
77. 1-bromobutane	298.15	168.10	[9]	147.0 ± 15.7	155.4 ± 22.9
78. 1-chlorobutane	298.15	174.60	[9]	146.2 ± 21.0	151.1 ± 10.9
79. pyrrolidine	298.15	156.50	[9]	141.3 ± 16.3	146.5 ± 19.4
80. N,N-dimethylacetamide	298.15	176.00	[9]	174.6 ± 31.7	182.3 ± 27.5
81. morpholine	293.15	173.88	[13]	160.6 ± 30.4	167.8 ± 30.0
82. pyridine	298.15	135.60	[9]	120.8 ± 23.3	125.9 ± 19.5
83. cyclopentanone	298.15	154.50	[9]	152.8 ± 32.9	159.1 ± 18.8
84. 1-cyclopropylethanone	298.15			158.4 ± 31.1	167.4 ± 18.2
85. pentane-2,4-dione	298.15	208.20	[9]	184.0 ± 53.4	197.2 ± 19.9
86. methyl 2-methylprop-2-enoate	298.15	189.82	[13]	178.1 ± 25.9	187.4 ± 29.4
87. pentanenitrile	298.15	189.70	[9]	167.8 ± 25.3	156.6 ± 22.0
88. ethyl propanoate	298.15	196.10	[9]	195.6 ± 34.6	203.0 ± 24.6
89. diethyl carbonate	298.15	212.40	[9]	219.5 ± 68.2	223.6 ± 24.1
90. pentan-1-ol	298.15	208.90	[9]	197.3 ± 35.2	207.3 ± 28.3
91. pentan-3-ol	298.15	247.72	[13]	200.7 ± 50.9	208.7 ± 25.9
92. 2-methylbutan-2-ol	298.15	244.30	[9]	204.2 ± 36.4	212.8 ± 33.9
93. pentane-1,5-diol	298.15	225.50	[9]	214.9 ± 82.7	228.2 ± 44.8
94. pentan-3-amine	298.15	205.13	[22]		206.7 ± 31.0
95. 1,2,3,4-tetrafluorobenzene	298.15	190.06	[23]	170.7 ± 8.8	173.4 ± 13.9
96. 1,2,3,5-tetrafluorobenzene	298.15	190.19	[23]	169.7 ± 19.5	176.0 ± 10.6
97. 1,3-difluorobenzene	298.15	159.10	[11]	140.5 ± 18.6	145.2 ± 12.3
98. 1,2-difluorobenzene	298.15	159.00	[11]	140.7 ± 14.0	146.4 ± 13.4

Table S8: Heat capacity at constant pressure c_P based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_P	Ref.	c_P	c_P
99. fluorobenzene	298.15	146.30	[9]	126.9 ± 12.4	155.6 ± 9.9
100. nitrobenzene	298.15	177.20	[9]	177.9 ± 26.7	174.9 ± 27.9
101. 2-chloroaniline	293.15	196.88	[13]	174.5 ± 29.7	175.2 ± 20.7
102. phenol	318.15	202.77	[13]	160.4 ± 17.0	167.4 ± 29.7
103. benzenethiol	298.15	173.55	[13]	153.1 ± 8.6	153.4 ± 19.9
104. 2-methylpyridine	298.15	159.20	[9]	154.7 ± 30.6	161.4 ± 10.6
105. 3-methylpyridine	298.15	159.00	[9]	153.7 ± 21.8	161.6 ± 23.6
106. 4-methylpyridine	298.15	159.00	[9]	154.3 ± 28.1	160.6 ± 25.7
107. cyclohexanone	298.15	179.30	[9]	182.4 ± 33.3	193.2 ± 20.3
109. hexan-2-one	298.15	213.17	[13]	203.8 ± 36.5	213.9 ± 36.8
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15	255.56	[13]	246.4 ± 124.1	249.4 ± 28.7
111. cyclohexanamine	298.15	200.84	[22]	207.9 ± 63.1	216.7 ± 40.7
112. 2-propan-2-yloxypropane	298.15	216.10	[9]	221.6 ± 44.7	225.5 ± 25.4
113. 1-methoxy-2-(2-methoxyethoxy)ethane	298.15	226.00	[9]	267.9 ± 46.0	273.6 ± 53.0
114. triethyl phosphate	298.15			325.4 ± 390.7	333.3 ± 60.5
115. N,N-diethylethanamine	298.15	224.40	[9]	221.5 ± 42.9	228.9 ± 30.9
116. N-propan-2-ylpropan-2-amine	298.15	226.35	[13]	230.0 ± 44.9	235.7 ± 33.7
117. trifluoromethylbenzene	298.15	188.80	[13]	185.2 ± 16.4	184.3 ± 18.1
118. benzonitrile	288.15	163.00	[13]	150.4 ± 26.0	165.2 ± 13.2
119. benzaldehyde	298.15	172.00	[9]	161.1 ± 14.0	169.5 ± 19.6
120. toluene	298.15	157.20	[9]	153.5 ± 21.1	161.7 ± 8.4
121. methoxybenzene	298.15	208.60	[9]	177.3 ± 28.1	179.6 ± 22.2
122. phenylmethanol	297.15	216.44	[13]	182.8 ± 23.5	188.8 ± 55.4
123. 2-methylphenol	308.15	234.03	[13]	194.2 ± 36.4	201.1 ± 24.4
125. 4-methylphenol	313.15	229.41	[13]	195.6 ± 20.1	203.5 ± 24.5
126. diethyl propanedioate	293.15	284.24	[13]	281.3 ± 68.0	293.6 ± 38.6
127. 2,4-dimethylpentan-3-one	298.15	235.51	[13]	244.2 ± 54.5	251.1 ± 44.3
128. heptan-2-one	298.15	243.60	[9]	235.3 ± 63.3	247.5 ± 42.5
129. ethenylbenzene	298.15	182.50	[9]	164.0 ± 22.5	171.2 ± 22.3
130. 1-phenylethanone	298.15	204.60	[9]	195.8 ± 21.9	202.7 ± 25.5
131. methyl benzoate	298.15	221.30	[9]	214.4 ± 43.8	221.7 ± 51.5
132. methyl 2-hydroxybenzoate	298.15	247.51	[13]	237.3 ± 37.0	250.1 ± 37.8

Table S8: Heat capacity at constant pressure c_P based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_P	Ref.	c_P	c_P
133. ethylbenzene	298.15	185.50	[9]	182.8 ± 31.1	191.8 ± 22.6
134. 1,2-dimethylbenzene	298.15	188.00	[9]	189.6 ± 23.1	200.6 ± 25.7
135. 1,2-dimethoxybenzene	298.15			235.3 ± 35.0	238.2 ± 27.2
136. 2,4,6-trimethylpyridine	298.15	214.00	[9]	226.0 ± 199.7	235.2 ± 29.9
137. octan-1-ol	298.15	305.50	[9]	289.9 ± 113.2	304.8 ± 86.9
138. 1-butoxybutane	298.15	251.90	[9]	280.2 ± 95.7	289.4 ± 38.3
139. N-butylbutan-1-amine	298.15	292.80	[9]	288.2 ± 48.1	301.3 ± 51.0
141. quinoline	298.15	200.00	[9]	190.6 ± 28.6	194.1 ± 15.1
142. (1-methylethyl)benzene	298.15	198.90	[9]	217.9 ± 37.3	226.4 ± 32.2
144. 2,6-dimethylheptan-4-one	298.15	297.30	[11]	300.0 ± 124.7	317.0 ± 55.5
145. 1-chloronaphthalene	298.15	222.14	[13]	208.2 ± 41.6	211.9 ± 35.1
146. phenoxybenzene	303.15	269.87	[13]	262.9 ± 71.8	270.2 ± 56.0

Table S9: Heat capacity at constant volume c_V (J/mol K) calculated (based on density of states) compared to the experimental c_P - Δc (J/mol K). Blue font indicates that the calculated value differs more than 25% from the experimental ones, a red font indicates that it differs by more than 50%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA
Name	T	c_V	Ref.	c_V	c_V
1. chloroform	298.15	116.98	[9]	94.2 ± 0.6	94.3 ± 0.1
2. dichloro(fluoro)methane	282.05			80.7 ± 0.1	78.9 ± 0.3
3. dibromomethane	298.15	104.88	[9]	83.1 ± 0.3	81.2 ± 0.5
4. dichloromethane	298.15	100.86	[9]	76.9 ± 0.1	70.3 ± 0.3
5. methanal	253.65			50.9 ± 0.1	57.1 ± 0.2
6. methanoic acid	298.15	98.99	[9]	74.8 ± 0.2	79.5 ± 0.2
7. bromomethane	276.65				59.2 ± 0.1
8. methanamide	298.15	107.59	[9]	83.0 ± 0.2	87.1 ± 0.1
9. nitromethane	298.15	105.78	[9]	101.9 ± 0.2	96.6 ± 0.1
10. methanol	298.15	81.46	[9]	73.4 ± 0.1	75.8 ± 0.4
11. 1,1,1,2,2-pentachloroethane	293.15			154.6 ± 0.3	154.8 ± 0.5
12. 1,1,2,2-tetrachloroethane	298.15	165.67	[9]	139.7 ± 0.2	135.3 ± 0.2
13. 1,1-dichloroethene	298.15			81.8 ± 0.2	86.6 ± 0.2
14. 1,1,2-trichloroethane	298.15	148.48	[9]	122.6 ± 0.3	119.7 ± 0.3
15. acetonitrile	298.15	91.38	[9]	74.7 ± 0.2	58.1 ± 0.3
16. 1,2-dibromoethane	298.15	135.98	[9]	105.0 ± 0.3	112.6 ± 0.3
17. 1,1-dichloroethane	298.15	126.18	[9]	106.9 ± 0.4	103.7 ± 0.4
18. 1,2-dichloroethane	298.15	128.88	[9]	104.4 ± 0.3	106.5 ± 0.2
19. methyl formate	298.15			100.1 ± 0.2	102.6 ± 0.3
20. bromoethane	298.15	99.71	[20]	84.4 ± 0.2	90.6 ± 0.4
21. chloroethane	273.15	101.16	[20]	82.9 ± 0.3	83.2 ± 0.5
...	285.45			83.1 ± 0.4	82.8 ± 0.5
22. 2-chloroethanol	293.15			117.6 ± 0.3	120.0 ± 0.2
23. ethanamide	358.15			133.0 ± 0.2	137.2 ± 0.2
24. N-methylformamide	298.15	123.78	[9]	115.0 ± 0.2	119.4 ± 0.2
25. nitroethane	298.15	138.48	[9]	131.7 ± 0.4	127.5 ± 0.2
27. ethanol	298.15	112.29	[9]	106.1 ± 0.2	109.0 ± 0.1
28. 1,2-ethanedithiol	298.15			133.5 ± 0.3	144.4 ± 0.3
29. methyldisulfanylmethane	298.15			126.8 ± 0.4	133.7 ± 0.3
30. methylsulfinylmethane	298.15	153.08	[9]	132.4 ± 0.1	131.9 ± 0.3

Table S9: Heat capacity at constant volume c_V based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_V	Ref.	c_V	c_V
31. methylsulfanylmethane	298.15			96.3 ± 0.2	105.6 ± 0.3
32. 2-aminoethanol	293.15			128.0 ± 0.1	133.5 ± 0.1
33. ethane-1,2-diamine	298.15	172.49	[9]	139.6 ± 0.2	143.4 ± 0.2
34. prop-2-enenitrile	298.15			83.4 ± 0.2	81.2 ± 0.3
...	350.45			89.3 ± 0.2	82.3 ± 0.2
35. 1,3-dioxolan-2-one	312.15			135.8 ± 0.3	142.4 ± 0.2
36. propanenitrile	298.15	119.68	[9]	105.0 ± 0.3	89.3 ± 0.2
37. 1,2-dibromopropane	298.15			136.9 ± 0.2	147.0 ± 0.2
38. 1,3-dichloropropane	298.15	159.43	[20]	136.2 ± 0.2	137.0 ± 0.2
39. (2R)-2-methyloxirane	298.15			103.0 ± 0.4	111.6 ± 0.4
40. propan-2-one	298.15	124.88	[9]	111.7 ± 0.4	117.3 ± 0.1
41. methyl acetate	298.15	143.88	[9]	133.3 ± 0.1	135.9 ± 0.3
42. 1,3-dioxolane	293.15			123.7 ± 0.2	124.2 ± 0.3
43. 2-iodopropane	298.15			123.5 ± 0.2	125.7 ± 0.3
44. 1-bromopropane	298.15	133.44	[20]	116.5 ± 0.5	122.8 ± 0.3
45. N,N-dimethylformamide	298.15	148.28	[9]	142.9 ± 0.2	148.8 ± 0.4
47. 1-nitropropane	298.15	175.28	[9]	161.7 ± 0.2	159.7 ± 0.2
48. 2-nitropropane	298.15	170.18	[9]	163.6 ± 0.3	163.6 ± 0.4
49. dimethoxymethane	298.15			144.1 ± 0.3	145.6 ± 0.4
50. propane-1,2,3-triol	293.15	216.69	[20]	171.2 ± 0.3	174.1 ± 0.2
51. propan-1-amine	298.15	162.77	[20]	138.4 ± 0.3	138.9 ± 0.4
52. propan-2-amine	298.15			142.5 ± 0.2	141.8 ± 0.2
54. ethylsulfanylethane	298.15			156.3 ± 0.8	167.8 ± 0.2
55. butane-1-thiol	298.15			161.2 ± 0.2	170.4 ± 0.3
56. butan-1-ol	298.15	176.99	[9]	168.1 ± 0.2	174.0 ± 0.4
58. butane-1,4-diol	298.15	202.19	[9]	185.1 ± 0.2	195.4 ± 0.4
59. (2-hydroxyethoxy)ethan-2-ol	288.15			197.6 ± 0.2	210.7 ± 0.1
60. N-ethylethanamine	298.15	176.67	[9]	161.7 ± 0.4	164.1 ± 0.2
61. butan-1-amine	298.15	187.97	[9]	170.5 ± 0.6	172.8 ± 0.5
62. 2-methylpropan-2-amine	298.15			180.0 ± 0.2	181.9 ± 0.1
64. pyrimidine	298.15			120.8 ± 0.3	124.6 ± 0.1
65. furan	298.15			97.3 ± 0.2	99.3 ± 0.4

Table S9: Heat capacity at constant volume c_V based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_V	Ref.	c_V	c_V
66. thiophene	298.15			104.4 ± 0.2	110.3 ± 0.0
67. 1H-pyrrole	298.15	128.19	[9]	113.8 ± 0.3	116.2 ± 0.2
68. ethenyl acetate	298.15			144.2 ± 0.5	150.8 ± 0.5
69. oxolan-2-one	293.15			140.5 ± 0.2	147.3 ± 0.3
70. acetyl acetate	293.15			172.0 ± 0.2	179.8 ± 0.2
71. 1,4-dichlorobutane	298.15	189.20	[20]	167.2 ± 0.3	169.3 ± 0.4
72. oxolane	298.15	123.87	[9]	131.6 ± 0.5	134.8 ± 0.4
73. ethoxyethene	293.15			130.3 ± 0.2	135.2 ± 0.4
74. ethyl acetate	298.15	167.67	[9]	164.5 ± 0.2	169.5 ± 0.4
76. thiolane	298.15			139.5 ± 0.2	147.2 ± 0.4
77. 1-bromobutane	298.15	168.07	[9]	147.0 ± 0.4	155.4 ± 0.2
78. 1-chlorobutane	298.15	174.59	[9]	146.2 ± 0.4	151.0 ± 0.3
79. pyrrolidine	298.15	156.48	[9]	141.3 ± 0.4	146.5 ± 0.4
80. N,N-dimethylacetamide	298.15	175.97	[9]	174.5 ± 0.2	182.2 ± 0.2
81. morpholine	293.15			160.5 ± 0.2	167.8 ± 0.2
82. pyridine	298.15	135.58	[9]	120.8 ± 0.3	125.9 ± 0.2
83. cyclopentanone	298.15			152.8 ± 0.2	159.1 ± 0.5
84. 1-cyclopropylethanone	298.15			158.4 ± 0.3	167.4 ± 0.6
85. pentane-2,4-dione	298.15			183.9 ± 0.3	197.2 ± 0.2
86. methyl 2-methylprop-2-enoate	298.15			178.1 ± 0.3	187.4 ± 0.3
87. pentanenitrile	298.15	189.68	[9]	167.8 ± 0.3	156.6 ± 0.4
88. ethyl propanoate	298.15	196.07	[9]	195.5 ± 0.8	202.9 ± 0.6
89. diethyl carbonate	298.15	212.37	[9]	219.5 ± 0.4	223.6 ± 0.4
90. pentan-1-ol	298.15	208.88	[9]	197.3 ± 0.3	207.2 ± 0.4
91. pentan-3-ol	298.15	247.69	[20]	200.6 ± 0.3	208.7 ± 0.2
92. 2-methylbutan-2-ol	298.15	244.28	[9]	204.2 ± 0.3	212.8 ± 0.3
93. pentane-1,5-diol	298.15	225.49	[9]	214.8 ± 0.1	228.2 ± 0.3
94. pentan-3-amine	298.15				206.6 ± 0.3
95. 1,2,3,4-tetrafluorobenzene	298.15			170.6 ± 0.3	173.3 ± 0.4
96. 1,2,3,5-tetrafluorobenzene	298.15			169.7 ± 0.4	175.9 ± 0.3
97. 1,3-difluorobenzene	298.15			140.5 ± 0.3	145.2 ± 0.2
98. 1,2-difluorobenzene	298.15			140.7 ± 0.5	146.3 ± 0.4

Table S9: Heat capacity at constant volume c_V based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_V	Ref.	c_V	c_V
99. fluorobenzene	298.15	146.28	[9]	126.9 ± 0.4	155.5 ± 0.1
100. nitrobenzene	298.15	177.17	[9]	177.9 ± 0.3	174.9 ± 0.3
101. 2-chloroaniline	293.15			174.4 ± 0.4	175.1 ± 0.3
102. phenol	318.15			160.4 ± 0.3	167.4 ± 0.2
103. benzenethiol	298.15			153.1 ± 0.4	153.4 ± 0.1
104. 2-methylpyridine	298.15			154.6 ± 0.6	161.4 ± 0.5
105. 3-methylpyridine	298.15			153.7 ± 0.2	161.6 ± 0.3
106. 4-methylpyridine	298.15	158.98	[9]	154.2 ± 0.5	160.6 ± 0.4
107. cyclohexanone	298.15	179.27	[9]	182.3 ± 0.5	193.2 ± 0.3
109. hexan-2-one	298.15	213.14	[20]	203.7 ± 0.2	213.9 ± 0.4
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15			246.4 ± 0.2	249.4 ± 0.4
111. cyclohexanamine	298.15			207.9 ± 0.1	216.7 ± 0.3
112. 2-propan-2-yloxypropane	298.15	216.06	[9]	221.6 ± 0.7	225.5 ± 0.5
113. 1-methoxy-2-(2-methoxyethoxy)ethane	298.15	225.95	[9]	267.8 ± 0.3	273.6 ± 0.5
114. triethyl phosphate	298.15			325.4 ± 0.2	333.2 ± 0.3
115. N,N-diethylethanamine	298.15	224.37	[9]	221.5 ± 0.5	228.8 ± 0.5
116. N-propan-2-ylpropan-2-amine	298.15	226.32	[20]	229.9 ± 0.5	235.6 ± 0.5
117. trifluoromethylbenzene	298.15			185.1 ± 0.5	184.2 ± 0.4
118. benzonitrile	288.15			150.3 ± 0.3	165.2 ± 0.2
119. benzaldehyde	298.15	172.00	[9]	161.1 ± 0.1	169.5 ± 0.5
120. toluene	298.15	157.18	[9]	153.5 ± 0.3	161.7 ± 0.4
121. methoxybenzene	298.15	208.57	[9]	177.3 ± 0.4	179.5 ± 0.3
122. phenylmethanol	297.15			182.7 ± 0.4	188.8 ± 0.3
123. 2-methylphenol	308.15			194.2 ± 0.2	201.0 ± 0.2
125. 4-methylphenol	313.15			195.6 ± 0.2	203.5 ± 0.4
126. diethyl propanedioate	293.15			281.2 ± 0.3	293.5 ± 0.4
127. 2,4-dimethylpentan-3-one	298.15			244.1 ± 0.4	251.1 ± 0.6
128. heptan-2-one	298.15	243.57	[9]	235.3 ± 0.8	247.4 ± 0.3
129. ethenylbenzene	298.15			163.9 ± 0.5	171.2 ± 0.3
130. 1-phenylethanone	298.15	204.57	[9]	195.8 ± 0.3	202.6 ± 0.3
131. methyl benzoate	298.15	221.26	[9]	214.4 ± 0.3	221.7 ± 0.4
132. methyl 2-hydroxybenzoate	298.15			237.2 ± 0.2	250.1 ± 0.4

Table S9: Heat capacity at constant volume c_V based on DoS - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_V	Ref.	c_V	c_V
133. ethylbenzene	298.15	185.47	[9]	182.7 ± 0.2	191.7 ± 0.3
134. 1,2-dimethylbenzene	298.15	187.98	[9]	189.6 ± 0.5	200.5 ± 0.3
135. 1,2-dimethoxybenzene	298.15			235.2 ± 0.4	238.1 ± 0.3
136. 2,4,6-trimethylpyridine	298.15			225.9 ± 0.7	235.2 ± 0.2
137. octan-1-ol	298.15	305.47	[9]	289.9 ± 0.5	304.7 ± 0.5
138. 1-butoxybutane	298.15			280.2 ± 0.7	289.3 ± 0.3
139. N-butylbutan-1-amine	298.15	292.76	[9]	288.2 ± 0.3	301.2 ± 0.5
141. quinoline	298.15	199.97	[9]	190.6 ± 0.3	194.0 ± 0.2
142. (1-methylethyl)benzene	298.15	198.88	[9]	217.9 ± 0.3	226.4 ± 0.3
144. 2,6-dimethylheptan-4-one	298.15			299.9 ± 0.5	316.9 ± 0.3
145. 1-chloronaphthalene	298.15	222.12	[20]	208.2 ± 0.4	211.9 ± 0.5
146. phenoxybenzene	303.15			262.9 ± 0.3	270.1 ± 0.6

Table S10: Classical heat capacity at constant pressure c_P^{class} (J/mol K) calculated and experimental. Blue font indicates that the calculated value differs more than 25% from the experimental ones, a red font indicates that it differs by more than 50%. The temperature in the calculations is noted in case it deviates from the one used in experiments.

	Experiment			GAFF	OPLS/AA
Name	T	c_P	Ref.	c_P^{class}	c_P^{class}
1. chloroform	298.15	117.00	[9]	140 ± 2	154 ± 4
2. dichloro(fluoro)methane	282.05	107.07	[13]	140 ± 2	137 ± 2
3. dibromomethane	293.15	104.62	[13]	126 ± 2	135 ± 1
...	298.15	104.90	[9]	121 ± 2	134 ± 2
4. dichloromethane	293.15	100.51	[13]	121 ± 1	123 ± 2
...	298.15	100.88	[13]	120 ± 2	133 ± 2
5. methanal	253.15	79.68	[22]	**226 ± 4**	94 ± 1
...	253.65	79.78	[22]	**230 ± 3**	94 ± 1
6. methanoic acid	293.15	99.03	[13]	**150 ± 2**	130 ± 2
...	298.15	99.00	[9]	140 ± 3	125 ± 2
7. bromomethane	276.65	78.75	[13]	**123 ± 1**	**119 ± 1**
8. methanamide	298.15	107.60	[9]	153 ± 2	**202 ± 3**
9. nitromethane	293.15	106.26	[13]	**163 ± 2**	155 ± 3
...	298.15	105.80	[9]	154 ± 2	157 ± 1
10. methanol	293.15	80.22	[13]	**142 ± 3**	**150 ± 2**
...	298.15	81.47	[9]	**142 ± 2**	**148 ± 2**
11. 1,1,1,2,2-pentachloroethane	293.15	173.96	[22]	190 ± 2	213 ± 2
12. 1,1,2,2-tetrachloroethane	293.15			193 ± 2	200 ± 3
...	298.15	165.70	[9]	193 ± 2	205 ± 4
13. 1,1-dichloroethene	293.15	110.53	[13]	**206 ± 3**	152 ± 2
...	298.15	111.33	[13]	**210 ± 3**	160 ± 2
14. 1,1,2-trichloroethane	293.15	150.05	[13]	190 ± 2	193 ± 3
...	298.15	148.50	[9]	197 ± 2	192 ± 3
15. acetonitrile	293.15	91.05	[13]	134 ± 2	125 ± 1
...	298.15	91.40	[9]	136 ± 2	123 ± 2
16. 1,2-dibromoethane	298.15	136.00	[9]	182 ± 3	203 ± 3
17. 1,1-dichloroethane	293.15	126.10	[13]	180 ± 2	183 ± 3
...	298.15	126.20	[9]	183 ± 3	172 ± 3
18. 1,2-dichloroethane	298.15	128.90	[9]	187 ± 2	189 ± 3
19. methyl formate	293.15	118.10	[13]	**187 ± 2**	170 ± 3
...	298.15	119.70	[9]	**191 ± 3**	176 ± 3

Table S10: Classical heat capacity at constant pressure - continued

Name	Experiment T	Experiment c_P	Ref.	GAFF c_P^{class}	OPLS/AA c_P^{class}
20. bromoethane	293.15	99.04	[13]	**178 ± 2**	**177 ± 4**
...	298.15	99.73	[13]	**174 ± 4**	**177 ± 2**
21. chloroethane	273.15	101.18	[13]	**177 ± 3**	**172 ± 3**
...	285.45	102.80	[13]	**175 ± 1**	**179 ± 2**
22. 2-chloroethanol	293.15	109.03	[13]	**232 ± 3**	**234 ± 3**
23. ethanamide	358.15	148.39	[13]	220 ± 4	**246 ± 4**
...	494.30	165.92	[13]	214 ± 2	201 ± 3
24. N-methylformamide	292.15			210 ± 5	208 ± 4
...	298.15	123.80	[9]	**212 ± 4**	**205 ± 2**
25. nitroethane	298.15	138.50	[9]	**220 ± 2**	**216 ± 5**
26. methoxymethane	240.00	102.17	[13]	**192 ± 4**	**202 ± 3**
27. ethanol	293.15	110.46	[13]	**206 ± 5**	**211 ± 5**
...	298.15	112.30	[9]	**209 ± 3**	**220 ± 4**
28. 1,2-ethanedithiol	293.15			228 ± 3	227 ± 3
...	298.15			230 ± 4	224 ± 4
29. methyldisulfanylmethane	293.15	145.55	[13]	**225 ± 4**	**219 ± 4**
...	298.15	145.96	[13]	**225 ± 3**	**221 ± 4**
30. methylsulfinylmethane	298.15	153.10	[9]	**235 ± 4**	**235 ± 2**
31. methylsulfanylmethane	293.15	117.60	[13]	**207 ± 3**	**199 ± 3**
...	298.15	118.10	[9]	**203 ± 3**	**202 ± 5**
32. 2-aminoethanol	293.15			284 ± 7	293 ± 4
...	320.00	164.75	[13]	**285 ± 8**	**286 ± 3**
33. ethane-1,2-diamine	293.15	172.24	[13]	**337 ± 9**	**333 ± 8**
...	298.15	172.50	[9]	**329 ± 9**	**333 ± 5**
34. prop-2-enenitrile	298.15	108.60	[9]	**205 ± 3**	130 ± 2
...	350.45	114.98	[13]	**198 ± 3**	135 ± 1
35. 1,3-dioxolan-2-one	312.15	133.84	[13]	**224 ± 4**	**208 ± 4**
36. propanenitrile	293.15	118.88	[13]	**201 ± 3**	**181 ± 3**
...	298.15	119.70	[9]	**201 ± 4**	**186 ± 3**
37. 1,2-dibromopropane	293.15	172.20	[22]	238 ± 4	253 ± 6
...	298.15	172.80	[22]	235 ± 4	250 ± 5
38. 1,3-dichloropropane	298.15	159.45	[13]	**240 ± 3**	**243 ± 3**

Table S10: Classical heat capacity at constant pressure - continued

Name	Experiment T	Experiment c_P	Experiment Ref.	GAFF c_P^{class}	OPLS/AA c_P^{class}
39. (2R)-2-methyloxirane	298.15			213 ± 4	203 ± 4
40. propan-2-one	298.15	124.90	[9]	**207 ± 3**	**195 ± 3**
41. methyl acetate	293.15	140.67	[13]	**240 ± 4**	**232 ± 4**
...	298.15	143.90	[9]	**244 ± 4**	**229 ± 4**
42. 1,3-dioxolane	293.15	120.32	[23]	**225 ± 3**	**225 ± 3**
...	298.15	118.00	[11]	**230 ± 4**	**235 ± 4**
43. 2-iodopropane	293.15	138.41	[13]	**230 ± 5**	**233 ± 3**
...	298.15	139.72	[13]	**221 ± 3**	**242 ± 5**
44. 1-bromopropane	293.15	132.65	[13]	**232 ± 4**	**238 ± 5**
...	298.15	133.47	[13]	**236 ± 3**	**231 ± 4**
45. N,N-dimethylformamide	298.15	148.30	[9]	**251 ± 6**	**247 ± 3**
46. N-methylacetamide	320.00			269 ± 5	274 ± 6
47. 1-nitropropane	298.15	175.30	[9]	**287 ± 6**	**277 ± 4**
48. 2-nitropropane	298.15	170.20	[9]	**284 ± 6**	**269 ± 4**
49. dimethoxymethane	293.15	160.40	[13]	**278 ± 4**	**287 ± 5**
...	298.15	161.50	[13]	**291 ± 6**	**277 ± 4**
50. propane-1,2,3-triol	293.15	216.70	[22]	290 ± 6	285 ± 5
...	320.00	229.32	[22]	**556 ± 6**	**353 ± 13**
51. propan-1-amine	293.15	162.40	[13]	**318 ± 9**	**319 ± 7**
...	298.15	162.79	[13]	**319 ± 7**	**325 ± 3**
52. propan-2-amine	293.15	163.27	[13]	**320 ± 4**	**321 ± 7**
...	298.15	163.81	[13]	**305 ± 5**	**324 ± 6**
53. 2-methylpropane	243.65	125.50	[13]	**283 ± 4**	**300 ± 9**
54. ethylsulfanylethane	293.15	170.32	[13]	**315 ± 10**	**312 ± 4**
...	298.15	171.40	[9]	**321 ± 10**	**320 ± 7**
55. butane-1-thiol	293.15			322 ± 5	314 ± 7
...	298.15	171.20	[11]	**325 ± 7**	**312 ± 7**
56. butan-1-ol	293.15	174.72	[13]	**319 ± 7**	**350 ± 4**
...	298.15	177.00	[9]	**323 ± 5**	**341 ± 8**
57. 2-methylpropan-2-ol	320.00	238.62	[13]	**395 ± 8**	**366 ± 7**
58. butane-1,4-diol	293.15	172.42	[13]	**408 ± 18**	**394 ± 9**
...	298.15	202.20	[9]	**371 ± 11**	**366 ± 7**
...	320.00	200.66	[13]	**364 ± 11**	**375 ± 12**

Table S10: Classical heat capacity at constant pressure - continued

Name	Experiment T	Experiment c_P	Experiment Ref.	GAFF c_P^{class}	OPLS/AA c_P^{class}
59. (2-hydroxyethoxy)ethan-2-ol	288.15	256.39	[22]	338 ± 9	**405 ± 13**
60. N-ethylethanamine	293.15	172.62	[13]	**367 ± 7**	**386 ± 6**
...	298.15	176.70	[9]	**366 ± 6**	**380 ± 4**
61. butan-1-amine	293.15	192.12	[13]	**400 ± 7**	**386 ± 6**
...	298.15	188.00	[9]	**406 ± 11**	**399 ± 10**
62. 2-methylpropan-2-amine	293.15	191.36	[13]	**383 ± 10**	**392 ± 8**
...	298.15	192.10	[13]	**359 ± 9**	**380 ± 7**
63. 2-(2-hydroxyethylamino)ethanol	320.00	275.72	[13]	387 ± 7	**439 ± 11**
64. pyrimidine	298.15	133.70	[9]	**222 ± 4**	**222 ± 3**
65. furan	293.15	113.61	[13]	**195 ± 4**	**188 ± 2**
...	298.15	114.80	[9]	**193 ± 4**	**190 ± 4**
66. thiophene	293.15	123.13	[13]	**196 ± 3**	**192 ± 4**
...	298.15	123.98	[13]	**196 ± 3**	**190 ± 2**
67. 1H-pyrrole	293.15	126.58	[13]	**315 ± 5**	**223 ± 5**
...	298.15	128.20	[9]	**322 ± 5**	**215 ± 4**
68. ethenyl acetate	298.15	171.47	[13]	**354 ± 6**	252 ± 5
69. oxolan-2-one	293.15	139.96	[22]	**253 ± 4**	**240 ± 4**
70. acetyl acetate	293.15	189.13	[13]	**293 ± 5**	**284 ± 3**
71. 1,4-dichlorobutane	298.15	189.23	[13]	**304 ± 5**	**309 ± 5**
72. oxolane	298.15	123.90	[9]	**261 ± 5**	**266 ± 5**
73. ethoxyethene	293.15	153.58	[13]	**355 ± 5**	**286 ± 4**
74. ethyl acetate	293.15	169.57	[13]	**314 ± 8**	**299 ± 6**
...	298.15	167.70	[9]	**311 ± 8**	**293 ± 7**
75. tetrahydrothiophene 1,1-dioxide	320.00	185.91	[13]	**331 ± 8**	**312 ± 4**
76. thiolane	293.15	138.69	[13]	**267 ± 4**	**262 ± 5**
...	298.15	139.80	[9]	**256 ± 4**	**268 ± 4**
77. 1-bromobutane	293.15	161.24	[13]	**304 ± 9**	**300 ± 6**
...	298.15	168.10	[9]	**305 ± 10**	**306 ± 5**
78. 1-chlorobutane	293.15			293 ± 4	293 ± 4
...	298.15	174.60	[9]	**301 ± 6**	**311 ± 5**
79. pyrrolidine	293.15	156.19	[13]	**324 ± 7**	**334 ± 5**
...	298.15	156.50	[9]	**303 ± 6**	**319 ± 5**

Table S10: Classical heat capacity at constant pressure - continued

Name	Experiment T	Experiment c_P	Ref.	GAFF c_P^{class}	OPLS/AA c_P^{class}
80. N,N-dimethylacetamide	298.15	176.00	[9]	**329 ± 6**	**309 ± 8**
81. morpholine	293.15	173.88	[13]	**334 ± 12**	**336 ± 9**
82. pyridine	293.15	131.65	[13]	**232 ± 5**	**226 ± 4**
...	298.15	135.60	[9]	**234 ± 6**	**232 ± 2**
83. cyclopentanone	293.15	148.02	[13]	**286 ± 4**	**274 ± 5**
...	298.15	154.50	[9]	**286 ± 6**	**288 ± 9**
84. 1-cyclopropylethanone	293.15			300 ± 5	358 ± 7
...	298.15			299 ± 5	385 ± 11
85. pentane-2,4-dione	298.15	208.20	[9]	**318 ± 5**	**326 ± 6**
86. methyl 2-methylprop-2-enoate	298.15	189.82	[13]	**354 ± 5**	**317 ± 6**
87. pentanenitrile	293.15	188.51	[13]	**316 ± 7**	**306 ± 5**
...	298.15	189.70	[9]	**306 ± 4**	**307 ± 5**
88. ethyl propanoate	298.15	196.10	[9]	**383 ± 7**	**363 ± 5**
89. diethyl carbonate	298.15	212.40	[9]	**386 ± 4**	**386 ± 7**
90. pentan-1-ol	293.15	205.78	[13]	**378 ± 8**	**419 ± 10**
...	298.15	208.90	[9]	**382 ± 11**	**407 ± 6**
...	320.00	225.74	[13]	**409 ± 6**	**420 ± 5**
91. pentan-3-ol	293.15	242.82	[13]	**435 ± 16**	**442 ± 7**
...	298.15	247.72	[13]	**446 ± 14**	**481 ± 10**
92. 2-methylbutan-2-ol	293.15	243.36	[13]	**383 ± 8**	**436 ± 5**
...	298.15	244.30	[9]	**378 ± 10**	**433 ± 8**
...	320.00	269.99	[13]	394 ± 8	**451 ± 8**
93. pentane-1,5-diol	293.15	224.40	[13]	**419 ± 8**	**417 ± 10**
...	298.15	225.50	[9]	**407 ± 11**	**484 ± 11**
94. pentan-3-amine	293.15	203.80	[22]	**437 ± 11**	**429 ± 6**
...	298.15	205.13	[22]	**448 ± 13**	**435 ± 8**
95. 1,2,3,4-tetrafluorobenzene	298.15	190.06	[23]	265 ± 4	270 ± 3
96. 1,2,3,5-tetrafluorobenzene	298.15	190.19	[23]	276 ± 6	**289 ± 4**
97. 1,3-difluorobenzene	293.15			263 ± 6	265 ± 3
...	298.15	159.10	[11]	**249 ± 3**	**260 ± 3**
98. 1,2-difluorobenzene	293.15			267 ± 5	269 ± 6
...	298.15	159.00	[11]	**249 ± 3**	**272 ± 7**

Table S10: Classical heat capacity at constant pressure - continued

Name	Experiment T	Experiment c_P	Experiment Ref.	GAFF c_P^{class}	OPLS/AA c_P^{class}
99. fluorobenzene	293.15	146.29	[13]	**265 ± 4**	**231 ± 5**
...	298.15	146.30	[9]	**247 ± 5**	**230 ± 3**
100. nitrobenzene	293.15	180.71	[13]	**312 ± 6**	**294 ± 4**
...	298.15	177.20	[9]	**304 ± 4**	**296 ± 6**
101. 2-chloroaniline	293.15	196.88	[13]	**321 ± 9**	**331 ± 6**
102. phenol	318.15	202.77	[13]	299 ± 4	**305 ± 7**
103. benzenethiol	293.15	172.65	[13]	**292 ± 3**	**277 ± 7**
...	298.15	173.55	[13]	**287 ± 6**	**277 ± 6**
104. 2-methylpyridine	293.15	157.42	[13]	**296 ± 6**	**289 ± 8**
...	298.15	159.20	[9]	**275 ± 6**	**281 ± 5**
105. 3-methylpyridine	293.15	157.68	[13]	**279 ± 3**	**281 ± 5**
...	298.15	159.00	[9]	**282 ± 5**	**291 ± 6**
106. 4-methylpyridine	293.15	157.83	[13]	**291 ± 5**	**288 ± 5**
...	298.15	159.00	[9]	**281 ± 5**	**283 ± 7**
107. cyclohexanone	293.15	182.28	[13]	**346 ± 10**	**338 ± 7**
...	298.15	179.30	[9]	**362 ± 9**	**363 ± 9**
108. (E)-hex-2-ene	293.15			359 ± 6	358 ± 6
109. hexan-2-one	298.15	213.17	[13]	**402 ± 6**	**398 ± 6**
110. 2,4,6-trimethyl-1,3,5-trioxane	293.15	255.56	[13]	374 ± 8	**418 ± 11**
111. cyclohexanamine	298.15	200.84	[22]	**475 ± 9**	**453 ± 13**
112. 2-propan-2-yloxypropane	298.15	216.10	[9]	**444 ± 13**	**432 ± 11**
113. 1-methoxy-2-(2-methoxyethoxy)ethane	293.15	273.08	[13]	**552 ± 10**	**529 ± 16**
...	298.15	226.00	[9]	**544 ± 10**	**541 ± 13**
114. triethyl phosphate	293.15			625 ± 19	539 ± 12
...	298.15			522 ± 14	557 ± 18
...	320.00			544 ± 11	544 ± 11
115. N,N-diethylethanamine	293.15	219.40	[13]	**450 ± 8**	**463 ± 13**
...	298.15	224.40	[9]	**447 ± 9**	**451 ± 6**
116. N-propan-2-ylpropan-2-amine	293.15	224.21	[13]	**448 ± 8**	**476 ± 11**
...	298.15	226.35	[13]	**458 ± 14**	**465 ± 11**
117. trifluoromethylbenzene	293.15	187.08	[13]	**322 ± 9**	**290 ± 9**
...	298.15	188.80	[13]	**316 ± 10**	**312 ± 5**

Table S10: Classical heat capacity at constant pressure - continued

Name	Experiment T	Experiment c_P	Experiment Ref.	GAFF c_P^{class}	OPLS/AA c_P^{class}
118. benzonitrile	288.15	163.00	[13]	**294 ± 7**	**248 ± 3**
119. benzaldehyde	298.15	172.00	[9]	**291 ± 7**	**289 ± 4**
120. toluene	298.15	157.20	[9]	**309 ± 8**	**292 ± 6**
121. methoxybenzene	293.15			339 ± 4	335 ± 4
...	298.15	208.60	[9]	**338 ± 9**	**333 ± 6**
122. phenylmethanol	297.15	216.44	[13]	**349 ± 6**	**378 ± 8**
123. 2-methylphenol	308.15	234.03	[13]	**361 ± 10**	**372 ± 13**
124. 3-methylphenol	320.00	233.79	[13]	**356 ± 6**	**380 ± 11**
125. 4-methylphenol	313.15	229.41	[13]	**348 ± 6**	**359 ± 13**
...	320.00	232.03	[13]	**355 ± 6**	**355 ± 7**
126. diethyl propanedioate	293.15	284.24	[13]	**501 ± 12**	**506 ± 11**
127. 2,4-dimethylpentan-3-one	293.15	233.78	[13]	**460 ± 8**	**457 ± 10**
...	298.15	235.51	[13]	**460 ± 5**	**442 ± 9**
128. heptan-2-one	293.15	241.05	[13]	**489 ± 12**	**465 ± 4**
...	298.15	243.60	[9]	**467 ± 6**	**455 ± 8**
129. ethenylbenzene	298.15	182.50	[9]	**331 ± 8**	**333 ± 8**
130. 1-phenylethanone	293.15			393 ± 7	356 ± 7
...	298.15	204.60	[9]	**392 ± 8**	**360 ± 6**
131. methyl benzoate	298.15	221.30	[9]	**368 ± 8**	**380 ± 9**
132. methyl 2-hydroxybenzoate	298.15	247.51	[13]	**401 ± 10**	**397 ± 10**
...	320.00	262.63	[13]	**421 ± 13**	**409 ± 9**
133. ethylbenzene	298.15	185.50	[9]	**372 ± 7**	**366 ± 8**
134. 1,2-dimethylbenzene	293.15	184.85	[13]	**348 ± 7**	**358 ± 7**
...	298.15	188.00	[9]	**362 ± 11**	**360 ± 11**
135. 1,2-dimethoxybenzene	298.15			441 ± 4	435 ± 6
136. 2,4,6-trimethylpyridine	295.15	213.05	[13]	**379 ± 12**	**390 ± 12**
...	298.15	214.00	[9]	**394 ± 9**	**385 ± 6**
137. octan-1-ol	298.15	305.50	[9]	**561 ± 11**	**607 ± 13**
...	320.00	333.97	[13]	**624 ± 19**	**773 ± 22**
138. 1-butoxybutane	293.15	276.56	[13]	**580 ± 11**	**562 ± 11**
...	298.15	251.90	[9]	**563 ± 16**	**561 ± 12**
139. N-butylbutan-1-amine	293.15			590 ± 14	632 ± 12
...	298.15	292.80	[9]	**612 ± 10**	**611 ± 9**

Table S10: Classical heat capacity at constant pressure - continued

	Experiment			GAFF	OPLS/AA
Name	T	c_P	Ref.	c_P^{class}	c_P^{class}
140. isoquinoline	303.15	197.45	[13]	**340 ± 8**	**319 ± 4**
...	320.00	203.57	[13]	**359 ± 6**	**378 ± 9**
141. quinoline	288.15	191.49	[13]	**369 ± 6**	**346 ± 6**
...	298.15	200.00	[9]	**362 ± 9**	**353 ± 9**
142. (1-methylethyl)benzene	298.15	198.90	[9]	**422 ± 10**	**407 ± 7**
143. 1,2,4-trimethylbenzene	293.15	213.10	[13]	**423 ± 15**	**413 ± 9**
...	298.15	214.94	[13]	**424 ± 13**	**413 ± 9**
144. 2,6-dimethylheptan-4-one	293.15			570 ± 13	558 ± 12
...	298.15	297.30	[11]	**552 ± 12**	**575 ± 18**
145. 1-chloronaphthalene	298.15	222.14	[13]	**357 ± 7**	**387 ± 11**
146. phenoxybenzene	303.15	269.87	[13]	**504 ± 15**	**445 ± 11**

4 Polynomial Fits to Experimental Data

Figure S2: (part 1) Polynomial curves fitted to dielectric constant measurements for different molecules. For parameters see Table 4 in the main text.

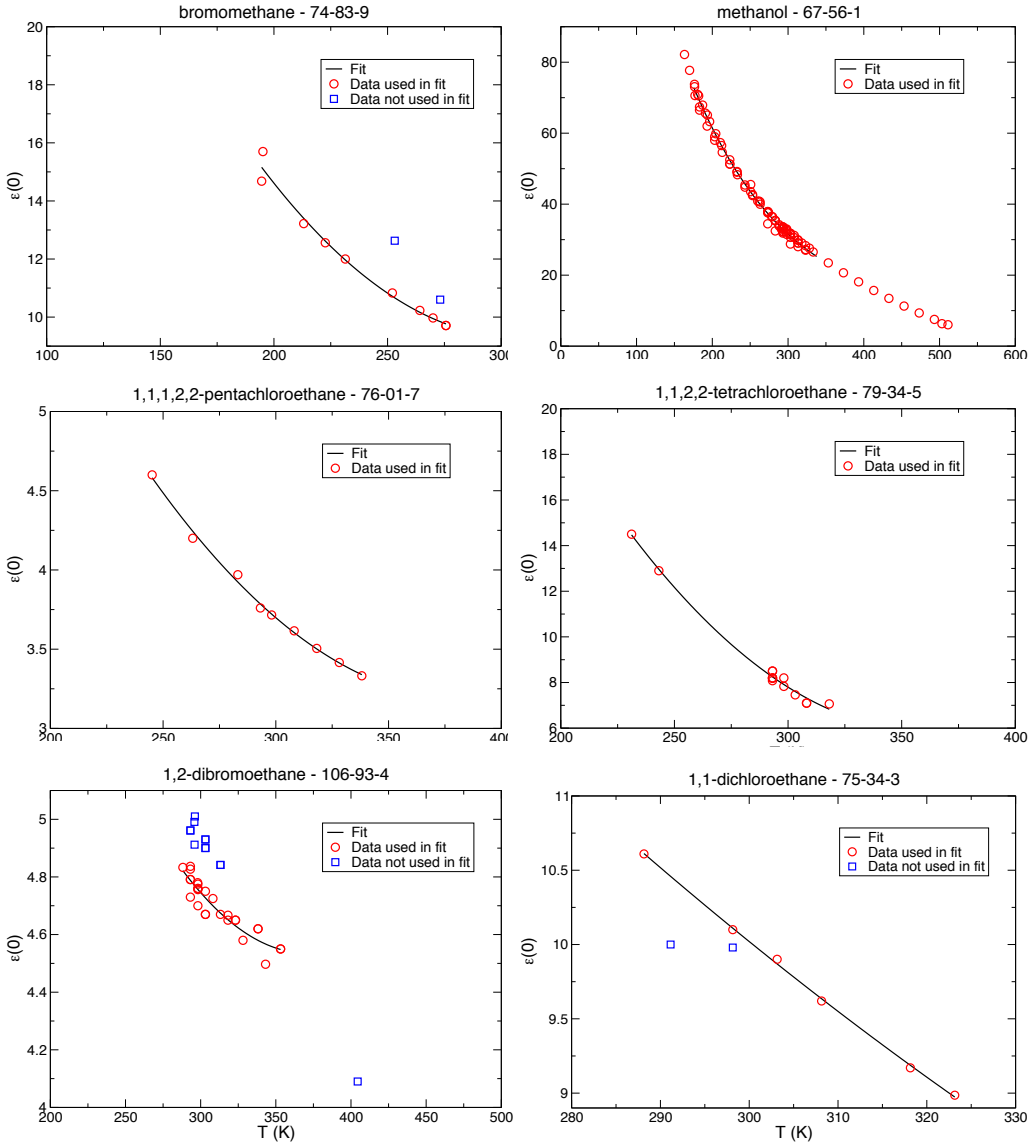

Figure S2: (part 2) Polynomial curves fitted to dielectric constant measurements for different molecules. For parameters see Table 4 in the main text.

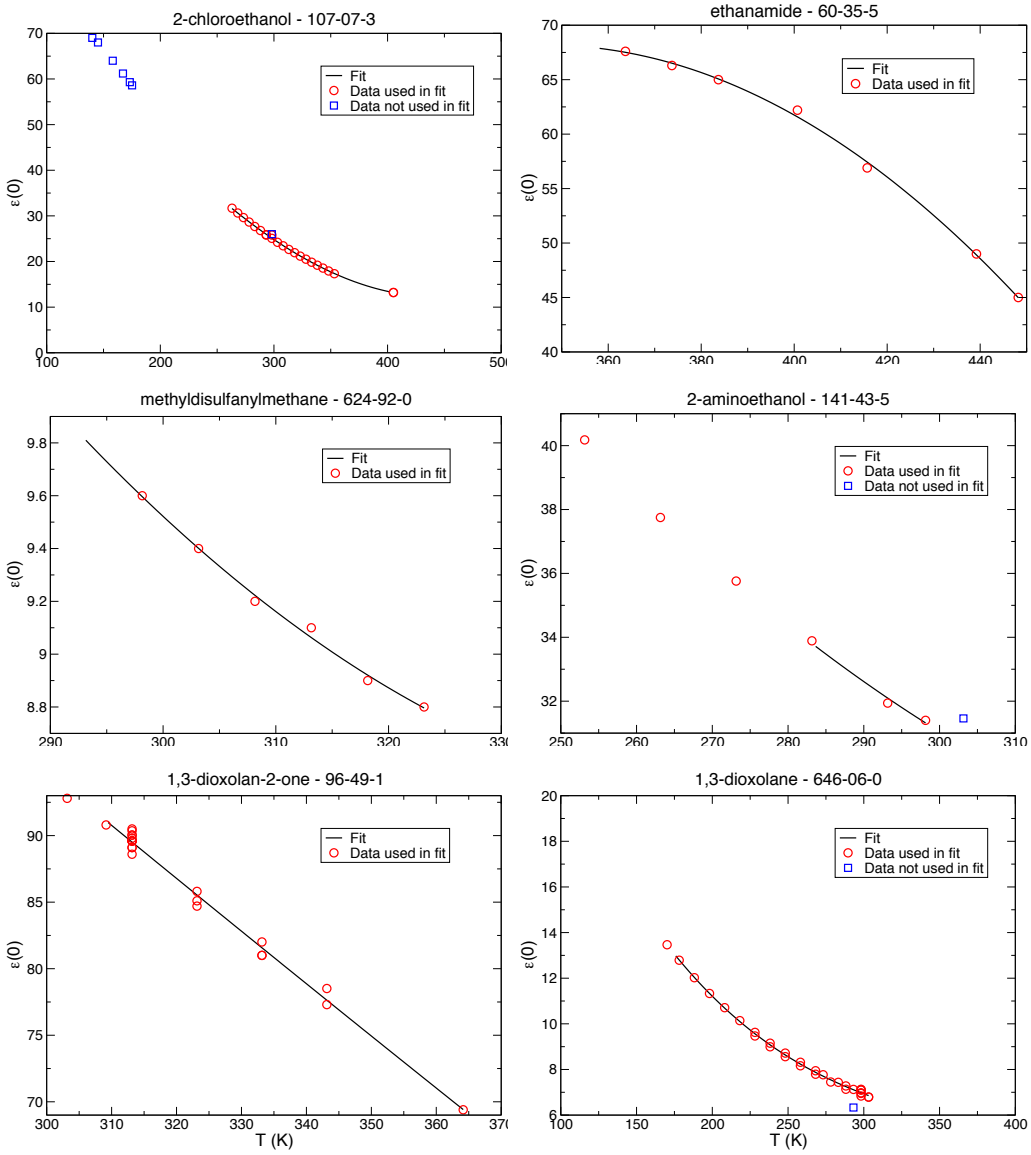

Figure S2: (part 3) Polynomial curves fitted to dielectric constant measurements for different molecules. For parameters see Table 4 in the main text.

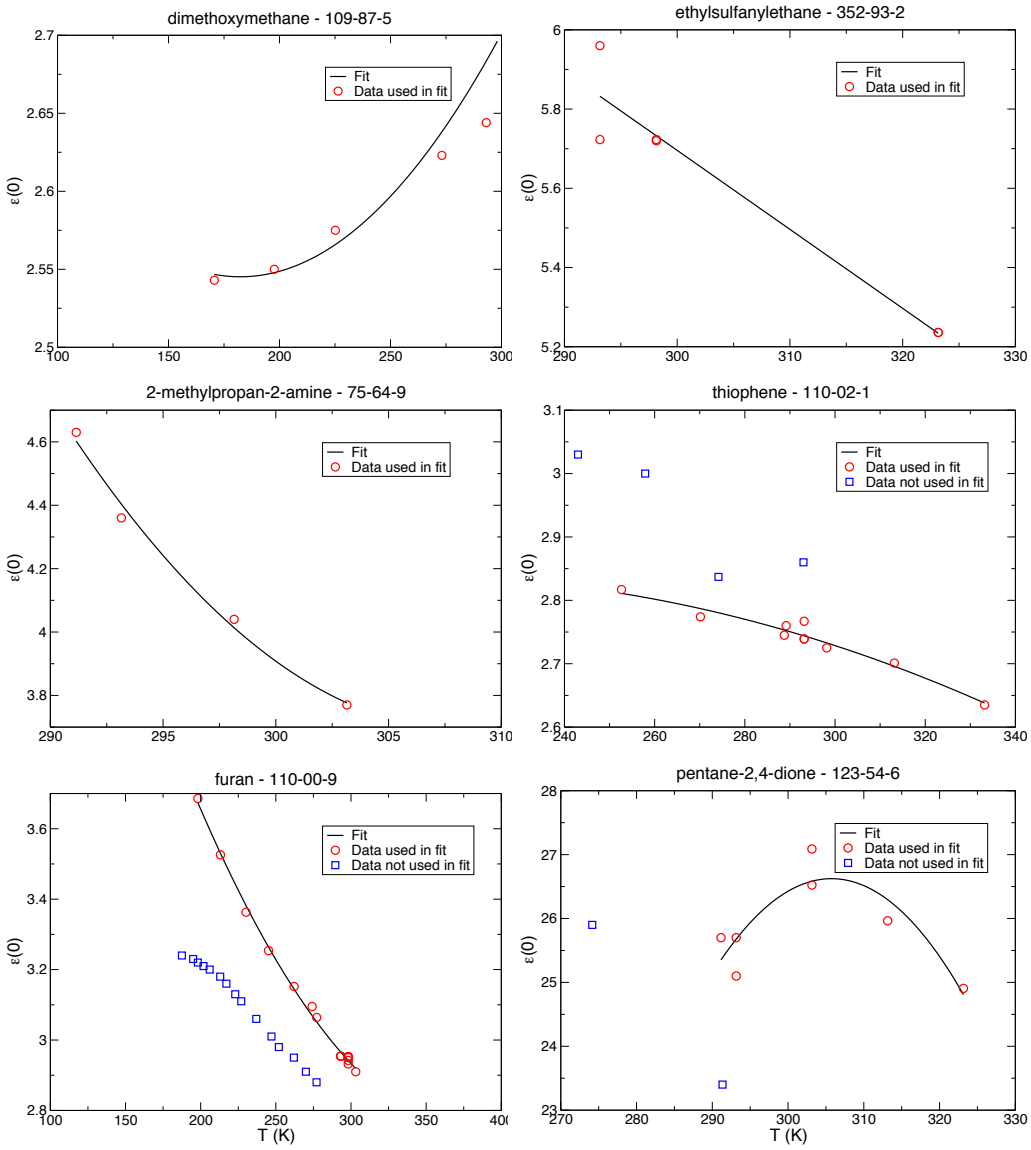

Figure S2: (part 4) Polynomial curves fitted to dielectric constant measurements for different molecules. For parameters see Table 4 in the main text.

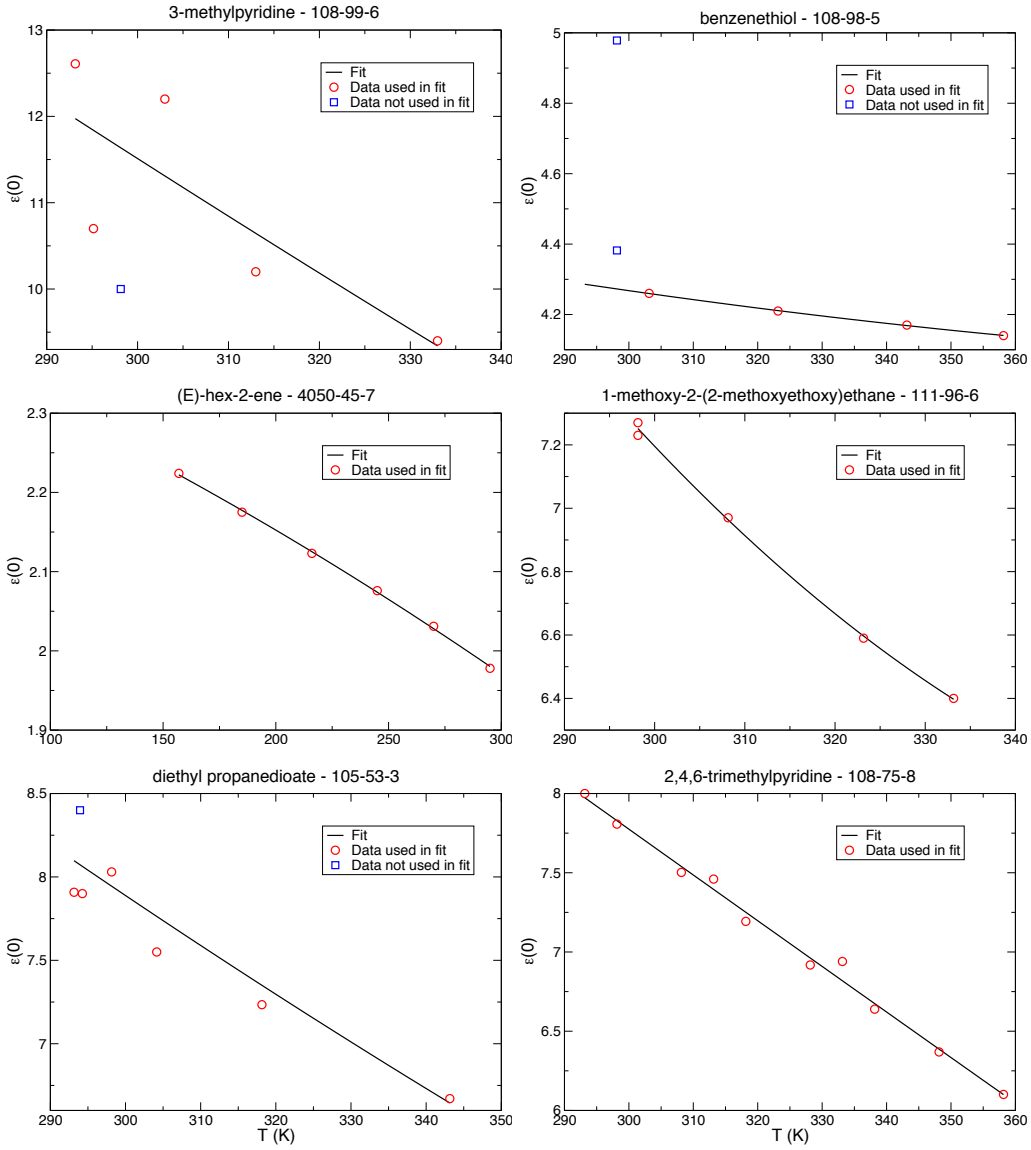

Figure S2: (part 5) Polynomial curves fitted to dielectric constant measurements for different molecules. For parameters see Table 4 in the main text.

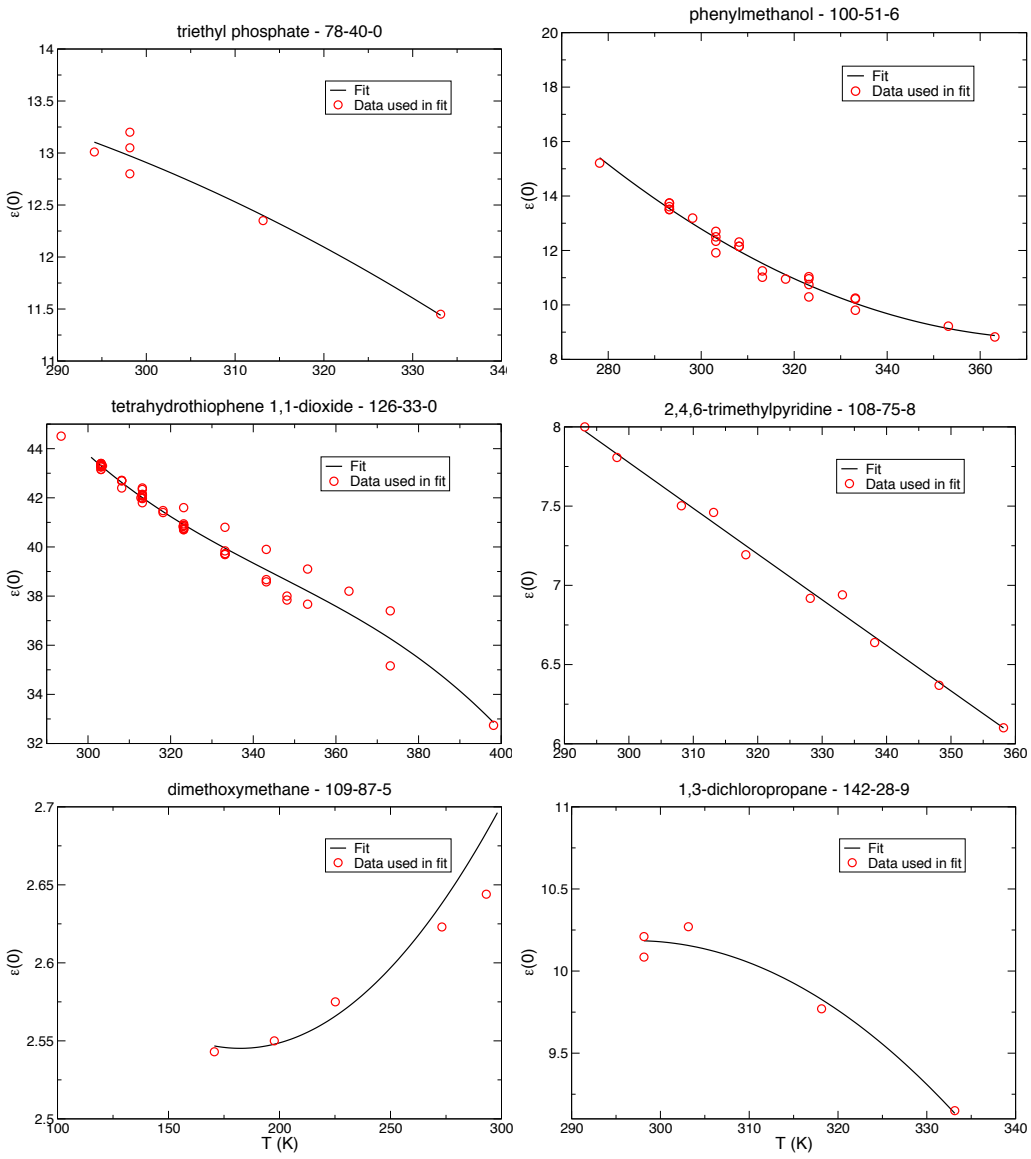

Figure S2: (part 6) Polynomial curves fitted to dielectric constant measurements for different molecules. For parameters see Table 4 in the main text.

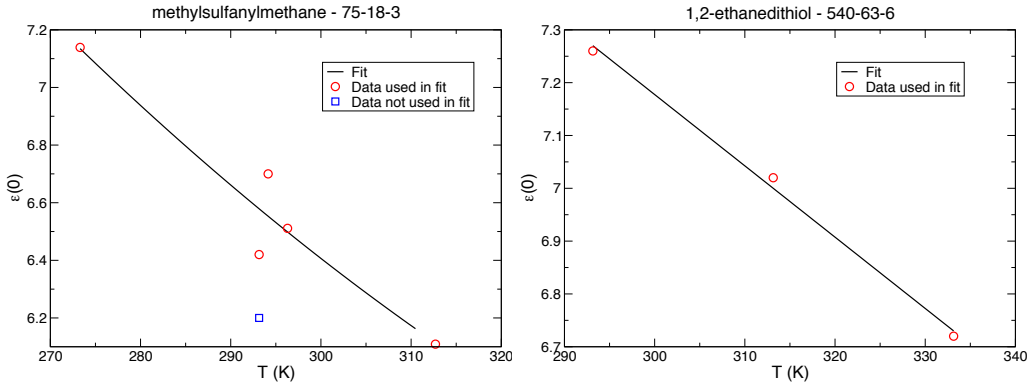

Table S11: References used for deriving fits of dielectric constants as a function of temperature to experimental data.

Molecule	References
ethylsulfanylethane	[19]
1,1-dichloroethane	[19]
2-aminoethanol	[24, 19, 25]
furan	[19, 26, 27, 28, 29]
2-chloroethanol	[30, 19, 31]
benzenethiol	[19, 32]
2,4,6-trimethylpyridine	[19]
1-methoxy-2-(2-methoxyethoxy)ethane	[19]
bromomethane	[19]
1,3-dioxolan-2-one	[19, 30, 23]
1,2-dibromoethane	[19, 23]
methanol	[19]
triethyl phosphate	[19]
2-methylpropan-2-amine	[19]
1,3-dichloropropane	[19, 33]
1,3-dioxolane	[34, 23, 35, 36, 37]
1,1,1,2,2-pentachloroethane	[19]
thiophene	[19]
dimethoxymethane	[19]
phenylmethanol	[19]
1,1,2,2-tetrachloroethane	[19, 23]
ethanamide	[19]
(E)-hex-2-ene	[19]
pentane-2,4-dione	[38, 39, 19, 40, 41, 42]
methylsulfanylmethane	[19, 23, 43]
1,2-ethanedithiol	[19]
diethyl propanedioate	[30, 44, 45]
methyldisulfanylmethane	[19]
3-methylpyridine	[32, 46, 19]
tetrahydrothiophene 1,1-dioxide	[19]

Figure S3: (part 1) Polynomial curves fitted to heat capacity at constant pressure measurements for different molecules. For parameters see Table 5 in the main text.

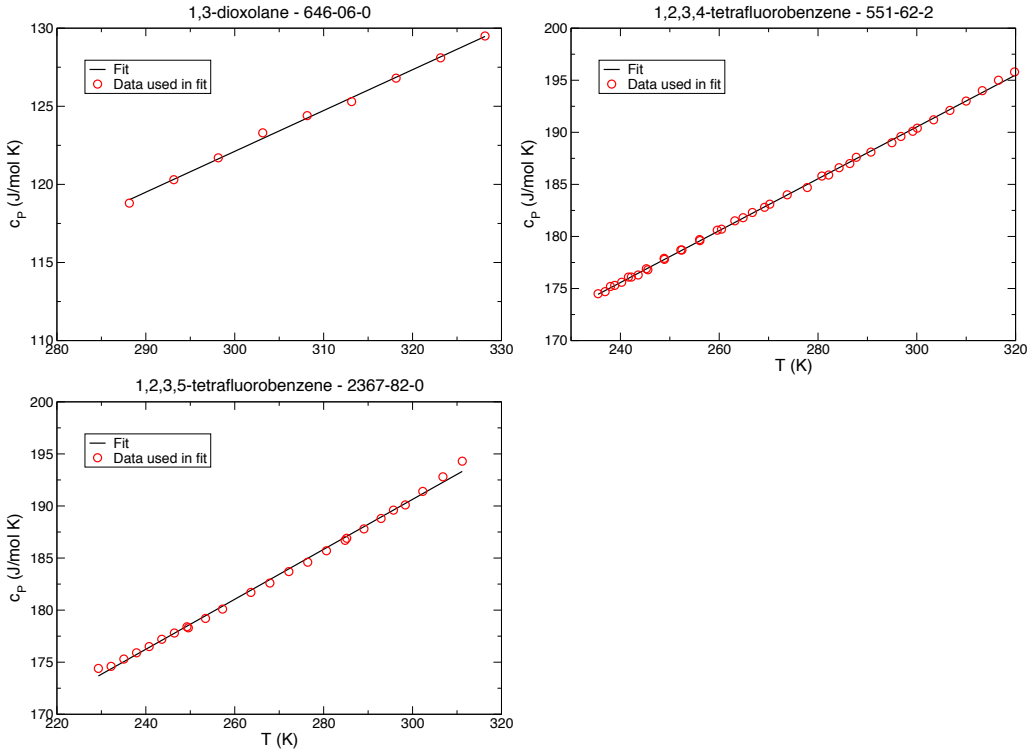

Table S12: References used for deriving fits of isothermal compressibilities as a function of temperature to experimental data.

Molecule	References
1,3-dioxolane	[23]
1,2,3,5-tetrafluorobenzene	[23]
1,2,3,4-tetrafluorobenzene	[23]

Figure S4: (part 1) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

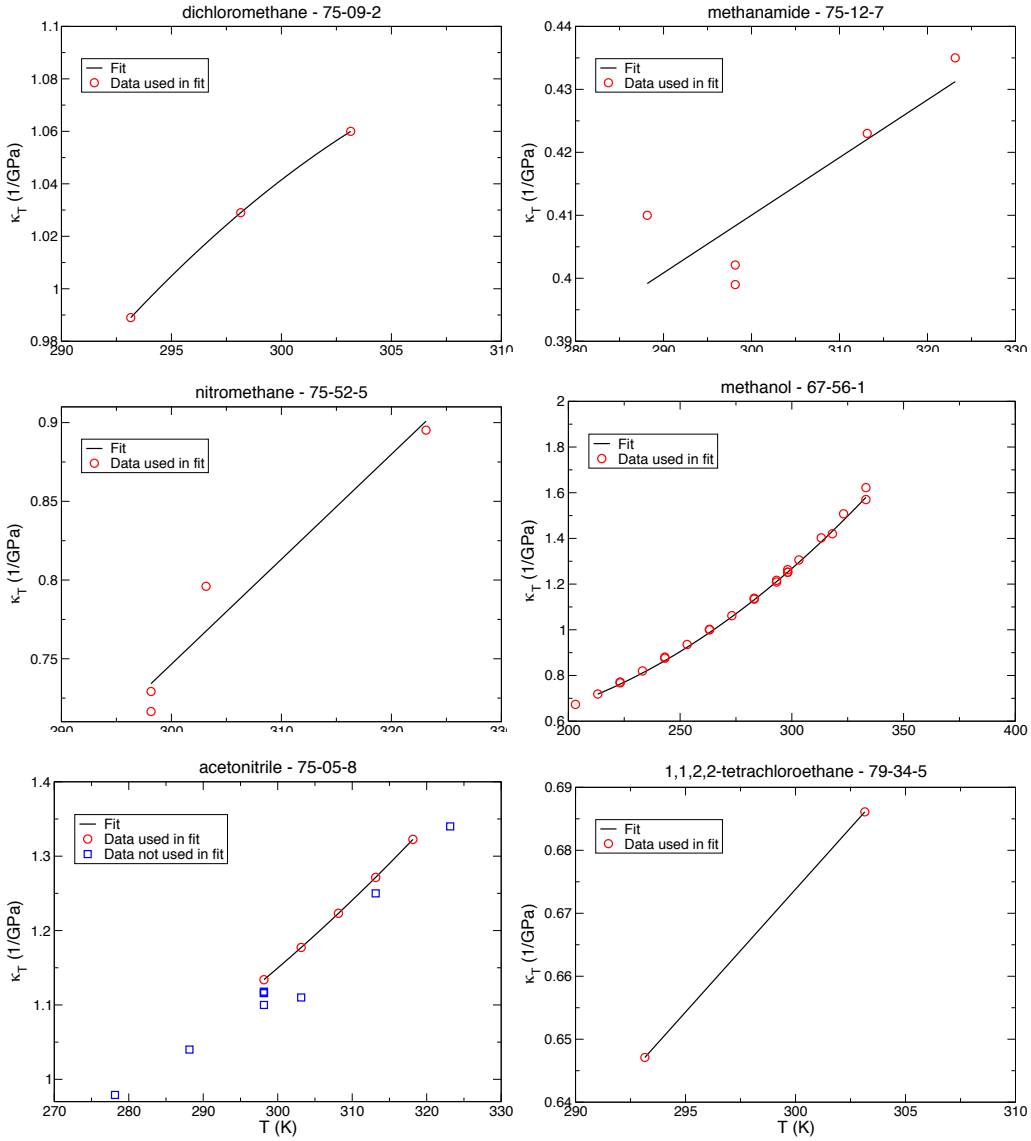

Figure S4: (part 2) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

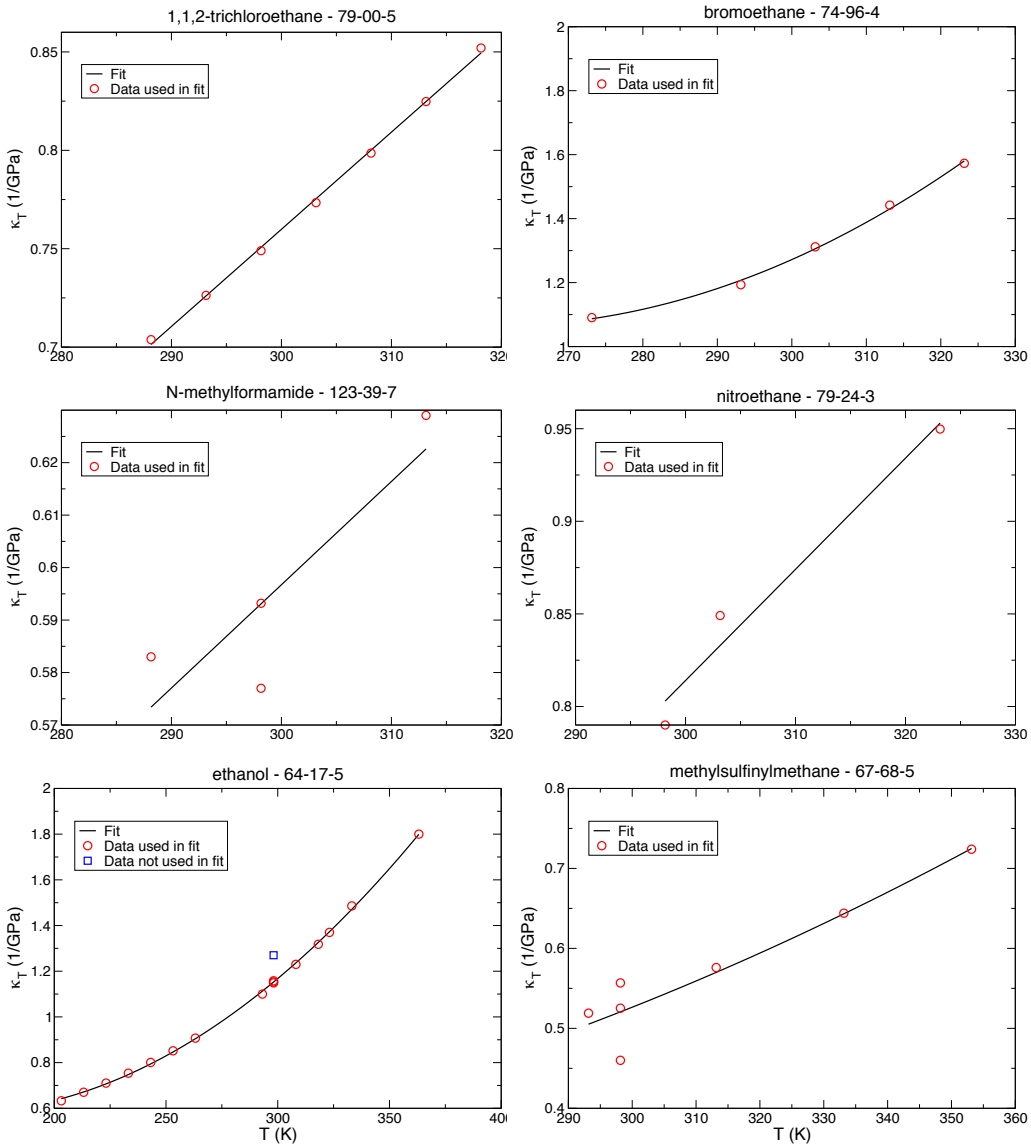

Figure S4: (part 3) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

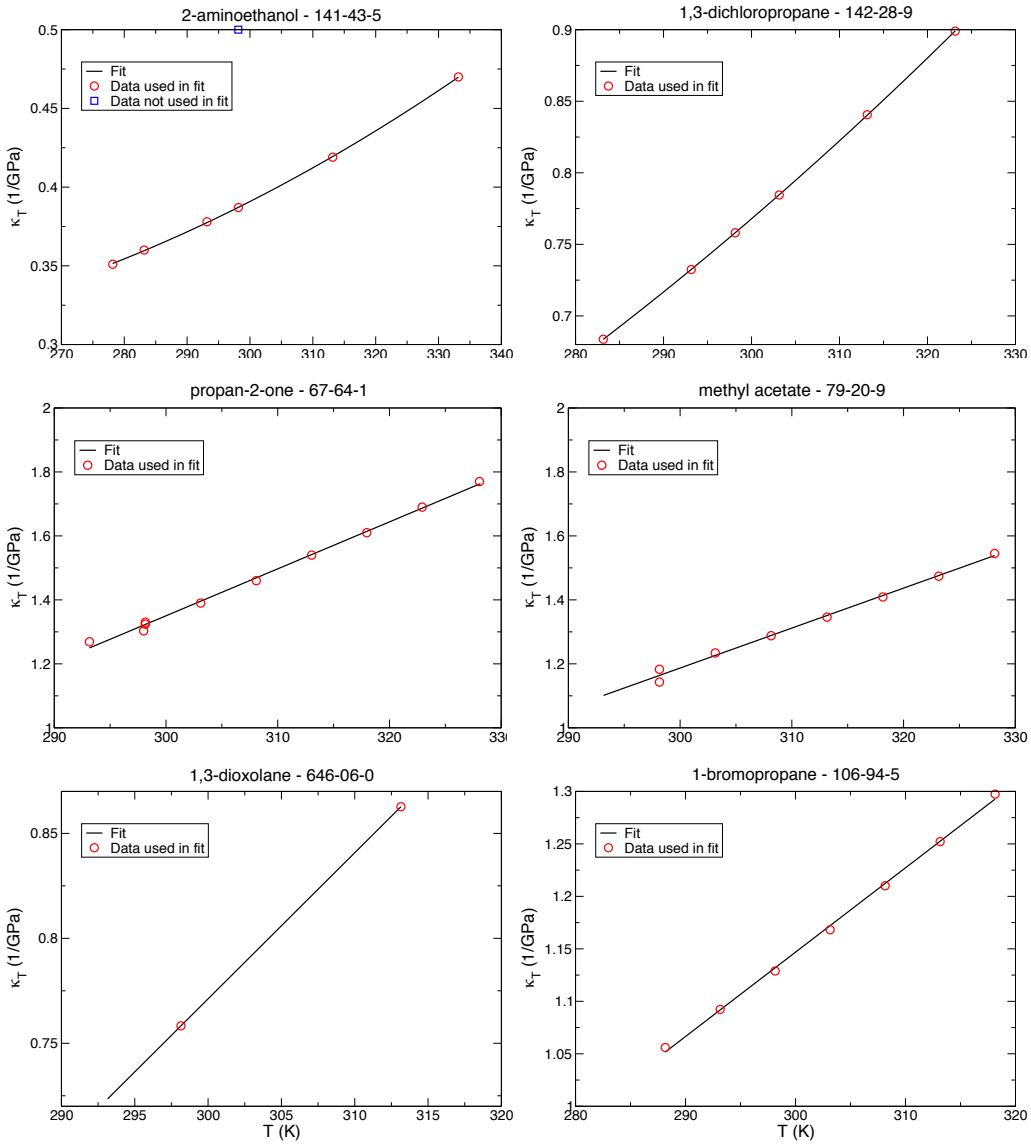

Figure S4: (part 4) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

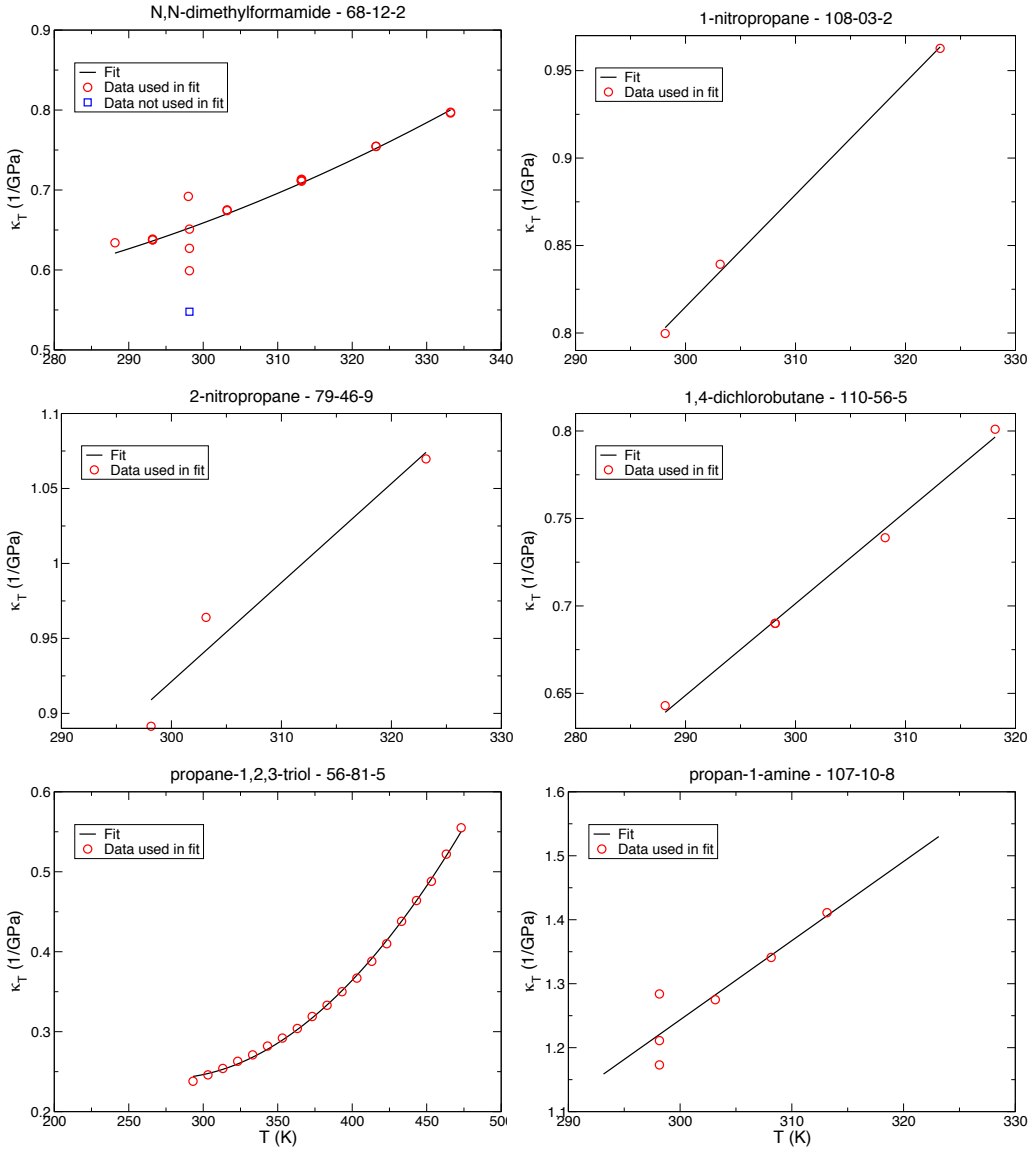

Figure S4: (part 5) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

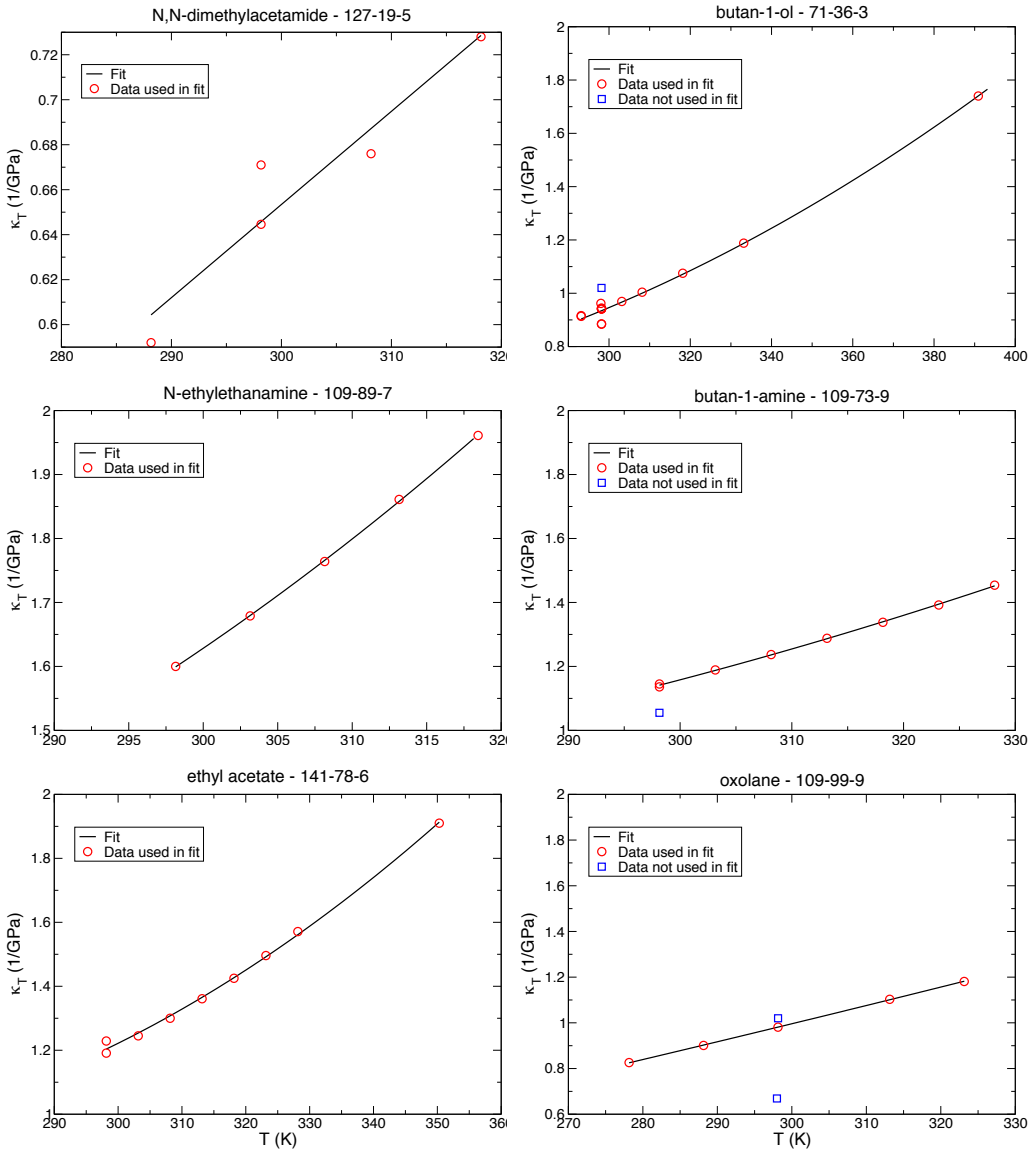

Figure S4: (part 6) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

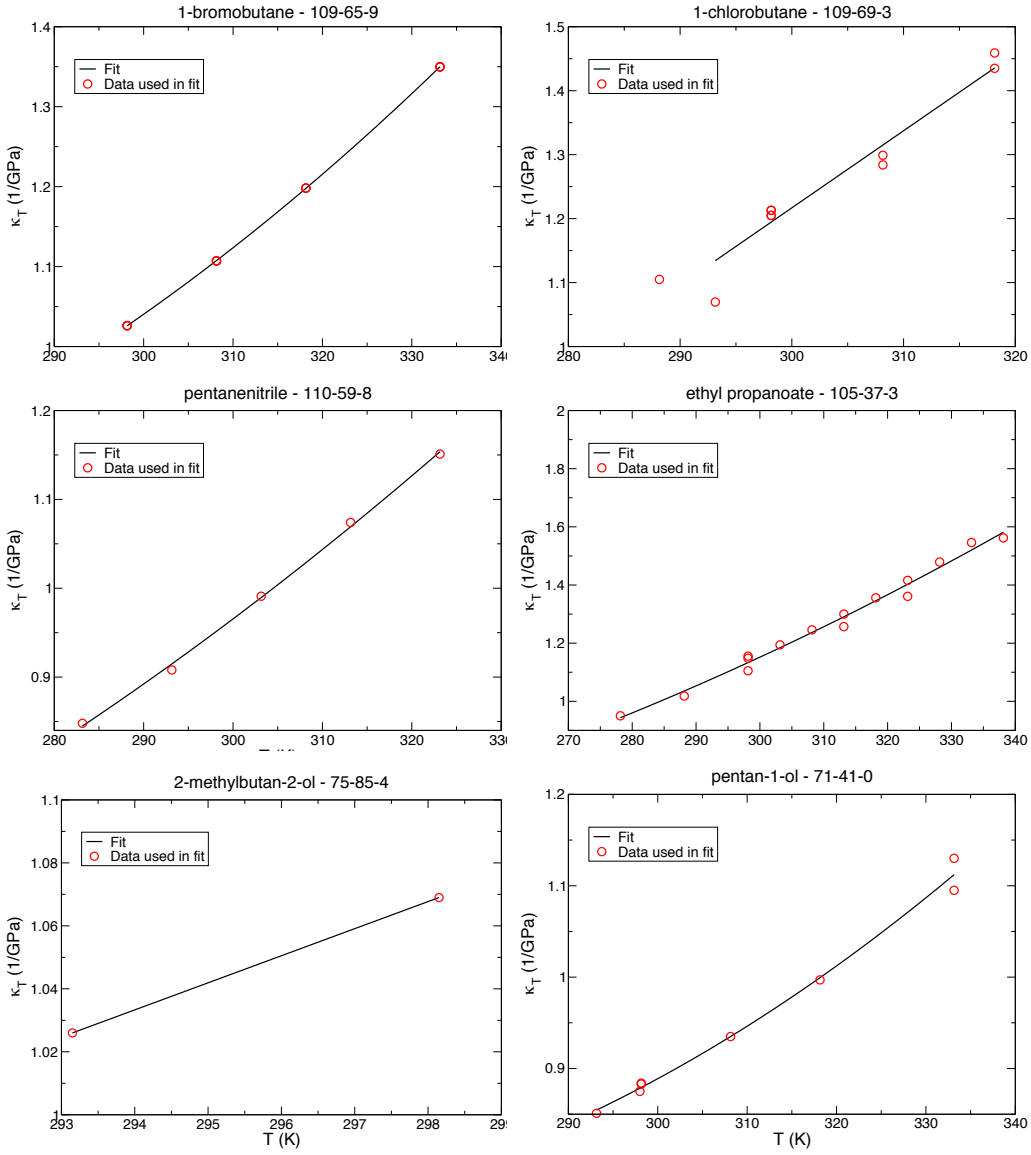

Figure S4: (part 7) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

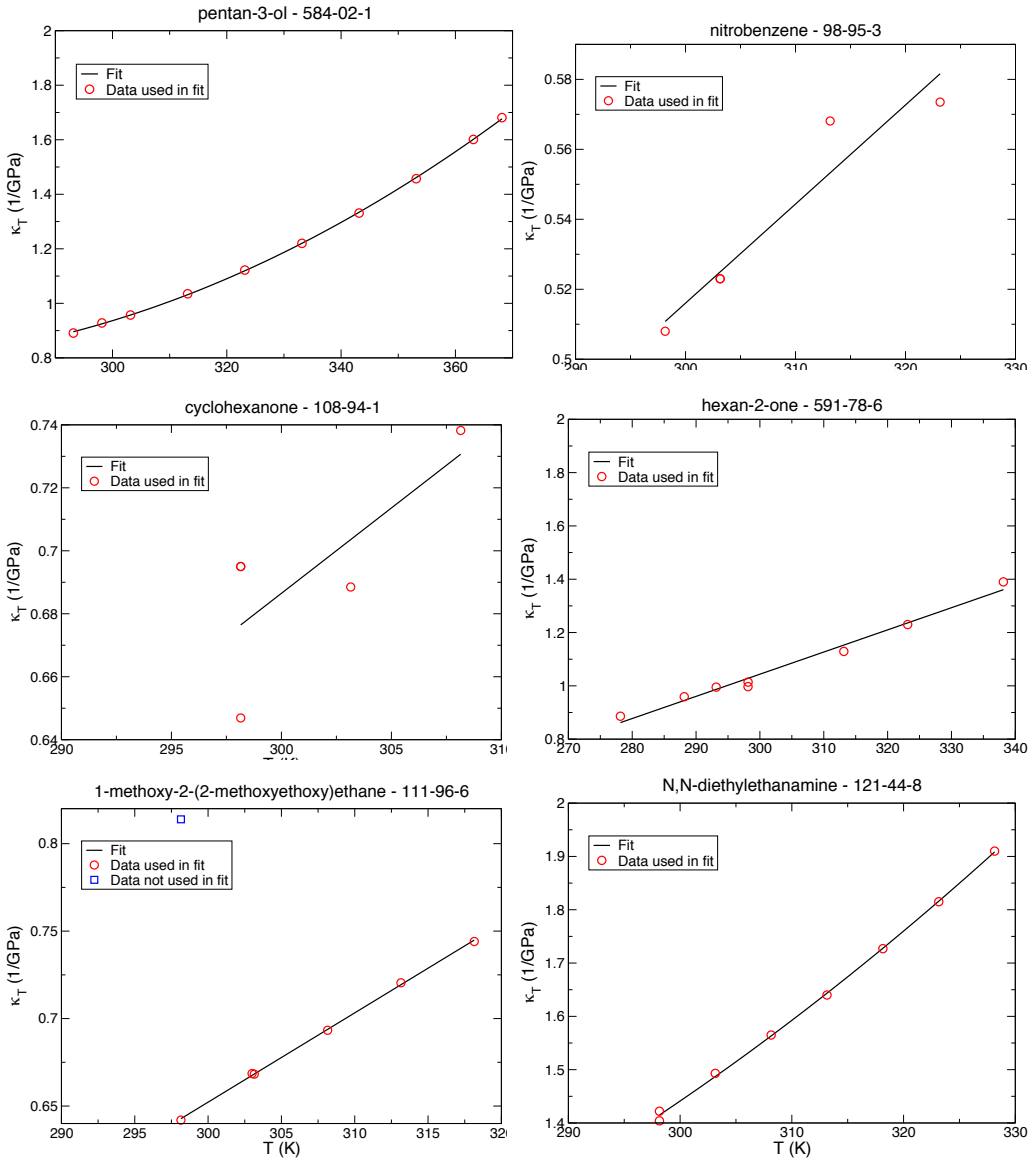

Figure S4: (part 8) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

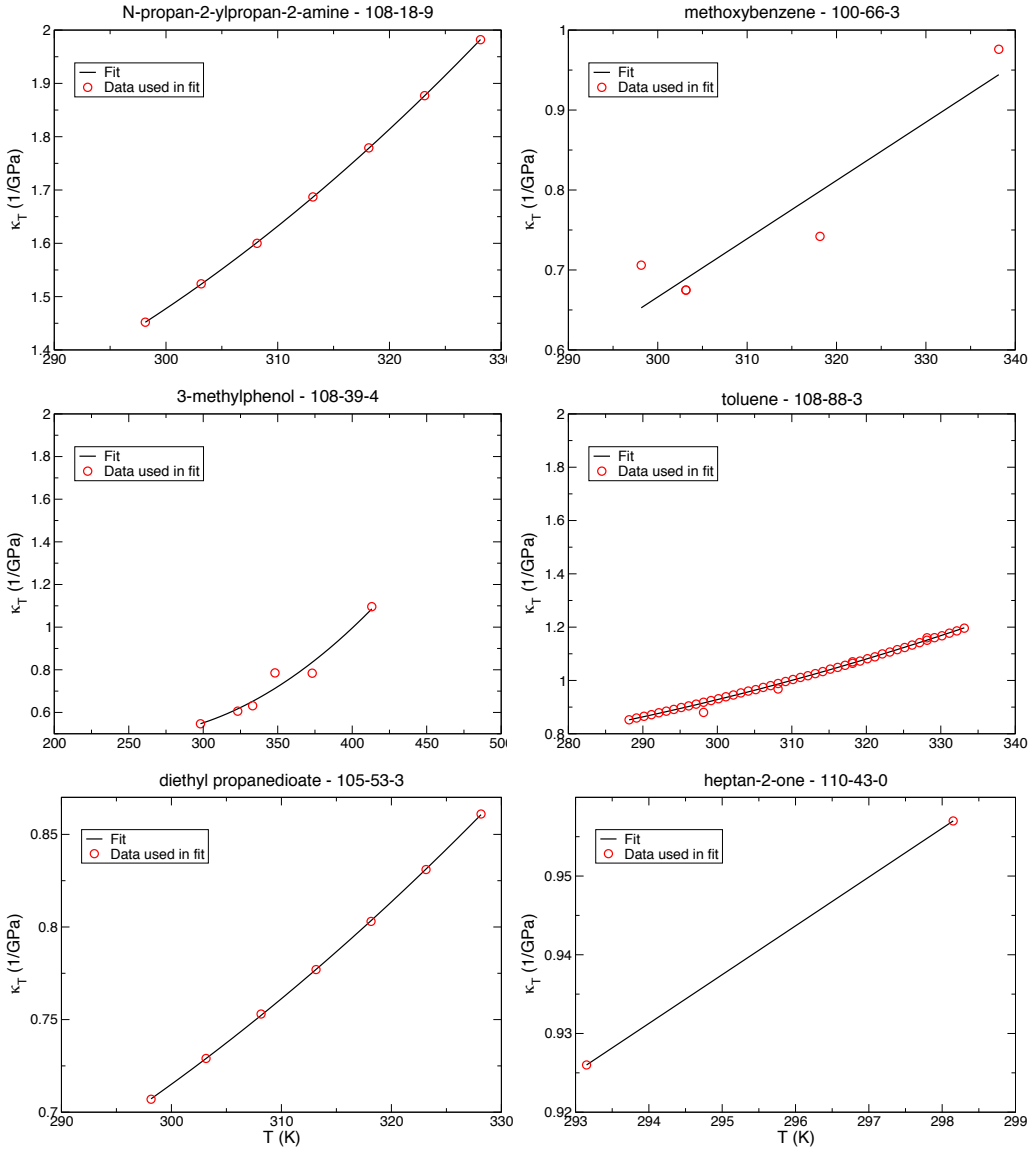

Figure S4: (part 9) Polynomial curves fitted to isothermal compressibility measurements for different molecules. For parameters see Table 6 in the main text.

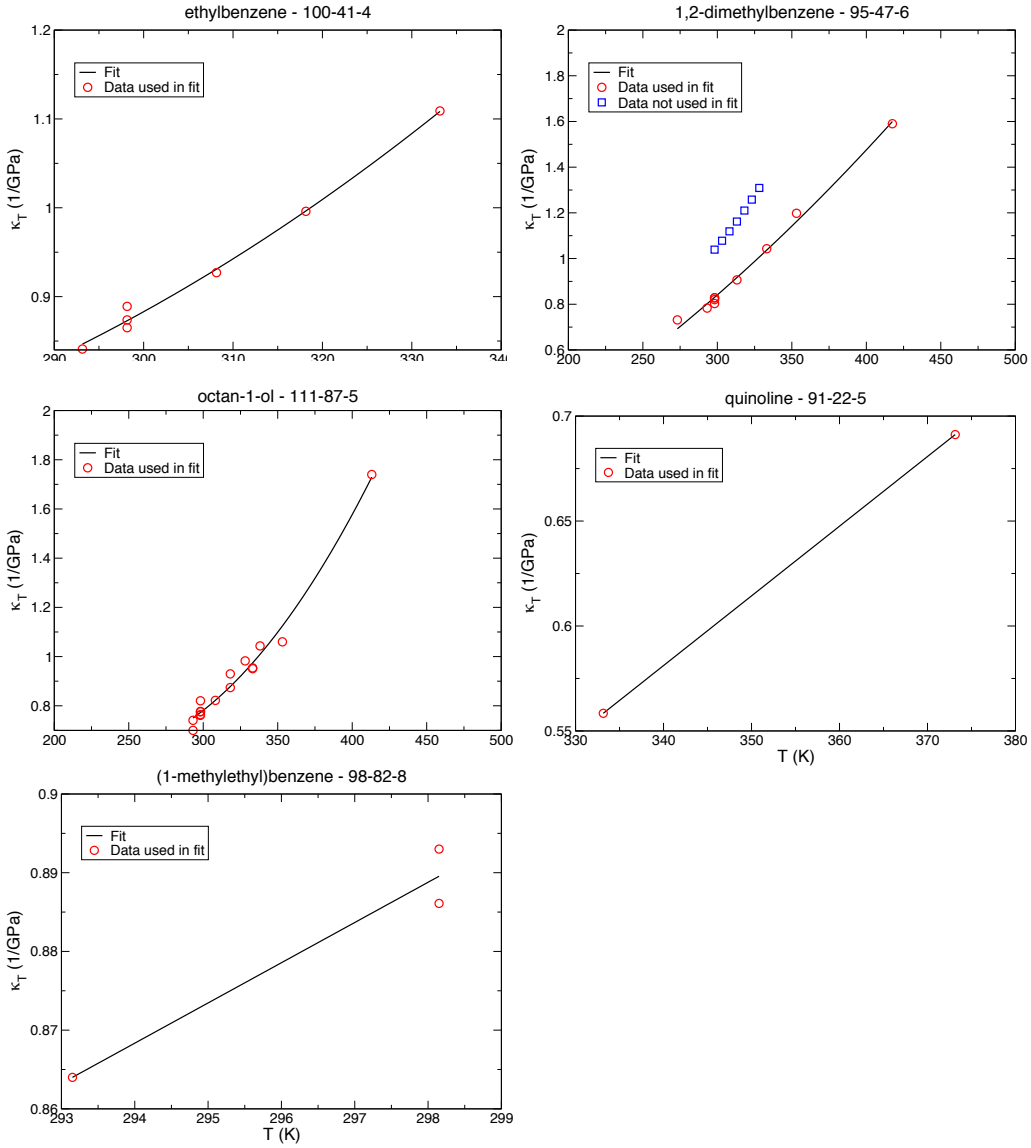

Table S13: References used for deriving fits of isothermal compressibilities as a function of temperature to experimental data.

Molecule	References
pentan-1-ol	[23]
1,4-dichlorobutane	[47]
2-aminoethanol	[23]
dichloromethane	[23]
methylsulfinylmethane	[23]
acetonitrile	[23]
1-chlorobutane	[23, 47]
ethanol	[23]
1-methoxy-2-(2-methoxyethoxy)ethane	[23]
hexan-2-one	[47]
heptan-2-one	[23]
N,N-diethylethanamine	[23]
nitromethane	[23, 47]
propane-1,2,3-triol	[23]
N,N-dimethylformamide	[23]
1,3-dioxolane	[23]
1,3-dichloropropane	[23]
nitrobenzene	[47]
1,2-dimethylbenzene	[23]
ethyl propanoate	[23]
1,1,2,2-tetrachloroethane	[23]
N-propan-2-ylpropan-2-amine	[23]
N-ethylethanamine	[23]
3-methylphenol	[23]
N-methylformamide	[23]
(1-methylethyl)benzene	[23]
diethyl propanedioate	[23]
octan-1-ol	[23]

Table S13: References used for deriving fits of isothermal compressibilities as a function of temperature to experimental data (continued).

Molecule	References
cyclohexanone	[23]
N,N-dimethylacetamide	[23, 47]
quinoline	[23]
pentan-3-ol	[23]
2-methylbutan-2-ol	[23]
methanamide	[23, 47]
propan-2-one	[47]
methoxybenzene	[23]
pentanenitrile	[23]
1-nitropropane	[47]
toluene	[23]
methanol	[23]
butan-1-ol	[23]
oxolane	[23]
1-bromopropane	[47]
2-nitropropane	[47]
ethylbenzene	[23]
methyl acetate	[23]
propan-1-amine	[23]
1-bromobutane	[23]
nitroethane	[47]
1,1,2-trichloroethane	[47]
bromoethane	[47]
butan-1-amine	[23]
ethyl acetate	[23]

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