Supplementary Material to

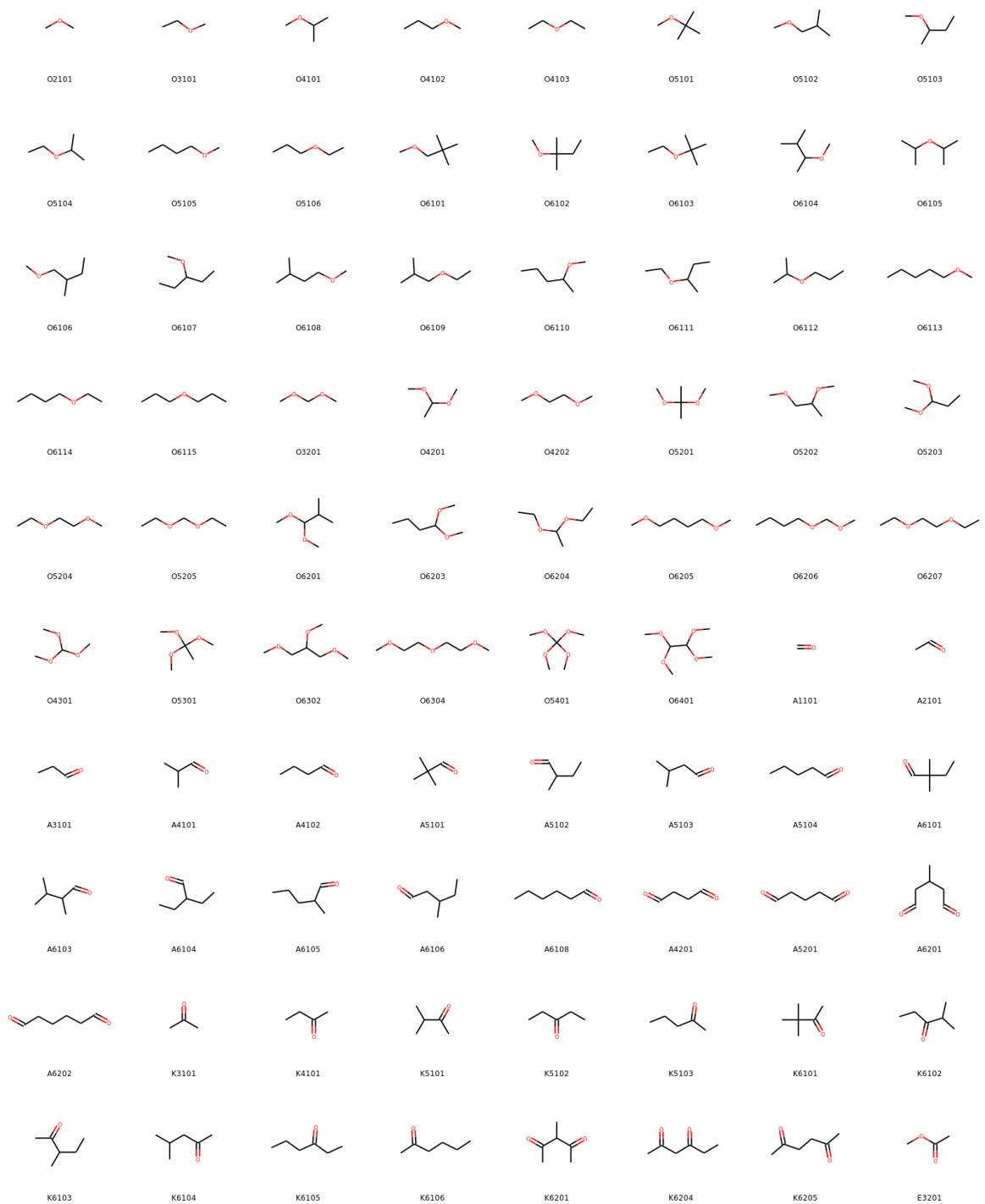
Systematic optimization of a fragment-based force field against experimental pure-liquid properties considering large compound families: Application to oxygen and nitrogen compounds.

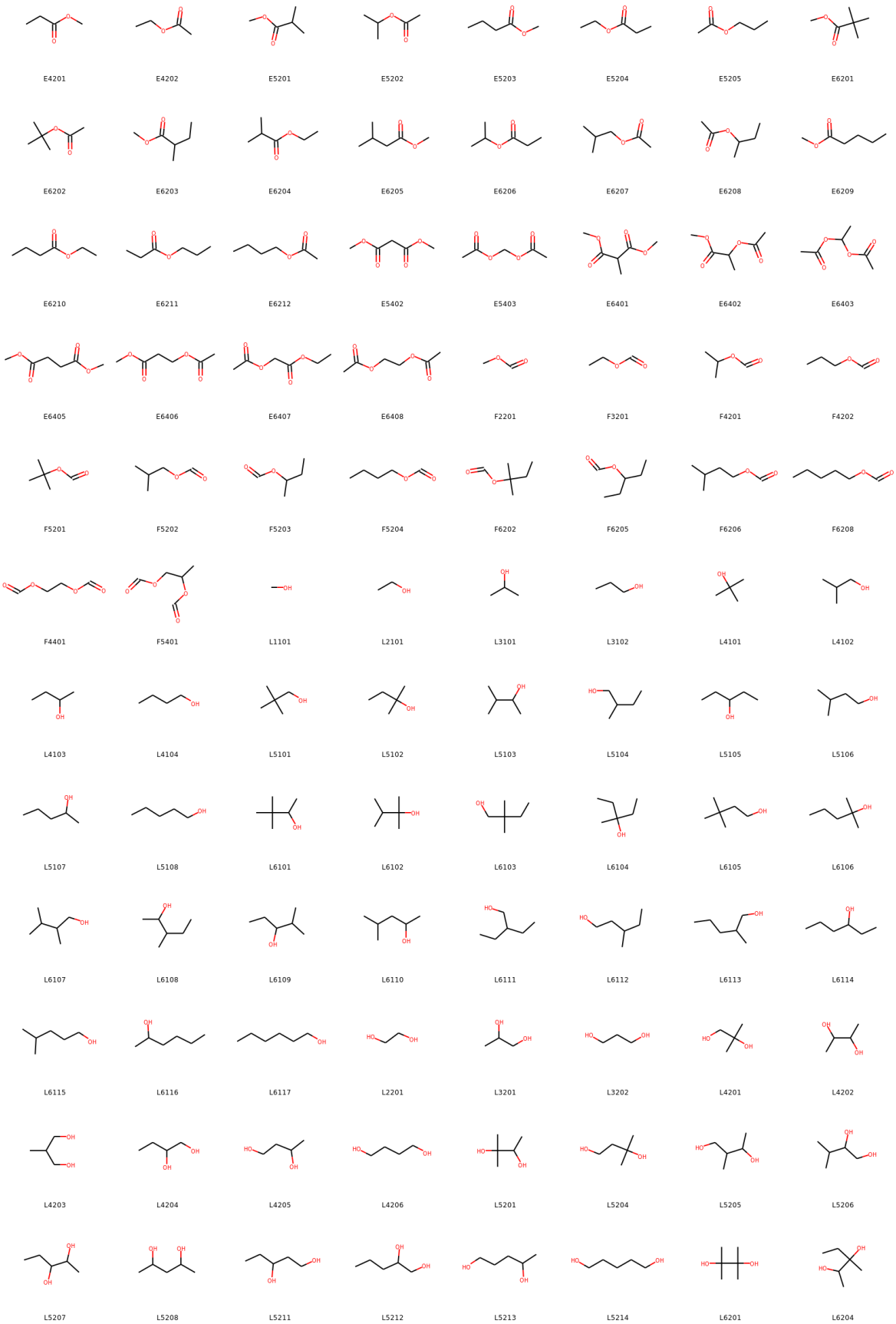
Marina P. Oliveira and Philippe H. Hünenberger

S.1 Compounds in the Calibration and Validation Sets

The structures of the compounds included in the calibration and validation sets are illustrated in Figs. S.1 and S.2, respectively.

Figure S.1: Structures of the $N_{\text{iso}}^{\text{cal}} = 339$ molecules with 1-6 carbon atom included in the calibration set. See Tab. S.1 for the corresponding names and CAS registry numbers.

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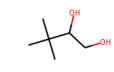

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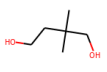

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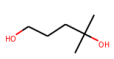

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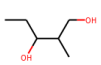

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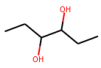

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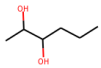

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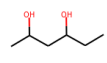

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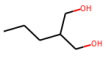

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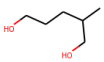

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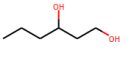

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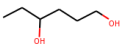

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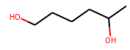

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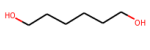

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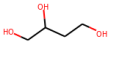

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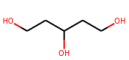

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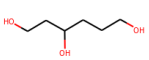

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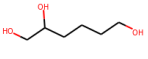

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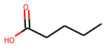

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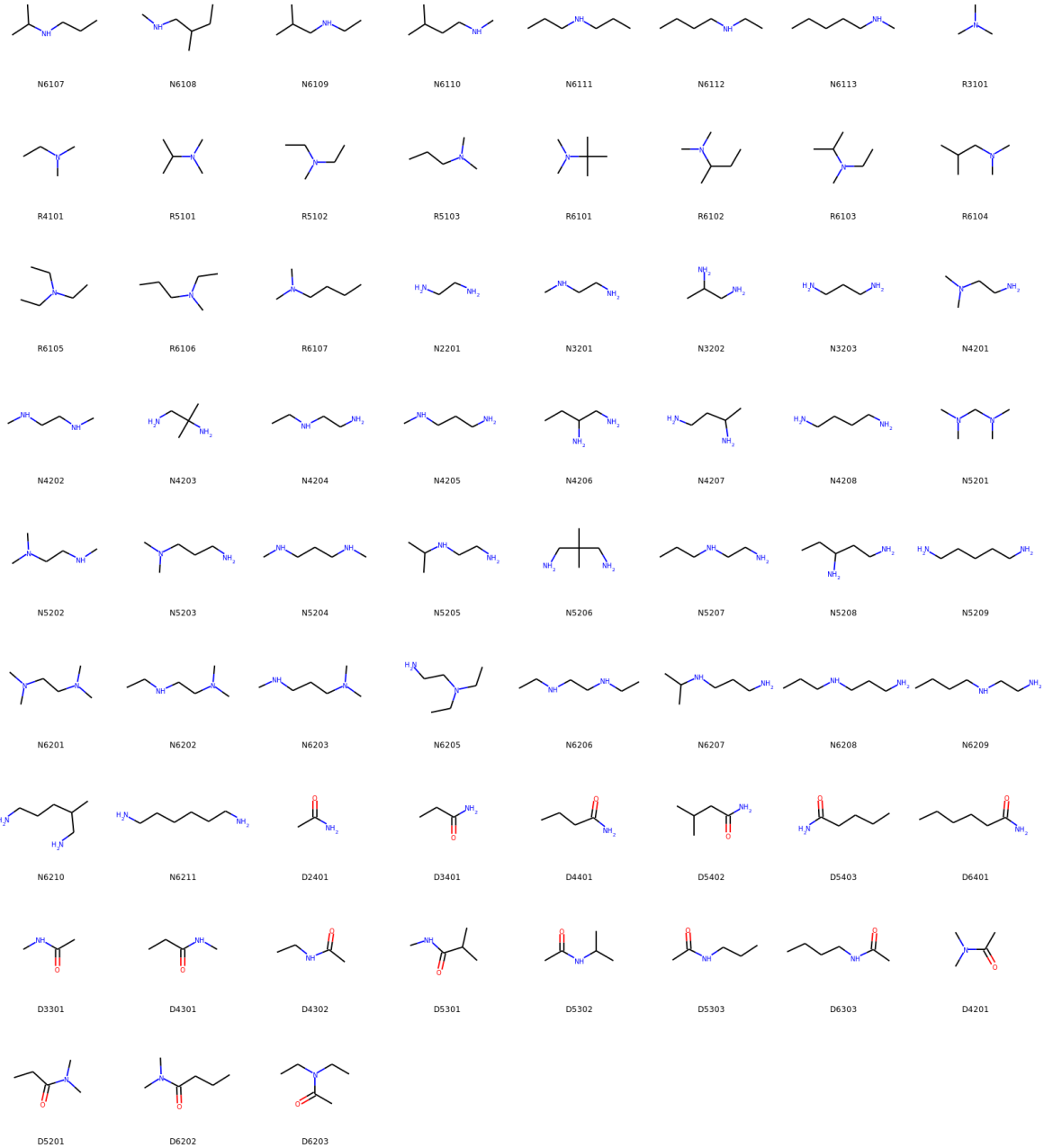
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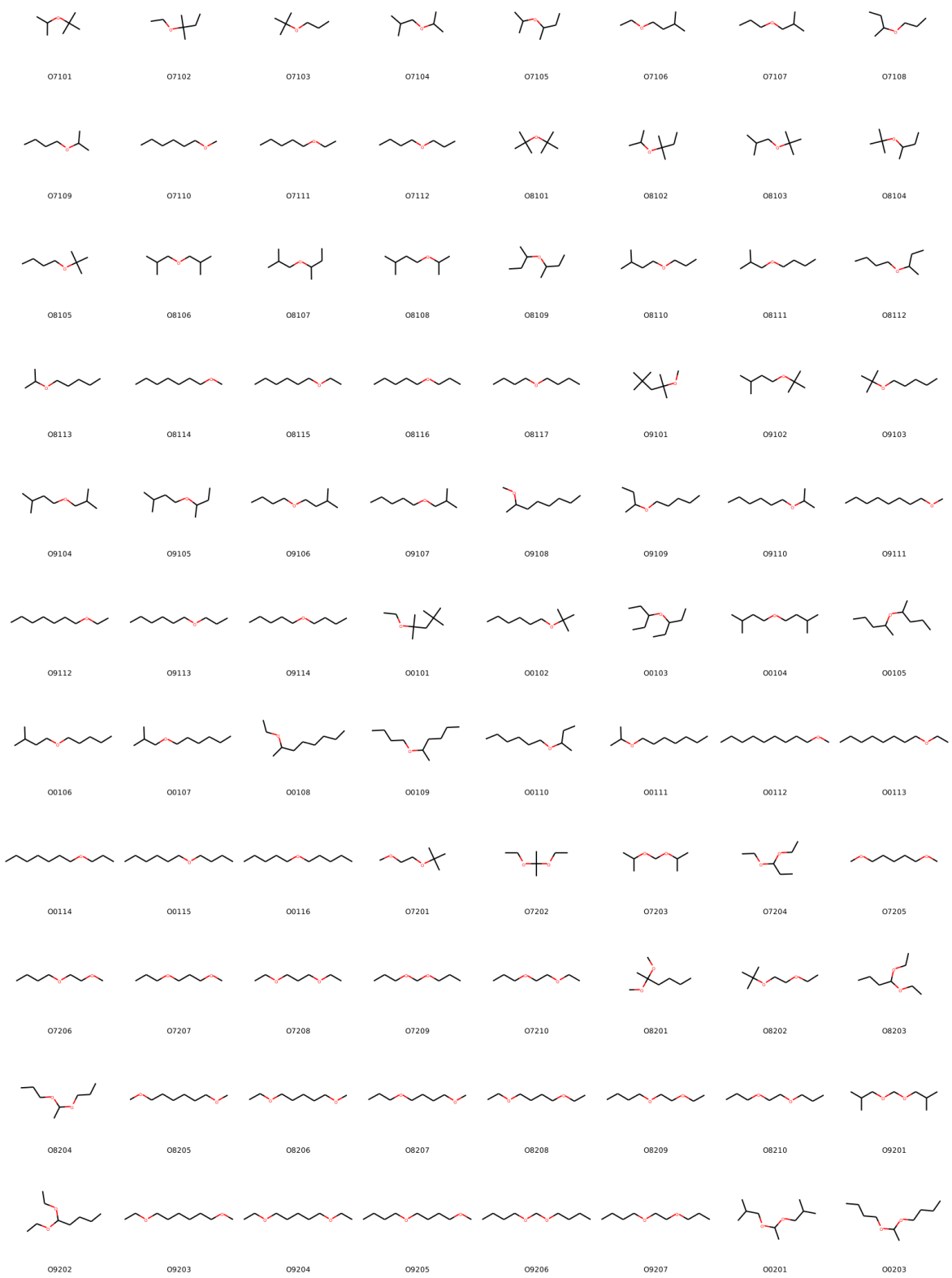
Figure S.2: Structures of the $N_{\text{iso}}^{\text{val}} = 836$ molecules with 7-10 carbon atoms included in the validation set. See Tab. S.1 for the corresponding names and CAS registry numbers.



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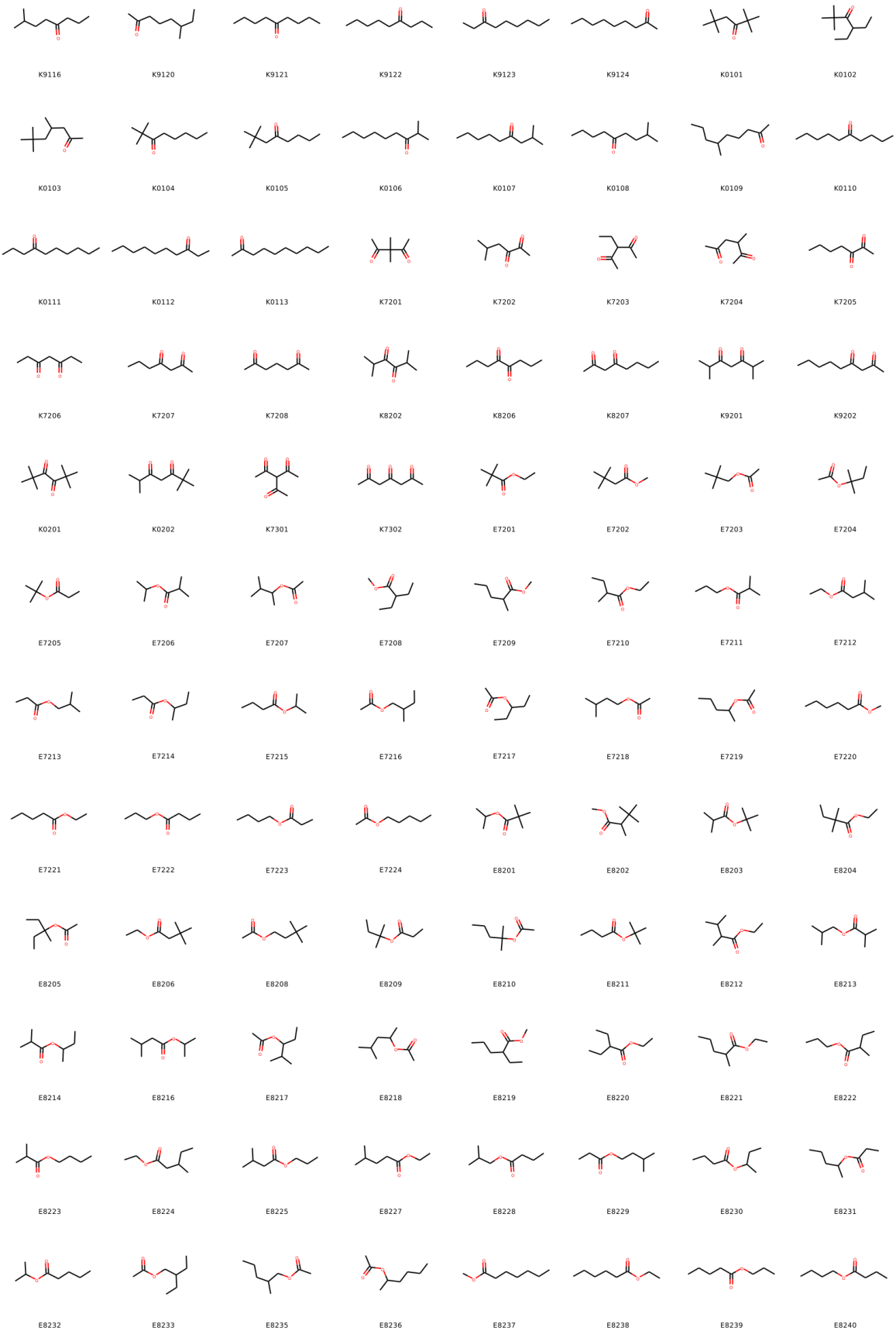
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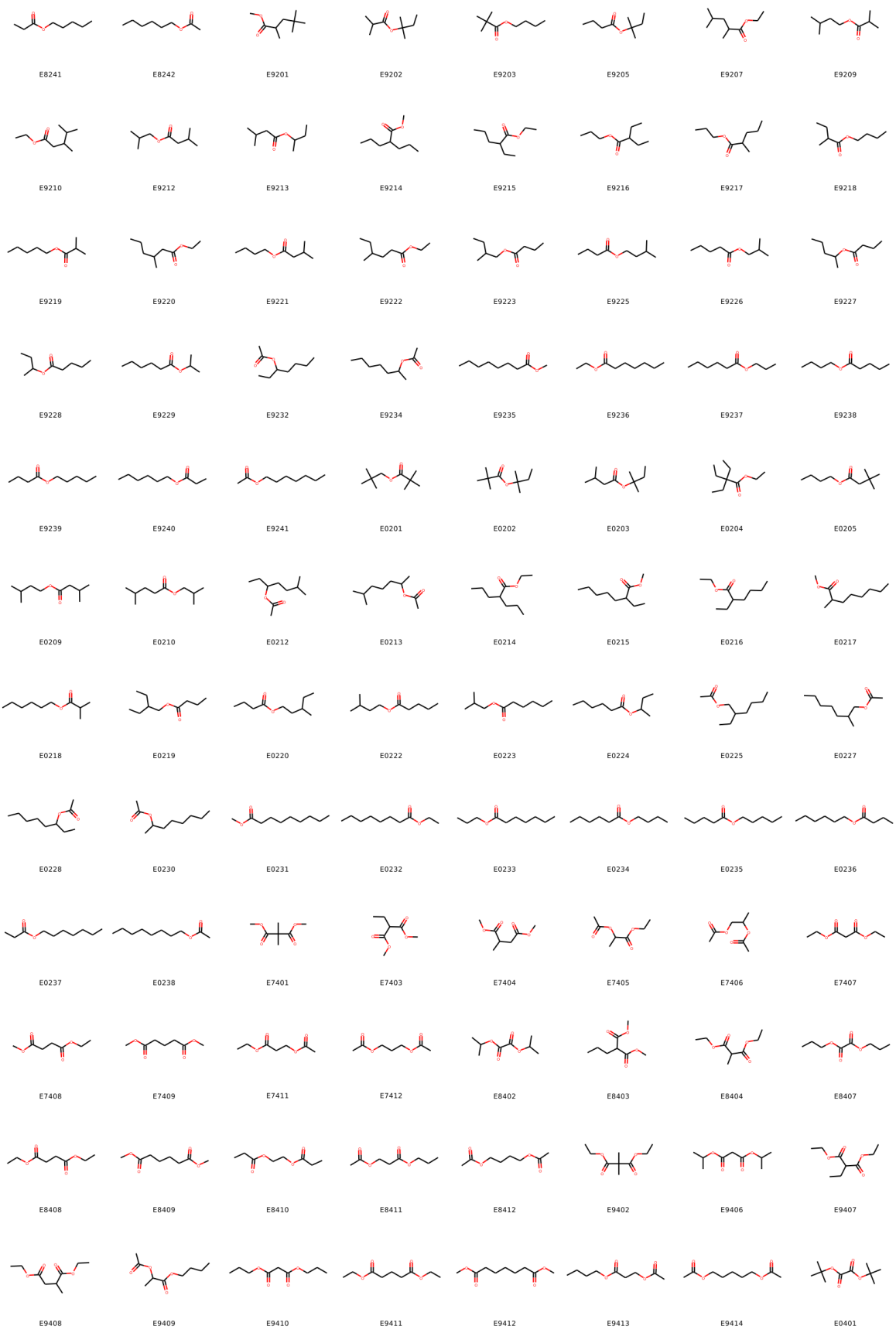
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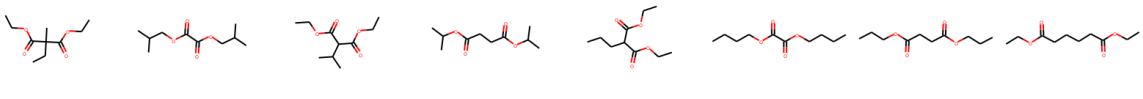
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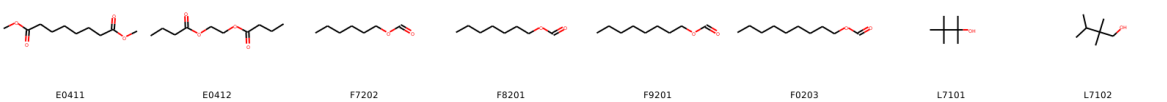
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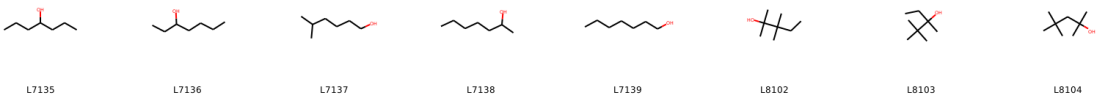
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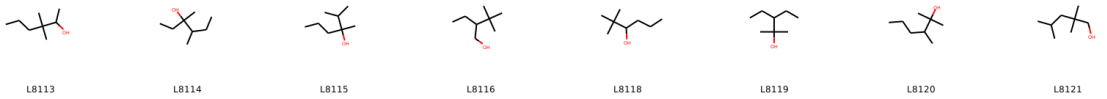
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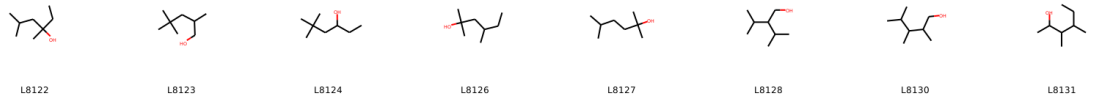
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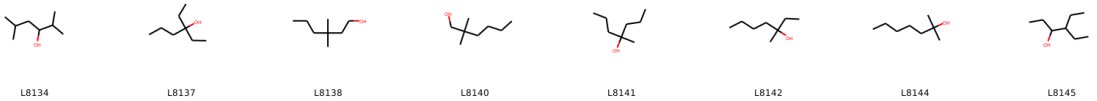
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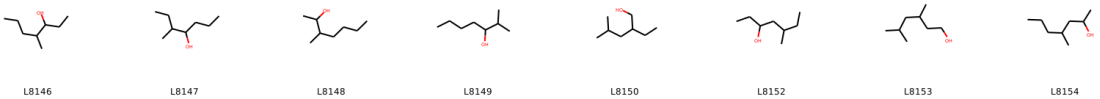
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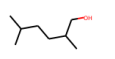
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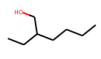
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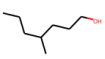
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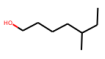
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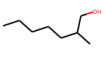
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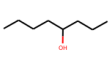
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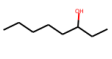
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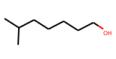
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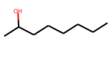
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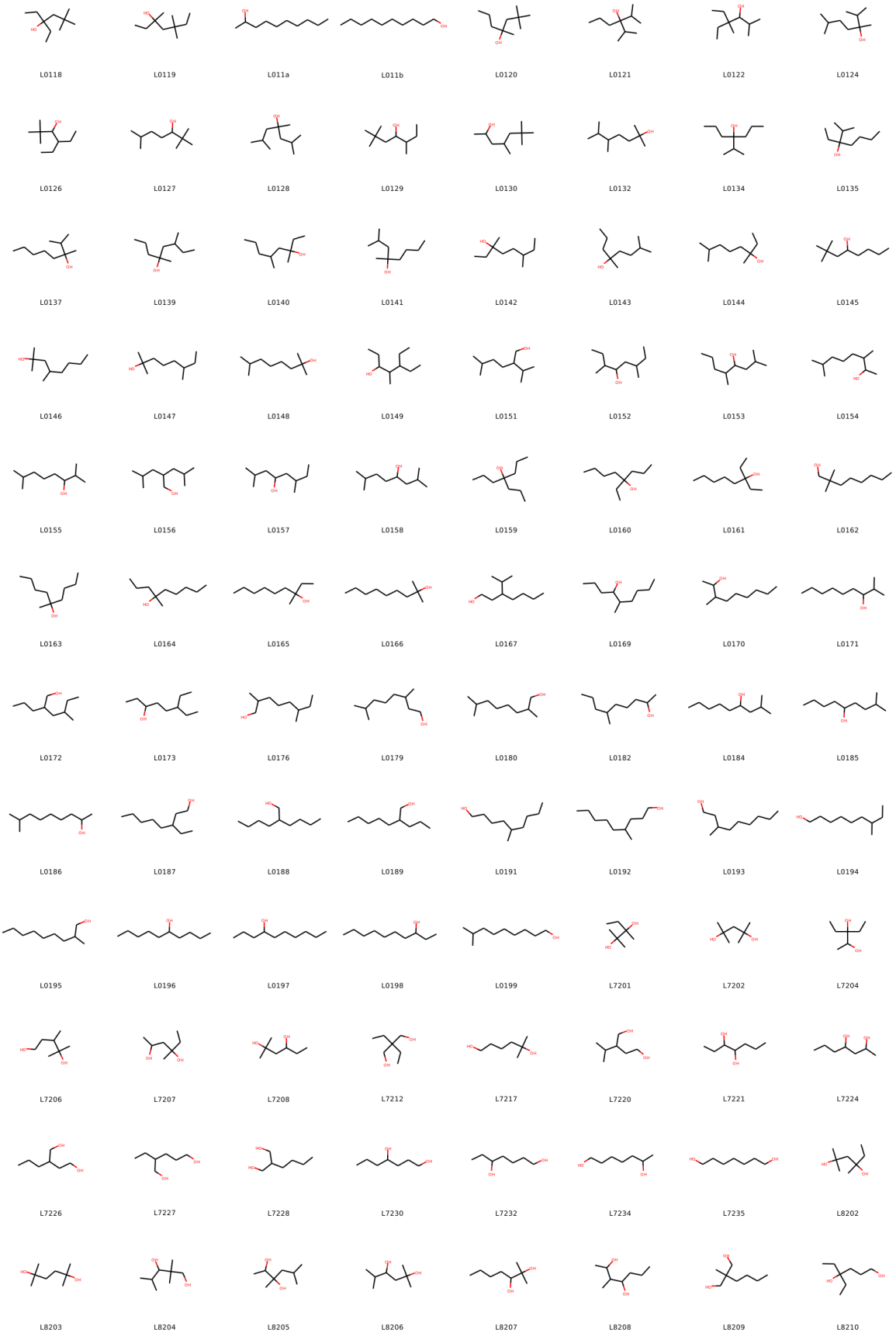
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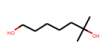

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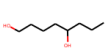

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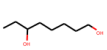

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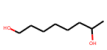

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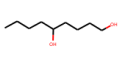

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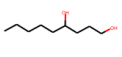

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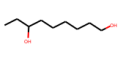

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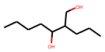

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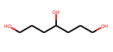

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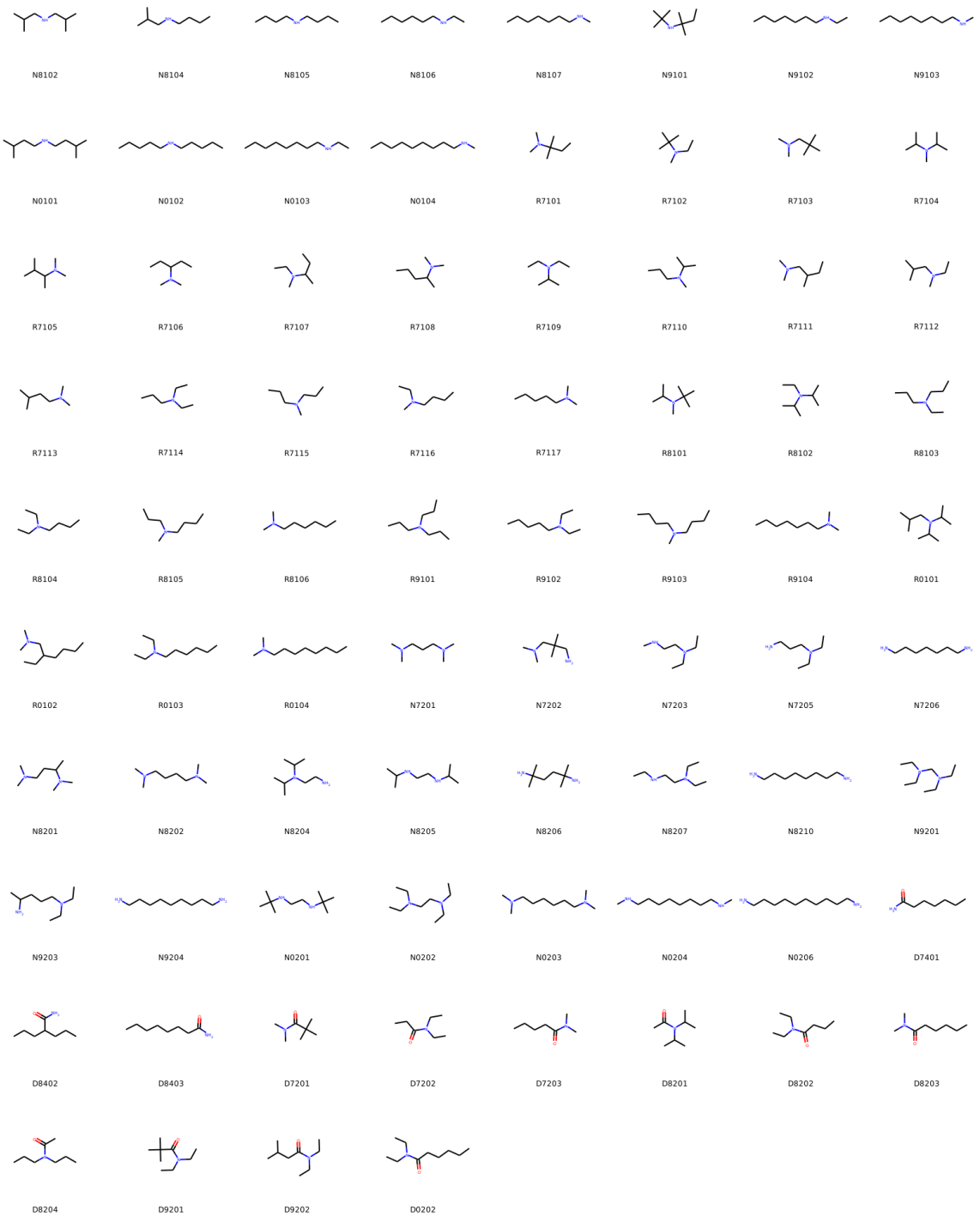
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S.2 Reference Experimental Data

The reference experimental data used in this work is reported in Tab. S.1. The $N_{\text{iso}}^{\text{sim}} = 1175$ molecules considered are referred to by their code, IUPAC name, CAS registry number, and whether they belong to the calibration (C) or validation (V) set. The structures of the compounds in these two sets are displayed in Figs. S.1 and S.2, respectively. For these molecules, simulations are performed at $N_{\text{sim}}^{\text{tot}} = 1405$ thermodynamic state points, with indicated pressure P and temperature T. Simulations of the same compound performed at different P, T-points are distinguished by an extra letter (a, b or c) appended to the molecule code. The quantities reported along with a literature source (Src) are the pure-liquid density ρ_{liq}, the vaporization enthalpy ΔH_{vap}, the melting point T_m and the boiling point T_b at $P^\circ = 1$ bar, the critical point T_c (pressure P_c unspecified), and the static relative dielectric permittivity ϵ. For ϵ, the column with the source contains either the experimental source or a dash to indicate an educated guess. In the latter case, the ϵ value is reported between parentheses.

Table S.1: Reference experimental data pertaining to the $N_{\mathrm{iso}}^{\mathrm{sim}} = 1175$ molecules (running index n_{iso}) and $N_{\mathrm{sim}}^{\mathrm{tot}} = 1405$ P,T-points (running index n_{sim}) considered in the simulations.

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1	1	C	O2101a	methoxymethane	115-10-6	1.0	248.12	735.04	[118]	21.56	[121]	131.66	[120]	248.31	[121]	400.10	[121]	6.18	[120]
2	1	C	O2101b	methoxymethane	115-10-6	9.06	298.28	661.92	[118]	-	-	131.66	[120]	248.31	[121]	400.10	[121]	6.18	[120]
3	1	C	O2101c	methoxymethane	115-10-6	5.77	298.15	-	-	17.75	[121]	131.66	[120]	248.31	[121]	400.10	[121]	6.18	[120]
4	2	C	O3101a	methoxyethane	540-67-0	1.0	273.15	726.00	[116]	-	-	160.15	[120]	280.50	[121]	437.80	[121]	(3.76)	-
5	2	C	O3101b	methoxyethane	540-67-0	1.82	298.15	691.94	[121]	-	-	160.15	[120]	280.50	[121]	437.80	[121]	(3.76)	-
6	2	C	O3101c	methoxyethane	540-67-0	1.0	280.5	-	-	31.22	[121]	160.15	[120]	280.50	[121]	437.80	[121]	(3.76)	-
7	3	C	O4101a	2-methoxypropane	598-53-8	1.0	298.15	708.95	[116]	26.40	[114]	-	-	303.92	[121]	464.48	[121]	(4.27)	-
8	4	C	O4102a	1-methoxypropane	557-17-5	1.0	298.15	719.22	[116]	27.90	[114]	-	-	311.72	[121]	476.25	[121]	(4.27)	-
9	5	C	O4103a	ethoxyethane	60-29-7	1.0	298.15	707.82	[116]	27.20	[114]	156.93	[120]	307.58	[121]	466.70	[121]	4.2666	[120]
10	6	C	O5101a	2-methoxy-2-methylpropane	1634-04-4	1.0	298.15	735.22	[116]	30.40	[114]	164.55	[120]	328.35	[121]	497.10	[121]	(3.76)	-
11	7	C	O5102a	1-methoxy-2-methylpropane	625-44-5	1.0	298.15	727.20	[116]	-	-	-	-	331.70	[121]	499.99	[121]	(3.76)	-
12	7	C	O5102b	1-methoxy-2-methylpropane	625-44-5	0.26	298.15	-	-	30.13	[121]	-	-	331.70	[121]	499.99	[121]	(3.76)	-
13	8	C	O5103a	2-methoxybutane	6795-87-5	1.0	298.15	736.70	[116]	-	-	-	-	332.15	[121]	499.99	[121]	(3.76)	-
14	8	C	O5103b	2-methoxybutane	6795-87-5	0.26	298.15	-	-	30.21	[121]	-	-	332.15	[121]	499.99	[121]	(3.76)	-
15	9	C	O5104a	2-ethoxypropane	625-54-7	1.0	298.15	717.30	[116]	30.00	[114]	-	-	326.15	[121]	499.99	[121]	(3.76)	-
16	10	C	O5105a	1-methoxybutane	628-28-4	1.0	298.15	739.40	[116]	32.50	[114]	157.45	[120]	343.35	[121]	512.74	[121]	(3.76)	-
17	11	C	O5106a	1-ethoxypropane	628-32-0	1.0	298.15	727.00	[116]	31.40	[114]	145.65	[120]	337.01	[121]	500.23	[121]	(3.76)	-
18	12	C	O6101a	1-methoxy-2,2-dimethylpropane	1118-00-9	0.08	298.15	753.94	[121]	-	-	-	-	356.15	[121]	526.03	[121]	(3.59)	-
19	13	C	O6102a	2-methoxy-2-methylbutane	994-05-8	1.0	298.15	765.90	[116]	35.00	[114]	-	-	359.45	[121]	526.03	[121]	(3.59)	-
20	14	C	O6103a	2-ethoxy-2-methylpropane	637-92-3	1.0	298.15	735.16	[116]	33.10	[114]	179.15	[120]	345.95	[121]	526.03	[121]	(3.59)	-
21	15	C	O6104a	2-methoxy-3-methylbutane	62016-49-3	1.0	298.15	754.20	[116]	-	-	-	-	356.15	[121]	526.03	[121]	(3.59)	-
22	16	C	O6105a	2-propan-2-yloxypropane	108-20-3	1.0	298.15	718.70	[116]	32.70	[114]	187.78	[120]	341.45	[121]	500.05	[121]	3.805	[120]
23	17	C	O6106a	1-methoxy-2-methylbutane	62016-48-2	0.07	298.15	746.09	[121]	-	-	-	-	363.15	[121]	526.03	[121]	(3.59)	-
24	18	C	O6107a	3-methoxypentane	36839-67-5	0.07	298.15	748.95	[121]	-	-	-	-	361.15	[121]	526.03	[121]	(3.59)	-
25	19	C	O6108a	1-methoxy-3-methylbutane	626-91-5	1.0	298.15	749.05	[116]	-	-	-	-	363.15	[121]	526.03	[121]	(3.59)	-
26	19	C	O6108b	1-methoxy-3-methylbutane	626-91-5	0.07	298.15	-	-	35.54	[121]	-	-	363.15	[121]	526.03	[121]	(3.59)	-
27	20	C	O6109a	1-ethoxy-2-methylpropane	627-02-1	1.0	298.15	734.03	[116]	-	-	-	-	354.25	[121]	526.03	[121]	(3.59)	-
28	20	C	O6109b	1-ethoxy-2-methylpropane	627-02-1	0.1	298.15	-	-	33.62	[121]	-	-	354.25	[121]	526.03	[121]	(3.59)	-
29	21	C	O6110a	2-methoxypentane	6795-88-6	0.06	298.15	749.89	[121]	35.61	[121]	-	-	364.15	[121]	526.03	[121]	(3.59)	-
30	22	C	O6111a	2-ethoxybutane	2679-87-0	1.0	298.15	738.30	[116]	-	-	-	-	354.35	[121]	526.03	[121]	(3.59)	-
31	22	C	O6111b	2-ethoxybutane	2679-87-0	0.11	298.15	-	-	32.63	[121]	-	-	354.35	[121]	526.03	[121]	(3.59)	-
32	23	C	O6112a	1-propan-2-yloxypropane	627-08-7	1.0	298.15	732.40	[116]	-	-	-	-	353.15	[121]	526.03	[121]	(3.59)	-
33	23	C	O6112b	1-propan-2-yloxypropane	627-08-7	0.09	298.15	-	-	33.98	[121]	-	-	353.15	[121]	526.03	[121]	(3.59)	-
34	24	C	O6113a	1-methoxypentane	628-80-8	1.0	298.15	755.20	[116]	-	-	-	-	372.15	[121]	546.49	[121]	(3.59)	-
35	24	C	O6113b	1-methoxypentane	628-80-8	0.04	298.15	-	-	36.44	[121]	-	-	372.15	[121]	546.49	[121]	(3.59)	-
36	25	C	O6114a	1-ethoxybutane	628-81-9	1.0	298.15	744.70	[116]	36.30	[114]	149.15	[120]	365.35	[121]	526.03	[121]	(3.59)	-
37	26	C	O6115a	1-propoxypropane	111-43-3	1.0	298.15	741.94	[116]	35.70	[114]	158.35	[120]	362.79	[121]	530.60	[121]	3.38	[120]
38	27	C	O3201a	dimethoxymethane	109-87-5	0.51	298.15	854.12	[121]	-	-	168.04	[120]	315.00	[121]	480.60	[121]	2.644	[120]
39	27	C	O3201b	dimethoxymethane	109-87-5	1.0	298.0	-	-	28.90	[114]	168.04	[120]	315.00	[121]	480.60	[121]	2.644	[120]
40	28	C	O4201a	1,1-dimethoxyethane	534-15-6	1.0	293.15	851.60	[116]	36.40	[114]	159.95	[120]	337.65	[121]	-	-	(7.30)	-
41	29	C	O4202a	1,2-dimethoxyethane	110-71-4	1.01	298.15	861.36	[118]	36.80	[114]	204.15	[120]	357.20	[121]	536.15	[121]	7.30	[120]
42	30	C	O5201a	2,2-dimethoxypropane	77-76-9	1.01	298.15	845.09	[118]	37.60	[114]	226.15	[120]	356.15	[121]	-	-	(2.53)	-
43	31	C	O5202a	1,2-dimethoxypropane	7778-85-0	1.0	369.05	-	-	31.46	[121]	-	-	369.05	[121]	-	-	(2.53)	-
44	32	C	O5203a	1,1-dimethoxypropane	4744-10-9	1.0	293.15	864.80	[120]	-	-	-	-	359.15	[121]	-	-	(2.53)	-
45	32	C	O5203b	1,1-dimethoxypropane	4744-10-9	1.0	359.15	-	-	30.53	[121]	-	-	359.15	[121]	-	-	(2.53)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
46	33	C	O5204a	1-ethoxy-2-methoxyethane	500005-27-6	1.0	298.15	846.00	[120]	39.80	[114]	-	-	375.25	[121]	-	-	(2.53)	-
47	34	C	O5205a	ethoxymethoxyethane	462-95-3	1.0	298.15	825.17	[116]	35.70	[114]	207.15	[120]	361.15	[121]	524.00	[121]	2.527	[120]
48	35	C	O6201a	1,1-dimethoxy-2-methylpropane	41632-89-7	1.0	293.15	844.60	[116]	-	-	-	-	-	-	-	-	(3.90)	-
49	36	C	O6203a	1,1-dimethoxybutane	4461-87-4	1.0	317.0	-	-	41.20	[114]	-	-	-	-	-	-	(3.90)	-
50	37	C	O6204a	1,1-diethoxyethane	105-57-7	1.01	298.15	821.96	[118]	39.60	[114]	167.05	[120]	376.75	[121]	539.70	[121]	(3.90)	-
51	38	C	O6205a	1,4-dimethoxybutane	13179-96-9	1.0	298.15	852.90	[116]	-	-	-	-	-	-	-	-	(3.90)	-
52	39	C	O6206a	1-(methoxymethoxy)butane	76050-97-0	1.0	340.0	-	-	38.60	[114]	-	-	-	-	-	-	(3.90)	-
53	40	C	O6207a	1,2-diethoxyethane	629-14-1	1.0	298.15	836.20	[116]	43.20	[114]	199.15	[120]	392.55	[121]	637.84	[121]	3.90	[120]
54	41	C	O4301a	trimethoxymethane	149-73-5	1.0	293.15	967.60	[120]	38.10	[114]	288.15	[120]	377.15	[121]	-	-	(6.00)	-
55	42	C	O5301a	1,1,1-trimethoxyethane	1445-45-0	1.0	298.15	943.80	[120]	-	-	-	-	381.15	[121]	-	-	(6.00)	-
56	42	C	O5301b	1,1,1-trimethoxyethane	1445-45-0	1.0	381.15	-	-	32.59	[121]	-	-	381.15	[121]	-	-	(6.00)	-
57	43	C	O6302a	1,2,3-trimethoxypropane	20637-49-4	1.0	421.15	-	-	36.36	[121]	-	-	421.15	[121]	-	-	(7.23)	-
58	44	C	O6304a	1-methoxy-2-(2-methoxyethoxy)ethane	111-96-6	1.0	298.15	939.24	[116]	48.00	[114]	209.15	[120]	432.91	[121]	608.00	[121]	7.23	[120]
59	45	C	O5401a	tetramethoxymethane	1850-14-2	1.0	298.15	1023.00	[120]	-	-	270.65	[120]	387.15	[121]	-	-	2.40	[120]
60	45	C	O5401b	tetramethoxymethane	1850-14-2	1.0	319.0	-	-	41.20	[114]	270.65	[120]	387.15	[121]	-	-	2.40	[120]
61	46	C	O6401a	1,1,2,2-tetramethoxyethane	2517-44-4	1.0	366.0	-	-	42.90	[114]	-	-	-	-	-	-	(5.01)	-
62	47	C	A1101a	formaldehyde	50-00-0	1.36	250.68	805.17	[121]	-	-	181.15	[120]	254.05	[121]	415.24	[121]	(2.0)	-
63	47	C	A1101b	formaldehyde	50-00-0	1.0	293.15	814.00	[117]	-	-	181.15	[120]	254.05	[121]	415.24	[121]	(2.0)	-
64	47	C	A1101c	formaldehyde	50-00-0	1.0	254.05	-	-	23.16	[121]	181.15	[120]	254.05	[121]	415.24	[121]	(2.0)	-
65	48	C	A2101a	acetaldehyde	75-07-0	1.0	298.15	772.00	[117]	26.90	[114]	149.75	[120]	293.55	[121]	466.00	[121]	21.0	[120]
66	49	C	A3101a	propanal	123-38-6	1.0	298.15	791.22	[117]	29.60	[114]	193.15	[120]	321.15	[121]	504.40	[121]	18.5	[120]
67	50	C	A4101a	2-methylpropanal	78-84-2	1.0	298.15	796.62	[117]	32.30	[114]	201.05	[120]	337.25	[121]	540.36	[121]	(13.45)	-
68	51	C	A4102a	butanal	123-72-8	1.0	298.15	796.60	[117]	33.70	[114]	176.29	[120]	347.95	[121]	537.20	[121]	13.45	[120]
69	52	C	A5101a	2,2-dimethylpropanal	630-19-3	0.14	298.15	783.10	[121]	-	-	274.15	[120]	347.15	[121]	570.01	[121]	9.051	[120]
70	52	C	A5101b	2,2-dimethylpropanal	630-19-3	1.0	322.0	-	-	34.20	[114]	274.15	[120]	347.15	[121]	570.01	[121]	9.051	[120]
71	53	C	A5102a	2-methylbutanal	96-17-3	0.06	298.15	804.11	[121]	34.75	[121]	-	-	365.15	[121]	570.01	[121]	(9.53)	-
72	54	C	A5103a	3-methylbutanal	590-86-3	1.0	298.15	794.21	[117]	-	-	222.15	[120]	365.75	[121]	570.01	[121]	(9.53)	-
73	54	C	A5103b	3-methylbutanal	590-86-3	0.06	298.15	-	-	34.82	[121]	222.15	[120]	365.75	[121]	570.01	[121]	(9.53)	-
74	55	C	A5104a	pentanal	110-62-3	1.0	298.15	806.23	[117]	38.10	[114]	191.65	[120]	376.15	[121]	566.10	[121]	10.00	[120]
75	56	C	A6101a	2,2-dimethylbutanal	2094-75-9	0.03	298.15	801.03	[121]	36.21	[121]	-	-	377.15	[121]	596.45	[121]	(13.51)	-
76	57	C	A6103a	2,3-dimethylbutanal	2109-98-0	1.0	298.15	809.70	[117]	-	-	-	-	386.15	[121]	596.45	[121]	(13.51)	-
77	58	C	A6104a	2-ethylbutanal	97-96-1	0.02	298.15	814.07	[121]	38.61	[121]	-	-	389.95	[121]	596.45	[121]	(13.51)	-
78	59	C	A6105a	2-methylpentanal	123-15-9	0.02	298.15	808.05	[121]	38.78	[121]	-	-	390.15	[121]	596.45	[121]	(13.51)	-
79	60	C	A6106a	3-methylpentanal	15877-57-3	0.01	299.47	806.65	[121]	-	-	-	-	395.15	[121]	596.45	[121]	(13.51)	-
80	61	C	A6108a	hexanal	66-25-1	1.01	298.15	833.12	[118]	42.30	[114]	214.95	[120]	401.45	[121]	591.00	[121]	(13.51)	-
81	62	C	A4201a	butanedial	638-37-9	1.0	293.15	1065.00	[120]	-	-	-	-	443.15	[121]	-	-	(9.0)	-
82	63	C	A5201b	pentanedial	111-30-8	1.0	342.0	-	-	56.20	[114]	259.15	[120]	461.15	[121]	660.00	[121]	(9.0)	-
83	64	C	A6201a	3-methylpentanedial	6280-15-5	1.0	439.15	-	-	38.07	[121]	-	-	439.15	[121]	-	-	(9.0)	-
84	65	C	A6202a	hexanedial	1072-21-5	1.0	292.15	1003.00	[120]	-	-	265.15	[120]	435.22	[121]	-	-	(9.0)	-
85	66	C	K3101a	propan-2-one	67-64-1	1.0	298.15	784.37	[117]	31.30	[114]	178.25	[120]	329.44	[121]	508.20	[121]	21.01	[120]
86	67	C	K4101a	butan-2-one	78-93-3	1.0	298.15	799.91	[117]	34.50	[114]	186.48	[120]	352.79	[121]	535.50	[121]	18.56	[120]
87	68	C	K5101a	3-methylbutan-2-one	563-80-4	1.0	298.15	809.36	[117]	36.80	[114]	180.02	[120]	367.55	[121]	553.40	[121]	10.37	[120]
88	69	C	K5102a	pentan-3-one	96-22-0	1.0	298.15	809.60	[117]	38.50	[114]	234.17	[120]	375.14	[121]	560.90	[121]	17.00	[120]
89	70	C	K5103a	pentan-2-one	107-87-9	1.0	298.15	801.76	[117]	38.30	[114]	196.32	[120]	375.46	[121]	561.08	[121]	15.45	[120]
90	71	C	K6101a	3,3-dimethylbutan-2-one	75-97-8	1.0	298.15	804.30	[117]	38.30	[114]	221.75	[120]	379.25	[120]	-	-	12.73	[120]
91	72	C	K6102a	2-methylpentan-3-one	565-69-5	1.0	298.15	806.60	[117]	39.80	[114]	-	-	386.55	[121]	587.45	[121]	(13.47)	-
92	73	C	K6103a	3-methylpentan-2-one	565-61-7	1.0	298.15	808.30	[117]	39.80	[114]	-	-	390.55	[121]	587.45	[121]	(13.47)	-
93	74	C	K6104a	4-methylpentan-2-one	108-10-1	1.0	298.15	796.30	[117]	41.00	[114]	188.15	[120]	389.65	[121]	574.60	[121]	13.11	[120]

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
94	75	C	K6105a	hexan-3-one	589-38-8	1.0	298.15	811.10	117	40.60	114	217.75	120	396.65	121	582.82	121	(13.47)	-
95	76	C	K6106a	hexan-2-one	591-78-6	1.0	298.15	807.14	117	42.20	114	217.70	120	400.85	121	587.61	121	14.56	120
96	77	C	K6201a	3-methylpentane-2,4-dione	815-57-6	0.01	332.77	946.77	121	46.75	121	-	-	444.65	121	629.00	121	(15.28)	-
97	78	C	K6204a	hexane-2,4-dione	3002-24-2	1.0	293.15	959.00	120	-	-	-	-	433.15	121	629.00	121	(15.28)	-
98	78	C	K6204b	hexane-2,4-dione	3002-24-2	0.01	323.57	-	-	44.21	121	-	-	433.15	121	629.00	121	(15.28)	-
99	79	C	K6205a	hexane-2,5-dione	110-13-4	0.01	350.77	884.64	121	-	-	267.65	120	467.15	121	629.00	121	(15.28)	-
100	79	C	K6205b	hexane-2,5-dione	110-13-4	1.0	401.0	-	-	50.10	114	267.65	120	467.15	121	629.00	121	(15.28)	-
101	80	C	E3201a	methyl acetate	79-20-9	1.01	298.15	927.50	118	32.30	114	174.95	120	330.09	121	506.55	121	7.07	120
102	81	C	E4201a	methyl propanoate	554-12-1	1.0	298.15	909.10	118	35.70	114	185.65	120	352.60	121	530.60	121	6.200	120
103	82	C	E4202a	ethyl acetate	141-78-6	1.0	298.15	894.27	116	35.10	114	189.35	120	350.21	121	523.30	121	6.0814	120
104	83	C	E5201a	methyl 2-methylpropanoate	547-63-7	1.0	298.15	883.30	116	37.30	114	188.55	120	365.65	121	540.70	121	(5.62)	-
105	84	C	E5202a	propan-2-yl acetate	108-21-4	1.0	298.15	869.00	116	37.00	114	199.75	120	361.65	121	532.00	121	(5.62)	-
106	85	C	E5203a	methyl butanoate	623-42-7	1.01	298.15	892.52	118	39.80	114	187.35	120	375.90	121	554.50	121	5.48	120
107	86	C	E5204a	ethyl propanoate	105-37-3	1.0	298.15	884.04	116	39.30	114	199.55	120	372.25	121	546.00	121	5.76	120
108	87	C	E5205a	propyl acetate	109-60-4	1.01	298.15	882.80	118	39.10	114	180.15	120	374.65	121	549.73	121	5.62	120
109	88	C	E6201a	methyl 2,2-dimethylpropanoate	598-98-1	1.0	293.15	850.00	116	38.80	114	-	-	374.25	121	-	-	(5.20)	-
110	89	C	E6202a	tert-butyl acetate	540-88-5	1.0	298.15	861.59	116	38.00	114	-	-	369.15	121	564.61	121	5.672	120
111	90	C	E6203a	methyl 2-methylbutanoate	868-57-5	1.0	293.15	884.70	116	-	-	-	-	-	-	-	-	(5.20)	-
112	91	C	E6204a	ethyl 2-methylpropanoate	97-62-1	1.0	298.15	864.04	116	39.80	114	175.35	120	383.00	121	553.15	121	(5.20)	-
113	92	C	E6205a	methyl 3-methylbutanoate	556-24-1	1.0	298.15	875.87	116	-	-	-	-	389.65	121	564.61	121	(5.20)	-
114	92	C	E6205b	methyl 3-methylbutanoate	556-24-1	0.02	298.15	-	-	39.41	121	-	-	389.65	121	564.61	121	(5.20)	-
115	93	C	E6206a	propan-2-yl propanoate	637-78-5	1.0	298.15	860.10	116	-	-	-	-	383.15	121	553.00	121	(5.20)	-
116	93	C	E6206b	propan-2-yl propanoate	637-78-5	0.03	298.15	-	-	38.40	121	-	-	383.15	121	553.00	121	(5.20)	-
117	94	C	E6207a	2-methylpropyl acetate	110-19-0	1.0	298.15	866.29	116	-	-	176.05	120	389.80	121	560.80	121	5.068	120
118	94	C	E6207b	2-methylpropyl acetate	110-19-0	0.02	298.15	-	-	39.52	121	176.05	120	389.80	121	560.80	121	5.068	120
119	95	C	E6208a	butan-2-yl acetate	105-46-4	1.0	298.15	866.05	116	40.70	114	174.25	120	385.15	121	564.61	121	5.135	120
120	96	C	E6209a	methyl pentanoate	624-24-8	1.0	298.15	885.17	116	43.70	114	-	-	400.55	121	564.61	121	4.992	120
121	97	C	E6210a	ethyl butanoate	105-54-4	1.0	298.15	873.78	116	42.00	114	176.15	120	394.65	121	571.00	121	5.18	120
122	98	C	E6211a	propyl propanoate	106-36-5	1.0	298.15	876.35	116	43.20	114	197.25	120	395.65	121	568.60	121	5.249	120
123	99	C	E6212a	butyl acetate	123-86-4	1.0	298.15	876.36	116	42.70	114	196.15	120	399.15	121	575.40	121	5.07	120
124	100	C	E5402a	dimethyl propanedioate	108-59-8	1.0	298.15	1146.71	116	57.50	114	211.15	120	454.55	121	-	-	9.82	120
125	101	C	E5403a	acetyloxymethyl acetate	628-51-3	1.0	298.15	1135.50	116	56.40	114	-	-	437.65	121	-	-	(9.82)	-
126	102	C	E6401a	dimethyl 2-methylpropanedioate	609-02-9	1.0	298.15	1093.63	116	-	-	-	-	447.15	121	-	-	(7.72)	-
127	102	C	E6401b	dimethyl 2-methylpropanedioate	609-02-9	1.0	293.0	-	-	57.80	114	-	-	447.15	121	-	-	(7.72)	-
128	103	C	E6402a	methyl 2-acetyloxypropanoate	6284-75-9	1.0	352.0	-	-	52.90	114	-	-	-	-	-	-	(7.72)	-
129	104	C	E6403a	1-acetyloxyethyl acetate	542-10-9	1.0	298.15	1070.00	120	59.00	114	292.05	120	442.15	121	635.00	121	(7.72)	-
130	105	C	E6405a	dimethyl butanedioate	106-65-0	1.0	298.15	1114.00	116	60.90	114	291.75	120	469.55	121	657.00	121	7.19	120
131	106	C	E6406a	methyl 3-acetyloxypropanoate	38003-42-8	1.0	350.0	-	-	68.00	114	-	-	-	-	-	-	(7.72)	-
132	107	C	E6407a	ethyl 2-acetyloxyacetate	623-86-9	1.0	452.15	-	-	39.31	121	-	-	452.15	121	-	-	(7.72)	-
133	108	C	E6408a	2-acetyloxyethyl acetate	111-55-7	1.0	298.15	1098.70	116	61.00	114	242.15	120	463.65	121	653.00	121	7.7	120
134	109	C	F2201a	methyl formate	107-31-3	1.0	298.15	966.82	116	28.40	114	173.45	120	304.90	121	487.20	121	9.20	120
135	110	C	F3201a	ethyl formate	109-94-4	1.0	298.15	915.87	116	31.50	114	193.55	120	327.46	121	508.40	121	8.57	120
136	111	C	F4201a	propan-2-yl formate	625-55-8	0.17	298.15	870.23	121	31.58	121	-	-	341.25	121	514.90	121	(6.92)	-
137	112	C	F4202a	propyl formate	110-74-7	1.0	298.15	899.89	116	36.60	114	180.25	120	353.97	121	538.00	121	6.92	120
138	113	C	F5201a	tert-butyl formate	762-75-4	0.09	298.15	871.91	121	33.63	121	-	-	355.95	121	540.95	121	(6.25)	-
139	114	C	F5202a	2-methylpropyl formate	542-55-2	1.0	298.15	875.70	116	-	-	177.65	120	371.22	121	551.35	121	6.41	120
140	114	C	F5202b	2-methylpropyl formate	542-55-2	0.05	298.15	-	-	36.15	121	177.65	120	371.22	121	551.35	121	6.41	120
141	115	C	F5203a	butan-2-yl formate	589-40-2	0.06	298.15	878.57	121	36.77	121	-	-	363.55	121	540.95	121	(6.25)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
142	116	C	F5204a	butyl formate	592-84-7	1.0	298.15	887.64	116	40.50	114	183.15	120	379.25	121	540.95	121	6.10	120
143	117	C	F6202a	2-methylbutan-2-yl formate	757-88-0	0.02	298.15	883.69	121	-	-	-	-	385.65	121	564.61	121	(5.57)	-
144	118	C	F6205a	pentan-3-yl formate	58368-67-5	0.02	298.15	874.27	121	-	-	-	-	393.76	121	564.61	121	(5.57)	-
145	119	C	F6206a	3-methylbutyl formate	110-45-2	1.0	298.15	877.00	116	-	-	179.65	120	397.15	120	564.61	121	5.44	120
146	119	C	F6206b	3-methylbutyl formate	110-45-2	0.01	298.85	-	-	40.77	121	179.65	120	397.15	120	564.61	121	5.44	120
147	120	C	F6208a	pentyl formate	638-49-3	1.0	298.15	880.37	116	45.20	114	200.15	120	406.60	121	576.00	121	5.7	120
148	121	C	F4401a	2-formyloxyethyl formate	629-15-2	1.0	273.15	1193.00	120	-	-	-	-	447.15	121	-	-	(6.0)	-
149	121	C	F4401b	2-formyloxyethyl formate	629-15-2	1.0	447.15	-	-	38.83	121	-	-	447.15	121	-	-	(6.0)	-
150	122	C	F5401a	2-formyloxypropyl formate	53818-14-7	1.0	348.15	-	-	29.51	121	-	-	348.15	121	-	-	(6.0)	-
151	123	C	L1101a	methanol	67-56-1	1.01	298.15	786.74	118	37.70	114	175.65	120	337.85	121	512.64	121	33.0	120
152	124	C	L2101a	ethanol	64-17-5	1.01	298.15	786.60	118	42.26	114	159.01	120	351.44	121	513.92	121	25.3	120
153	125	C	L3101a	propan-2-ol	67-63-0	1.0	298.15	781.23	115	44.40	114	185.24	120	355.41	121	508.31	121	20.18	120
154	126	C	L3102a	propan-1-ol	71-23-8	1.0	298.15	799.81	115	46.60	114	148.76	120	370.35	121	536.78	121	20.8	120
155	127	C	L4101a	2-methylpropan-2-ol	75-65-0	1.0	299.15	779.48	115	46.20	114	298.96	120	355.57	121	506.21	121	12.47	120
156	128	C	L4102a	2-methylpropan-1-ol	78-83-1	1.0	298.15	797.81	115	50.79	114	171.19	120	380.81	121	547.78	121	17.93	120
157	129	C	L4103a	butan-2-ol	78-92-2	1.01	298.15	803.01	118	48.50	114	184.71	120	372.70	121	536.05	121	17.26	120
158	130	C	L4104a	butan-1-ol	71-36-3	1.0	298.15	805.80	118	52.10	114	184.55	120	390.81	121	563.05	121	17.84	120
159	131	C	L5101a	2,2-dimethylpropan-1-ol	75-84-3	0.08	327.15	780.00	121	-	-	328.15	120	386.25	121	569.99	121	8.35	120
160	131	C	L5101b	2,2-dimethylpropan-1-ol	75-84-3	1.0	345.0	-	-	47.50	114	328.15	120	386.25	121	569.99	121	8.35	120
161	132	C	L5102a	2-methylbutan-2-ol	75-85-4	1.0	298.15	804.73	115	50.10	114	264.45	120	375.15	121	543.70	121	5.78	120
162	133	C	L5103a	3-methylbutan-2-ol	598-75-4	1.0	298.15	815.00	115	-	-	-	-	384.65	121	556.10	121	(11.99)	-
163	134	C	L5104a	2-methylbutan-1-ol	137-32-6	1.0	298.15	815.20	115	54.10	114	-	-	401.85	121	575.40	121	(11.99)	-
164	135	C	L5105a	pentan-3-ol	584-02-1	1.0	298.15	815.40	115	52.90	114	203.25	120	388.45	121	559.60	121	13.35	120
165	136	C	L5106a	3-methylbutan-1-ol	123-51-3	1.0	298.15	806.90	115	55.30	114	155.95	120	404.35	121	577.20	121	15.63	120
166	137	C	L5107a	pentan-2-ol	6032-29-7	1.01	298.15	805.30	118	53.60	114	200.15	120	392.15	121	560.30	121	13.71	120
167	138	C	L5108a	pentan-1-ol	71-41-0	1.0	298.15	811.34	115	56.90	114	195.57	120	410.95	121	588.10	121	15.13	120
168	139	C	L6101a	3,3-dimethylbutan-2-ol	464-07-3	0.01	298.15	813.91	121	-	-	-	-	393.15	121	596.03	121	(8.51)	-
169	139	C	L6101b	3,3-dimethylbutan-2-ol	464-07-3	1.0	298.0	-	-	53.80	114	-	-	393.15	121	596.03	121	(8.51)	-
170	140	C	L6102a	2,3-dimethylbutan-2-ol	594-60-5	1.0	298.15	818.59	115	54.00	114	262.65	120	391.75	121	596.03	121	(8.51)	-
171	141	C	L6103a	2,2-dimethylbutan-1-ol	1185-33-7	1.0	298.15	824.50	115	55.7	114	-	-	409.95	121	596.03	121	10.5	120
172	141	C	L6103b	2,2-dimethylbutan-1-ol	1185-33-7	1.0	313.0	-	-	52.10	114	-	-	409.95	121	596.03	121	10.5	120
173	142	C	L6104a	3-methylpentan-3-ol	77-74-7	1.0	298.15	823.80	115	-	-	249.55	120	395.56	121	575.60	121	4.322	120
174	143	C	L6105a	3,3-dimethylbutan-1-ol	624-95-3	1.0	298.15	809.70	115	58.00	114	213.15	120	416.15	121	596.03	121	(8.51)	-
175	144	C	L6106a	2-methylpentan-2-ol	590-36-3	1.0	298.15	809.45	115	54.70	114	170.15	120	394.56	121	559.50	121	(8.51)	-
176	145	C	L6107a	2,3-dimethylbutan-1-ol	19550-30-2	1.0	298.15	823.70	115	-	-	-	-	422.15	121	596.03	121	(8.51)	-
177	145	C	L6107b	2,3-dimethylbutan-1-ol	19550-30-2	1.0	339.0	-	-	51.40	114	-	-	422.15	121	596.03	121	(8.51)	-
178	146	C	L6108a	3-methylpentan-2-ol	565-60-6	1.0	298.15	824.73	115	58.20	114	-	-	407.36	121	596.03	121	(8.51)	-
179	147	C	L6109a	2-methylpentan-3-ol	565-67-3	1.0	298.15	820.13	115	56.00	114	-	-	399.66	121	596.03	121	(8.51)	-
180	148	C	L6110a	4-methylpentan-2-ol	108-11-2	1.0	298.15	803.04	115	-	-	183.15	120	404.85	121	574.40	121	(8.51)	-
181	148	C	L6110b	4-methylpentan-2-ol	108-11-2	1.0	308.0	-	-	49.60	114	183.15	120	404.85	121	574.40	121	(8.51)	-
182	149	C	L6111a	2-ethylbutan-1-ol	97-95-0	1.0	298.15	829.27	115	60.30	114	-	-	419.65	121	596.03	121	6.19	120
183	150	C	L6112a	3-methylpentan-1-ol	589-35-5	1.0	298.15	820.50	115	61.70	114	-	-	425.55	121	596.03	121	(8.51)	-
184	151	C	L6113a	2-methylpentan-1-ol	105-30-6	1.0	298.15	820.63	115	59.40	114	-	-	421.15	121	604.40	121	(8.51)	-
185	152	C	L6114a	hexan-3-ol	623-37-0	1.0	298.15	814.49	115	58.60	114	-	-	408.55	121	596.03	121	(8.51)	-
186	153	C	L6115a	4-methylpentan-1-ol	626-89-1	1.0	298.15	809.72	115	-	-	-	-	424.95	121	603.50	121	(8.51)	-
187	153	C	L6115b	4-methylpentan-1-ol	626-89-1	1.0	313.0	-	-	63.90	114	-	-	424.95	121	603.50	121	(8.51)	-
188	154	C	L6116a	hexan-2-ol	626-93-7	1.0	298.15	810.34	115	58.30	114	-	-	413.04	121	585.90	121	(8.51)	-
189	155	C	L6117a	hexan-1-ol	111-27-3	1.0	298.15	815.54	115	59.60	114	226.75	120	430.15	121	610.30	121	13.03	120

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
190	156	C	L2201a	ethane-1,2-diol	107-21-1	1.0	298.15	1109.94	[115]	64.80	[114]	260.15	[120]	470.45	[121]	720.00	[121]	41.4	[120]
191	157	C	L3201a	propane-1,2-diol	57-55-6	1.0	298.15	1032.52	[115]	62.20	[114]	213.15	[120]	460.75	[121]	700.17	[121]	27.5	[120]
192	158	C	L3202a	propane-1,3-diol	504-63-2	1.0	298.15	1050.30	[115]	69.80	[114]	245.55	[120]	487.55	[121]	724.00	[121]	35.1	[120]
193	159	C	L4201a	2-methylpropane-1,2-diol	558-43-0	1.0	298.15	989.60	[115]	-	-	-	-	451.15	[121]	728.82	[121]	(30.35)	-
194	160	C	L4202a	butane-2,3-diol	513-85-9	1.0	298.15	999.80	[115]	-	-	-	-	455.15	[121]	728.82	[121]	(30.35)	-
195	160	C	L4202b	butane-2,3-diol	513-85-9	1.0	332.0	-	-	58.40	[114]	-	-	455.15	[121]	728.82	[121]	(30.35)	-
196	161	C	L4203a	2-methylpropane-1,3-diol	2163-42-0	1.0	293.15	1009.00	[115]	71.30	[114]	182.15	[120]	487.15	[121]	728.82	[121]	(30.35)	-
197	162	C	L4204a	butane-1,2-diol	584-03-2	1.0	298.15	999.22	[115]	-	-	-	-	464.15	[121]	680.00	[121]	(30.35)	-
198	163	C	L4205a	butane-1,3-diol	107-88-0	1.0	298.15	1000.20	[115]	72.60	[114]	196.15	[120]	480.15	[121]	676.00	[121]	28.8	[120]
199	164	C	L4206a	butane-1,4-diol	110-63-4	1.0	298.15	1015.40	[115]	76.60	[114]	293.58	[120]	501.15	[121]	728.82	[121]	31.9	[120]
200	165	C	L5201a	2-methylbutane-2,3-diol	5396-58-7	1.0	298.15	968.80	[115]	-	-	-	-	447.15	[121]	754.49	[121]	(22.21)	-
201	166	C	L5204a	3-methylbutane-1,3-diol	2568-33-4	1.0	293.15	964.50	[115]	-	-	-	-	472.15	[121]	754.49	[121]	24.56	[122]
202	167	C	L5205a	2-methylbutane-1,3-diol	684-84-4	1.0	293.15	991.70	[115]	-	-	-	-	473.15	[121]	754.49	[121]	(22.21)	-
203	168	C	L5206a	3-methylbutane-1,2-diol	50468-22-9	1.0	294.65	984.20	[115]	-	-	-	-	473.15	[121]	754.49	[121]	(22.21)	-
204	169	C	L5207a	pentane-2,3-diol	42027-23-6	1.0	292.15	979.80	[120]	-	-	-	-	460.65	[121]	754.49	[121]	17.37	[120]
205	170	C	L5208a	pentane-2,4-diol	625-69-4	1.0	298.15	956.00	[115]	72.50	[114]	-	-	472.15	[121]	754.49	[121]	24.69	[120]
206	171	C	L5211a	pentane-1,3-diol	3174-67-2	1.0	293.15	981.00	[115]	-	-	-	-	494.15	[121]	754.49	[121]	(22.21)	-
207	172	C	L5212a	pentane-1,2-diol	5343-92-0	1.0	297.15	969.10	[115]	74.60	[114]	-	-	482.15	[121]	754.49	[121]	(22.21)	-
208	173	C	L5213a	pentane-1,4-diol	626-95-9	1.0	293.15	989.50	[115]	-	-	-	-	497.00	[121]	754.49	[121]	26.74	[120]
209	174	C	L5214a	pentane-1,5-diol	111-29-5	1.0	298.15	989.71	[115]	86.80	[114]	253.15	[120]	512.15	[121]	754.49	[121]	26.2	[120]
210	175	C	L6201a	2,3-dimethylbutane-2,3-diol	76-09-5	0.002	316.45	970.40	[121]	-	-	316.45	[120]	445.95	[121]	777.84	[121]	(25.86)	-
211	176	C	L6204a	3-methylpentane-2,3-diol	63521-37-9	1.0	298.15	963.80	[115]	-	-	-	-	505.76	[121]	777.84	[121]	(25.86)	-
212	177	C	L6205a	3,3-dimethylbutane-1,2-diol	59562-82-2	1.0	323.15	940.00	[115]	-	-	-	-	478.65	[121]	777.84	[121]	(25.86)	-
213	178	C	L6206a	2,3-dimethylbutane-1,3-diol	24893-35-4	1.0	298.15	964.50	[115]	-	-	-	-	480.00	[121]	777.84	[121]	(25.86)	-
214	179	C	L6207a	2-methylpentane-2,3-diol	7795-80-4	1.0	293.15	962.70	[115]	-	-	-	-	505.76	[121]	777.84	[121]	(25.86)	-
215	180	C	L6208a	2-methylpentane-2,4-diol	107-41-5	1.0	298.15	918.53	[115]	68.60	[114]	223.15	[120]	470.65	[121]	777.84	[121]	25.86	[120]
216	181	C	L6209a	3-methylpentane-2,4-diol	5683-44-3	1.0	287.15	990.60	[115]	-	-	-	-	484.65	[121]	777.84	[121]	(25.86)	-
217	182	C	L6210a	2-ethyl-2-methylpropane-1,3-diol	77-84-9	1.0	323.15	958.20	[115]	-	-	-	-	498.95	[121]	777.84	[121]	(25.86)	-
218	183	C	L6212a	2,2-dimethylbutane-1,4-diol	32812-23-0	1.0	277.15	996.00	[115]	-	-	-	-	480.00	[121]	777.84	[121]	(25.86)	-
219	184	C	L6213a	3-methylpentane-1,3-diol	33879-72-0	1.0	293.15	969.00	[115]	-	-	-	-	482.98	[121]	777.84	[121]	(25.86)	-
220	185	C	L6215a	4-methylpentane-1,4-diol	1462-10-8	1.0	293.15	964.50	[115]	-	-	-	-	494.35	[121]	777.84	[121]	(25.86)	-
221	186	C	L6216a	2-propan-2-ylpropane-1,3-diol	2612-27-3	1.0	293.15	976.80	[115]	-	-	-	-	496.94	[121]	777.84	[121]	(25.86)	-
222	187	C	L6217a	2-ethylbutane-1,3-diol	66553-17-1	1.0	298.15	967.70	[115]	-	-	-	-	480.00	[121]	777.84	[121]	(25.86)	-
223	188	C	L6218a	2,3-dimethylbutane-1,4-diol	57716-80-0	1.0	293.15	977.10	[115]	-	-	-	-	-	-	-	-	(25.86)	-
224	189	C	L6219a	2-methylpentane-1,3-diol	149-31-5	1.0	295.15	973.70	[115]	-	-	-	-	493.45	[121]	777.84	[121]	(25.86)	-
225	190	C	L6220a	hexane-3,4-diol	922-17-8	1.0	273.15	799.30	[115]	-	-	-	-	496.94	[121]	777.84	[121]	(25.86)	-
226	191	C	L6221a	hexane-2,3-diol	617-30-1	1.0	288.15	989.00	[115]	-	-	-	-	478.15	[121]	777.84	[121]	(25.86)	-
227	192	C	L6222a	hexane-2,4-diol	19780-90-6	1.0	294.15	951.60	[115]	-	-	-	-	484.15	[121]	777.84	[121]	(25.86)	-
228	193	C	L6223a	hexane-2,5-diol	2935-44-6	1.0	323.15	939.80	[115]	-	-	316.15	[120]	493.95	[121]	777.84	[121]	(25.86)	-
229	194	C	L6224a	2-propylpropane-1,3-diol	2612-28-4	1.0	298.15	963.60	[115]	-	-	-	-	474.16	[121]	777.84	[121]	(25.86)	-
230	195	C	L6225a	3-methylpentane-1,5-diol	4457-71-0	1.0	293.15	972.60	[115]	-	-	-	-	521.55	[121]	777.84	[121]	(25.86)	-
231	196	C	L6226a	2-methylpentane-1,5-diol	42856-62-2	1.0	293.15	971.90	[115]	-	-	-	-	496.94	[121]	777.84	[121]	(25.86)	-
232	197	C	L6227a	hexane-1,3-diol	21531-91-9	1.0	295.15	958.00	[115]	-	-	-	-	508.15	[121]	777.84	[121]	(25.86)	-
233	198	C	L6228a	hexane-1,4-diol	16432-53-4	1.0	289.45	982.00	[115]	-	-	-	-	529.15	[121]	777.84	[121]	(25.86)	-
234	199	C	L6230a	hexane-1,5-diol	928-40-5	1.0	298.15	964.00	[115]	-	-	-	-	510.15	[121]	777.84	[121]	(25.86)	-
235	200	C	L6231a	hexane-1,6-diol	629-11-8	1.0	318.15	968.30	[115]	-	-	314.65	[120]	516.15	[121]	777.84	[121]	(25.86)	-
236	200	C	L6231b	hexane-1,6-diol	629-11-8	1.0	342.0	-	-	87.00	[114]	314.65	[120]	516.15	[121]	777.84	[121]	(25.86)	-
237	201	C	L3301a	propane-1,2,3-triol	56-81-5	1.0	298.15	1258.30	[115]	-	-	291.35	[120]	563.15	[121]	850.00	[121]	46.53	[120]

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
238	201	C	L3301b	propane-1,2,3-triol	56-81-5	1.0	308.0	-	-	85.80	[114]	291.35	[120]	563.15	[121]	850.00	[121]	46.53	[120]
239	202	C	L4302a	butane-1,2,4-triol	3068-00-6	1.0	298.15	1184.00	[115]	-	-	-	-	-	-	697.00	[121]	(39.02)	-
240	203	C	L5303a	pentane-1,3,5-triol	4328-94-3	1.0	298.15	1103.60	[115]	-	-	-	-	460.64	[121]	-	-	(39.02)	-
241	204	C	L6306a	hexane-1,3,6-triol	18990-98-2	1.0	293.15	1104.10	[115]	-	-	-	-	-	-	-	-	(31.50)	-
242	205	C	L6307a	hexane-1,2,6-triol	106-69-4	1.0	298.15	1099.98	[115]	-	-	-	-	472.47	[121]	-	-	31.5	[120]
243	206	C	C1201a	formic acid	64-18-6	1.0	298.15	1213.6	[117]	46.3	[114]	281.45	[120]	373.71	[121]	588.00	[121]	51.1	[120]
244	207	C	C2201a	acetic acid	64-19-7	1.01	298.15	1043.50	[118]	50.30	[114]	290.15	[120]	391.05	[121]	591.95	[121]	6.20	[120]
245	208	C	C3201a	propanoic acid	79-09-4	1.01	298.15	988.10	[118]	54.90	[114]	252.65	[120]	414.32	[121]	600.81	[121]	3.44	[120]
246	209	C	C4201a	2-methylpropanoic acid	79-31-2	1.0	298.15	943.89	[117]	56.30	[114]	227.15	[120]	427.55	[120]	-	-	2.58	[120]
247	210	C	C4202a	butanoic acid	107-92-6	1.0	298.15	952.94	[117]	58.20	[114]	268.03	[120]	436.85	[120]	615.70	[121]	2.98	[120]
248	211	C	C5201a	2,2-dimethylpropanoic acid	75-98-9	1.0	309.82	907.45	[117]	-	-	309.15	[120]	436.95	[121]	630.95	[121]	(2.66)	-
249	211	C	C5201b	2,2-dimethylpropanoic acid	75-98-9	1.0	320.0	-	-	57.60	[114]	309.15	[120]	436.95	[121]	630.95	[121]	(2.66)	-
250	212	C	C5202a	2-methylbutanoic acid	116-53-0	1.0	298.15	934.70	[117]	-	-	-	-	450.15	[120]	630.95	[121]	(2.66)	-
251	213	C	C5203a	3-methylbutanoic acid	503-74-2	1.0	298.15	924.06	[117]	61.20	[114]	243.55	[120]	448.25	[121]	629.09	[121]	(2.66)	-
252	214	C	C5204a	pentanoic acid	109-52-4	1.0	298.15	934.40	[117]	63.00	[114]	239.52	[120]	458.65	[121]	639.16	[121]	2.661	[120]
253	215	C	C6201a	2,2-dimethylbutanoic acid	595-37-9	1.0	293.15	927.47	[117]	-	-	258.15	[120]	459.15	[121]	654.61	[121]	(2.72)	-
254	215	C	C6201b	2,2-dimethylbutanoic acid	595-37-9	1.0	370.0	-	-	59.40	[114]	258.15	[120]	459.15	[121]	654.61	[121]	(2.72)	-
255	216	C	C6202a	3,3-dimethylbutanoic acid	1070-83-3	1.0	298.05	908.00	[117]	64.00	[114]	279.15	[120]	457.15	[120]	654.61	[121]	2.85	[120]
256	217	C	C6203a	2,3-dimethylbutanoic acid	14287-61-7	1.0	293.15	927.45	[117]	-	-	-	-	464.85	[121]	654.61	[121]	(2.72)	-
257	218	C	C6204a	2-ethylbutanoic acid	88-09-5	1.0	298.15	923.50	[117]	-	-	241.35	[120]	466.15	[120]	654.61	[121]	2.72	[120]
258	218	C	C6204b	2-ethylbutanoic acid	88-09-5	1.0	388.0	-	-	58.20	[114]	241.35	[120]	466.15	[120]	654.61	[121]	2.72	[120]
259	219	C	C6205a	2-methylpentanoic acid	97-61-0	1.0	298.15	918.22	[117]	-	-	-	-	-	-	654.61	[121]	(2.72)	-
260	220	C	C6206a	3-methylpentanoic acid	105-43-1	1.0	298.15	923.00	[117]	-	-	-	-	-	-	654.61	[121]	(2.72)	-
261	221	C	C6207a	4-methylpentanoic acid	646-07-1	1.0	298.15	917.00	[117]	-	-	240.15	[120]	473.65	[121]	654.61	[121]	(2.72)	-
262	221	C	C6207b	4-methylpentanoic acid	646-07-1	1.0	354.0	-	-	91.70	[114]	240.15	[120]	473.65	[121]	654.61	[121]	(2.72)	-
263	222	C	C6208a	hexanoic acid	142-62-1	1.0	298.15	922.88	[117]	69.20	[114]	269.05	[120]	478.85	[121]	660.20	[121]	2.600	[120]
264	223	C	M1101a	methanamine	74-89-5	1.0	266.85	694.21	[117]	26.11	[121]	179.73	[120]	266.82	[121]	430.05	[121]	16.7	[120]
265	223	C	M1101b	methanamine	74-89-5	3.52	298.15	655.00	[121]	-	-	179.73	[120]	266.82	[121]	430.05	[121]	16.7	[120]
266	224	C	M2101a	ethanamine	75-04-7	1.0	288.15	688.56	[117]	27.35	[121]	192.15	[120]	289.73	[121]	456.15	[121]	8.7	[120]
267	225	C	M3101a	propan-2-amine	75-31-0	1.01	298.15	683.94	[118]	28.40	[114]	178.03	[120]	305.55	[121]	471.85	[121]	5.6268	[120]
268	226	C	M3102a	propan-1-amine	107-10-8	1.01	298.15	712.76	[118]	31.30	[114]	188.37	[120]	321.65	[121]	496.95	[121]	5.08	[120]
269	227	C	M4101a	2-methylpropan-2-amine	75-64-9	1.0	298.15	690.07	[117]	29.60	[114]	206.23	[120]	317.55	[121]	483.90	[121]	(4.71)	-
270	228	C	M4102a	butan-2-amine	13952-84-6	1.01	298.15	717.81	[118]	32.60	[114]	-	-	336.15	[121]	514.30	[121]	(4.71)	-
271	229	C	M4103a	2-methylpropan-1-amine	78-81-9	1.0	298.15	729.14	[117]	33.80	[114]	187.15	[120]	340.88	[121]	522.40	[121]	(4.71)	-
272	230	C	M4104a	butan-1-amine	109-73-9	1.0	298.15	736.83	[117]	35.60	[114]	224.15	[120]	350.55	[121]	531.90	[121]	4.71	[120]
273	231	C	M5101a	2-methylbutan-2-amine	594-39-8	0.11	298.15	727.59	[121]	32.49	[121]	168.15	[120]	350.15	[121]	557.66	[121]	(4.27)	-
274	232	C	M5102a	2,2-dimethylpropan-1-amine	5813-64-9	0.1	298.15	728.07	[121]	33.38	[121]	-	-	350.15	[121]	557.66	[121]	(4.27)	-
275	233	C	M5103a	3-methylbutan-2-amine	598-74-3	0.08	298.15	753.00	[121]	33.88	[121]	223.15	[120]	357.15	[121]	557.66	[121]	(4.27)	-
276	234	C	M5104a	pentan-3-amine	616-24-0	1.0	291.35	711.30	[117]	-	-	-	-	362.15	[121]	557.66	[121]	(4.27)	-
277	234	C	M5104b	pentan-3-amine	616-24-0	0.06	298.15	-	-	34.61	[121]	-	-	362.15	[121]	557.66	[121]	(4.27)	-
278	235	C	M5105a	2-methylbutan-1-amine	96-15-1	1.0	298.15	750.50	[117]	-	-	-	-	368.65	[121]	557.66	[121]	(4.27)	-
279	235	C	M5105b	2-methylbutan-1-amine	96-15-1	0.04	298.15	-	-	35.61	[121]	-	-	368.65	[121]	557.66	[121]	(4.27)	-
280	236	C	M5106a	pentan-2-amine	63493-28-7	0.05	298.15	735.70	[121]	34.82	[121]	-	-	364.85	[121]	557.66	[121]	(4.27)	-
281	237	C	M5107a	3-methylbutan-1-amine	107-85-7	1.0	298.15	744.30	[117]	-	-	-	-	370.15	[121]	557.66	[121]	(4.27)	-
282	237	C	M5107b	3-methylbutan-1-amine	107-85-7	0.04	298.15	-	-	35.13	[121]	-	-	370.15	[121]	557.66	[121]	(4.27)	-
283	238	C	M5108a	pentan-1-amine	110-58-7	0.04	298.15	751.00	[121]	-	-	222.15	[120]	377.65	[121]	557.66	[121]	4.27	[120]
284	238	C	M5108b	pentan-1-amine	110-58-7	1.0	298.0	-	-	40.10	[114]	222.15	[120]	377.65	[121]	557.66	[121]	4.27	[120]
285	239	C	M6101a	2,3-dimethylbutan-2-amine	4358-75-2	0.03	298.15	760.06	[121]	-	-	-	-	377.65	[121]	589.15	[121]	(4.08)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
286	240	C	M6102a	3,3-dimethylbutan-2-amine	3850-30-4	0.04	298.15	760.06	121	36.13	121	253.15	120	375.15	121	589.15	121	(4.08)	-
287	241	C	M6103a	3-methylpentan-3-amine	3495-46-3	0.01	300.86	757.89	121	-	-	-	-	398.45	121	589.15	121	(4.08)	-
288	242	C	M6104a	2,2-dimethylbutan-1-amine	41781-17-3	0.02	298.15	760.06	121	-	-	-	-	386.65	121	589.15	121	(4.08)	-
289	243	C	M6105a	2-methylpentan-2-amine	53310-02-4	0.03	298.15	743.00	121	36.13	121	-	-	377.15	121	589.15	121	(4.08)	-
290	244	C	M6106a	3,3-dimethylbutan-1-amine	15673-00-4	0.01	306.83	753.09	121	-	-	-	-	405.98	121	589.15	121	(4.08)	-
291	245	C	M6107a	2-methylpentan-3-amine	54287-41-1	0.01	308.71	741.67	121	-	-	-	-	408.33	121	589.15	121	(4.08)	-
292	246	C	M6108a	3-methylpentan-2-amine	35399-81-6	0.01	308.71	741.67	121	-	-	-	-	408.33	121	589.15	121	(4.08)	-
293	247	C	M6109a	2,3-dimethylbutan-1-amine	66553-05-7	0.03	298.15	752.75	121	-	-	-	-	378.15	121	589.15	121	(4.08)	-
294	248	C	M6110a	4-methylpentan-2-amine	108-09-8	0.02	298.15	745.70	121	37.37	121	-	-	381.65	121	589.15	121	(4.08)	-
295	249	C	M6111a	2-ethylbutan-1-amine	617-79-8	0.01	309.07	751.27	121	-	-	398.15	120	408.77	121	589.15	121	(4.08)	-
296	250	C	M6112a	hexan-3-amine	16751-58-9	0.01	309.07	761.11	121	-	-	-	-	408.77	121	589.15	121	(4.08)	-
297	251	C	M6113a	2-methylpentan-1-amine	13364-16-4	0.01	302.05	759.81	121	-	-	-	-	400.00	121	589.15	121	(4.08)	-
298	252	C	M6114a	3-methylpentan-1-amine	42245-37-4	0.01	298.15	767.00	121	-	-	-	-	395.15	121	589.15	121	(4.08)	-
299	253	C	M6115a	hexan-2-amine	5329-79-3	0.01	305.93	756.67	121	38.22	121	-	-	403.15	121	589.15	121	(4.08)	-
300	254	C	M6116a	4-methylpentan-1-amine	5344-20-7	0.01	301.25	767.49	121	39.81	121	-	-	397.05	121	589.15	121	(4.08)	-
301	255	C	M6117a	hexan-1-amine	111-26-2	1.0	298.15	762.99	117	45.00	114	252.15	120	404.65	121	589.15	121	4.08	120
302	256	C	N2101a	N-methylmethanamine	124-40-3	1.0	282.82	667.93	117	27.20	114	180.15	120	280.03	121	437.20	121	(3.12)	-
303	256	C	N2101b	N-methylmethanamine	124-40-3	1.96	298.15	649.96	121	-	-	180.15	120	280.03	121	437.20	121	(3.12)	-
304	257	C	N3101a	N-methylethanamine	624-78-2	0.65	298.15	684.00	121	26.66	121	-	-	309.15	121	475.00	121	(3.12)	-
305	258	C	N4101a	N-methylpropan-2-amine	4747-21-1	1.0	288.15	740.00	117	30.70	114	-	-	323.55	121	482.40	121	(3.68)	-
306	259	C	N4102a	N-ethylethanamine	109-89-7	1.0	298.15	701.20	117	31.20	114	223.15	120	328.60	121	496.60	121	3.680	120
307	260	C	N4103a	N-methylpropan-1-amine	627-35-0	0.2	298.15	711.93	121	31.15	121	-	-	336.15	121	482.40	121	(3.68)	-
308	261	C	N5101a	N,2-dimethylpropan-2-amine	14610-37-8	1.0	298.15	727.00	117	32.30	114	-	-	350.15	121	517.66	121	(3.12)	-
309	262	C	N5102a	N-methylbutan-2-amine	7713-69-1	0.1	298.15	719.96	121	33.32	121	-	-	351.65	121	517.66	121	(3.12)	-
310	263	C	N5103a	N,2-dimethylpropan-1-amine	625-43-4	0.12	298.15	729.96	121	-	-	-	-	346.15	121	517.66	121	(3.12)	-
311	264	C	N5104a	N-ethylpropan-2-amine	19961-27-4	0.13	298.15	719.96	121	-	-	-	-	349.15	121	517.66	121	(3.12)	-
312	264	C	N5104b	N-ethylpropan-2-amine	19961-27-4	1.0	298.0	-	-	33.10	114	-	-	349.15	121	517.66	121	(3.12)	-
313	265	C	N5105a	N-ethylpropan-1-amine	20193-20-8	0.11	298.15	726.66	121	31.88	121	-	-	353.45	121	517.66	121	(3.12)	-
314	266	C	N5106a	N-methylbutan-1-amine	110-68-9	0.05	298.15	728.09	121	-	-	-	-	364.25	121	517.66	121	(3.12)	-
315	266	C	N5106b	N-methylbutan-1-amine	110-68-9	1.0	298.0	-	-	38.10	114	-	-	364.25	121	517.66	121	(3.12)	-
316	267	C	N6101a	N,2,2-trimethylpropan-1-amine	26153-91-3	0.02	298.15	740.06	121	-	-	-	-	383.62	121	549.15	121	(2.92)	-
317	268	C	N6102a	N-ethyl-2-methylpropan-2-amine	4432-77-3	1.0	298.15	716.10	117	-	-	-	-	351.15	121	549.15	121	(2.92)	-
318	268	C	N6102b	N-ethyl-2-methylpropan-2-amine	4432-77-3	0.1	298.15	-	-	34.09	121	-	-	351.15	121	549.15	121	(2.92)	-
319	269	C	N6103a	N,3-dimethylbutan-2-amine	34317-39-0	0.02	298.15	740.06	121	-	-	-	-	386.41	121	549.15	121	(2.92)	-
320	270	C	N6104a	N-propan-2-ylpropan-2-amine	108-18-9	1.0	298.15	712.27	117	34.50	114	212.15	120	357.05	121	523.10	121	(2.92)	-
321	271	C	N6105a	N-methylpentan-3-amine	52317-98-3	0.03	298.15	740.06	121	37.35	121	-	-	381.15	121	549.15	121	(2.92)	-
322	272	C	N6106a	N-ethylbutan-2-amine	21035-44-9	0.04	298.15	729.77	121	-	-	-	-	371.15	121	549.15	121	(2.92)	-
323	272	C	N6106b	N-ethylbutan-2-amine	21035-44-9	1.0	298.0	-	-	37.90	114	-	-	371.15	121	549.15	121	(2.92)	-
324	273	C	N6107a	N-propan-2-ylpropan-1-amine	21968-17-2	0.04	298.15	723.16	121	-	-	-	-	371.45	121	549.15	121	(2.92)	-
325	273	C	N6107b	N-propan-2-ylpropan-1-amine	21968-17-2	1.0	298.0	-	-	37.30	114	-	-	371.45	121	549.15	121	(2.92)	-
326	274	C	N6108a	N,2-dimethylbutan-1-amine	51932-19-5	0.02	298.15	740.06	121	-	-	-	-	386.41	121	549.15	121	(2.92)	-
327	275	C	N6109a	N-ethyl-2-methylpropan-1-amine	13205-60-2	0.04	298.15	730.04	121	36.13	121	-	-	371.15	121	549.15	121	(2.92)	-
328	276	C	N6110a	N,3-dimethylbutan-1-amine	4104-44-3	1.0	295.15	739.00	117	-	-	-	-	-	-	-	-	(2.92)	-
329	277	C	N6111a	N-propylpropan-1-amine	142-84-7	1.0	298.15	734.90	117	40.00	114	210.15	120	382.00	121	550.00	121	2.923	120
330	278	C	N6112a	N-ethylbutan-1-amine	13360-63-9	0.02	298.15	735.42	121	-	-	-	-	381.15	121	549.15	121	(2.92)	-
331	278	C	N6112b	N-ethylbutan-1-amine	13360-63-9	1.0	298.0	-	-	40.20	114	-	-	381.15	121	549.15	121	(2.92)	-
332	279	C	N6113a	N-methylpentan-1-amine	25419-06-1	0.02	298.15	743.01	121	39.93	121	-	-	390.55	121	549.15	121	(2.92)	-
333	280	C	R3101a	N,N-dimethylmethanamine	75-50-3	1.0	273.15	655.70	117	22.91	121	156.05	120	276.02	121	433.25	121	2.440	120

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
334	280	C	R3101b	N,N-dimethylmethanamine	75-50-3	2.33	298.15	628.94	121	-	-	156.05	120	276.02	121	433.25	121	2.440	120
335	281	C	R4101a	N,N-dimethylethanamine	598-56-1	1.0	298.15	669.40	117	-	-	133.15	120	310.15	121	500.00	121	(2.41)	-
336	281	C	R4101b	N,N-dimethylethanamine	598-56-1	0.67	298.15	-	-	26.68	121	133.15	120	310.15	121	500.00	121	(2.41)	-
337	282	C	R5101a	N,N-dimethylpropan-2-amine	996-35-0	1.0	298.15	710.60	117	31.90	114	-	-	339.18	121	517.66	121	(2.41)	-
338	283	C	R5102a	N-ethyl-N-methylethanamine	616-39-7	1.0	298.15	701.55	117	31.80	114	77.15	120	339.15	121	517.66	121	(2.41)	-
339	284	C	R5103a	N,N-dimethylpropan-1-amine	926-63-6	0.21	298.15	695.57	121	31.14	121	-	-	339.15	121	517.66	121	(2.41)	-
340	285	C	R6101a	N,N,2-trimethylpropan-2-amine	918-02-5	1.0	298.15	737.60	117	34.80	114	-	-	363.15	121	549.15	121	(2.42)	-
341	286	C	R6102a	N,N-dimethylbutan-2-amine	921-04-0	0.05	298.15	733.93	121	35.36	121	-	-	367.15	121	549.15	121	(2.42)	-
342	287	C	R6103a	N-ethyl-N-methylpropan-2-amine	39198-07-7	0.06	298.15	721.46	121	35.05	121	-	-	364.65	121	549.15	121	(2.42)	-
343	288	C	R6104a	N,N,2-trimethylpropan-1-amine	7239-24-9	0.1	298.15	719.96	121	33.08	121	-	-	354.15	121	549.15	121	(2.42)	-
344	289	C	R6105a	N,N-diethylethanamine	121-44-8	1.01	298.15	723.01	118	-	-	158.45	120	361.92	121	535.15	121	2.418	120
345	289	C	R6105b	N,N-diethylethanamine	121-44-8	0.06	298.15	-	-	34.91	121	158.45	120	361.92	121	535.15	121	2.418	120
346	290	C	R6106a	N-ethyl-N-methylpropan-1-amine	4458-32-6	0.06	298.15	718.00	121	35.05	121	-	-	364.65	121	549.15	121	(2.42)	-
347	291	C	R6107a	N,N-dimethylbutan-1-amine	927-62-8	0.06	298.15	716.01	121	35.29	121	-	-	367.15	121	549.15	121	(2.42)	-
348	292	C	N2201a	ethane-1,2-diamine	107-15-3	0.02	298.15	892.82	121	-	-	284.29	120	390.41	121	593.00	121	13.82	120
349	292	C	N2201b	ethane-1,2-diamine	107-15-3	1.0	298.0	-	-	45.00	114	284.29	120	390.41	121	593.00	121	13.82	120
350	293	C	N3201a	N'-methylethane-1,2-diamine	109-81-9	1.0	298.15	841.00	120	-	-	-	-	388.15	121	-	-	(13.82)	-
351	293	C	N3201b	N'-methylethane-1,2-diamine	109-81-9	1.0	388.15	-	-	33.25	121	-	-	388.15	121	-	-	(13.82)	-
352	294	C	N3202a	propane-1,2-diamine	78-90-0	0.02	298.15	856.00	121	-	-	-	-	392.45	121	585.03	121	(13.82)	-
353	294	C	N3202b	propane-1,2-diamine	78-90-0	1.0	298.0	-	-	44.20	114	-	-	392.45	121	585.03	121	(13.82)	-
354	295	C	N3203a	propane-1,3-diamine	109-76-2	1.0	298.15	884.00	120	50.20	114	262.25	120	412.95	121	608.00	121	(13.82)	-
355	296	C	N4201a	N',N'-dimethylethane-1,2-diamine	108-00-9	1.0	298.15	803.00	120	-	-	-	-	378.65	121	-	-	(13.82)	-
356	296	C	N4201b	N',N'-dimethylethane-1,2-diamine	108-00-9	1.0	378.65	-	-	31.11	121	-	-	378.65	121	-	-	(13.82)	-
357	297	C	N4202a	N,N'-dimethylethane-1,2-diamine	110-70-3	1.0	288.15	828.00	120	-	-	-	-	393.15	121	-	-	(13.82)	-
358	297	C	N4202b	N,N'-dimethylethane-1,2-diamine	110-70-3	1.0	393.15	-	-	34.96	121	-	-	393.15	121	-	-	(13.82)	-
359	298	C	N4203a	2-methylpropane-1,2-diamine	811-93-8	1.0	298.15	841.00	120	45.80	114	-	-	396.15	121	-	-	(13.82)	-
360	299	C	N4204a	N'-ethylethane-1,2-diamine	110-72-5	1.0	298.15	837.00	120	-	-	-	-	402.15	121	-	-	(13.82)	-
361	299	C	N4204b	N'-ethylethane-1,2-diamine	110-72-5	1.0	373.0	-	-	43.00	114	-	-	402.15	121	-	-	(13.82)	-
362	300	C	N4205a	N'-methylpropane-1,3-diamine	6291-84-5	1.0	298.0	-	-	53.10	114	-	-	413.15	121	-	-	(13.82)	-
363	301	C	N4206a	butane-1,2-diamine	4426-48-6	1.0	298.0	-	-	46.90	114	-	-	-	-	-	-	(13.82)	-
364	302	C	N4207a	butane-1,3-diamine	590-88-5	1.0	419.15	-	-	43.72	121	-	-	419.15	121	-	-	(13.82)	-
365	303	C	N4208a	butane-1,4-diamine	110-60-1	1.0	298.15	877.00	120	55.20	114	295.05	120	431.65	121	-	-	(13.82)	-
366	304	C	N5201a	N,N,N',N'-tetramethylmethanediamine	51-80-9	1.0	291.15	749.10	120	-	-	-	-	356.15	121	-	-	(13.82)	-
367	304	C	N5201b	N,N,N',N'-tetramethylmethanediamine	51-80-9	1.0	298.0	-	-	33.10	114	-	-	356.15	121	-	-	(13.82)	-
368	305	C	N5202a	N,N',N'-trimethylethane-1,2-diamine	142-25-6	1.0	390.15	-	-	29.68	121	-	-	390.15	121	-	-	(13.82)	-
369	306	C	N5203a	N',N'-dimethylpropane-1,3-diamine	109-55-7	1.0	293.15	827.20	120	42.20	114	-	-	406.65	121	-	-	(13.82)	-
370	307	C	N5204a	N,N'-dimethylpropane-1,3-diamine	111-33-1	1.0	418.15	-	-	36.90	121	-	-	418.15	121	-	-	(13.82)	-
371	308	C	N5205a	N'-propan-2-ylethane-1,2-diamine	19522-67-9	1.0	409.15	-	-	34.34	121	-	-	409.15	121	-	-	(13.82)	-
372	309	C	N5206a	2,2-dimethylpropane-1,3-diamine	7328-91-8	1.0	426.15	-	-	39.41	121	-	-	426.15	121	-	-	(13.82)	-
373	310	C	N5207a	N'-propylethane-1,2-diamine	111-39-7	1.0	421.65	-	-	37.97	121	-	-	421.65	121	-	-	(13.82)	-
374	311	C	N5208a	pentane-1,3-diamine	589-37-7	1.0	298.0	-	-	54.90	114	-	-	437.15	121	-	-	(13.82)	-
375	312	C	N5209a	pentane-1,5-diamine	462-94-2	1.0	298.15	873.00	120	58.70	114	284.95	120	452.15	121	-	-	(13.82)	-
376	313	C	N6201a	N,N,N',N'-tetramethylethane-1,2-diamine	110-18-9	1.0	298.15	770.00	120	41.40	114	215.15	120	394.15	121	-	-	(13.82)	-
377	314	C	N6202a	N-ethyl-N',N'-dimethylethane-1,2-diamine	123-83-1	1.0	298.15	738.00	120	-	-	-	-	407.65	121	-	-	(13.82)	-
378	314	C	N6202b	N-ethyl-N',N'-dimethylethane-1,2-diamine	123-83-1	1.0	407.65	-	-	35.09	121	-	-	407.65	121	-	-	(13.82)	-
379	315	C	N6203a	N,N',N'-trimethylpropane-1,3-diamine	4543-96-8	1.0	414.15	-	-	30.57	121	-	-	414.15	121	-	-	(13.82)	-
380	316	C	N6205a	N',N'-diethylethane-1,2-diamine	100-36-7	1.0	293.15	828.00	120	45.80	114	-	-	417.15	121	-	-	(13.82)	-
381	317	C	N6206a	N,N'-diethylethane-1,2-diamine	111-74-0	1.0	293.15	828.00	120	-	-	-	-	419.15	121	-	-	(13.82)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
382	317	C	N6206b	N,N'-diethylethane-1,2-diamine	111-74-0	1.0	419.15	-	-	31.73	121	-	-	419.15	121	-	-	(13.82)	-
383	318	C	N6207a	N'-propan-2-ylpropane-1,3-diamine	3360-16-5	1.0	435.15	-	-	35.84	121	-	-	435.15	121	-	-	(13.82)	-
384	319	C	N6208a	N'-propylpropane-1,3-diamine	23764-31-0	1.0	442.15	-	-	37.88	121	-	-	442.15	121	-	-	(13.82)	-
385	320	C	N6209a	N'-butylethane-1,2-diamine	19522-69-1	1.0	431.15	-	-	34.75	121	-	-	431.15	121	-	-	(13.82)	-
386	321	C	N6210a	2-methylpentane-1,5-diamine	15520-10-2	1.0	298.0	-	-	60.90	114	-	-	466.15	121	-	-	(13.82)	-
387	322	C	N6211a	hexane-1,6-diamine	124-09-4	1.0	298.0	-	-	63.10	114	311.95	120	475.04	121	-	-	(13.82)	-
388	323	C	D2401a	acetamide	60-35-5	0.004	354.2	1001.97	121	-	-	353.31	120	494.3	121	761.00	121	67.6	120
389	323	C	D2401b	acetamide	60-35-5	1.0	396.0	-	-	63.80	114	353.31	120	494.3	121	761.00	121	67.6	120
390	324	C	D3401a	propanamide	79-05-0	1.01	355.65	963.20	118	-	-	353.05	120	486.15	121	-	-	(43.86)	-
391	324	C	D3401b	propanamide	79-05-0	1.0	390.0	-	-	63.90	114	353.05	120	486.15	121	-	-	(43.86)	-
392	325	C	D4401a	butanamide	541-35-5	1.0	393.15	885.00	120	-	-	389.15	120	489.15	121	-	-	(43.86)	-
393	326	C	D5402a	3-methylbutanamide	541-46-8	1.0	499.15	-	-	43.80	121	410.15	120	499.15	121	-	-	(20.13)	-
394	327	C	D5403a	pentanamide	626-97-1	1.0	383.15	873.50	120	-	-	377.15	120	498.15	121	-	-	(20.13)	-
395	328	C	D6401a	hexanamide	628-02-4	1.0	528.15	-	-	46.59	121	374.15	120	528.15	121	-	-	(43.86)	-
396	329	C	D3301a	N-methylacetamide	79-16-3	1.01	308.15	949.70	118	-	-	303.75	120	478.15	121	718.00	121	179.0	120
397	329	C	D3301b	N-methylacetamide	79-16-3	1.0	348.0	-	-	59.60	114	303.75	120	478.15	121	718.00	121	179.0	120
398	330	C	D4301a	N-methylpropanamide	1187-58-2	1.0	298.15	930.50	120	66.60	114	242.25	120	421.15	121	-	-	177.11	122
399	331	C	D4302a	N-ethylacetamide	625-50-3	1.0	277.15	942.00	120	-	-	-	-	478.15	121	-	-	129.0	122
400	331	C	D4302b	N-ethylacetamide	625-50-3	1.0	298.0	-	-	64.90	114	-	-	478.15	121	-	-	129.0	122
401	332	C	D5301a	N,2-dimethylpropanamide	2675-88-9	1.0	298.0	-	-	67.10	114	-	-	-	-	-	-	(141.44)	-
402	333	C	D5302a	N-propan-2-ylacetamide	1118-69-0	1.0	298.0	-	-	66.40	114	-	-	-	-	-	-	(141.44)	-
403	334	C	D5303a	N-propylacetamide	5331-48-6	1.0	298.0	-	-	69.80	114	-	-	-	-	-	-	(141.44)	-
404	335	C	D6303a	N-butylacetamide	1119-49-9	1.0	298.15	896.00	120	76.10	114	-	-	502.15	121	700.00	121	104.0	120
405	336	C	D4201a	N,N-dimethylacetamide	127-19-5	1.01	298.15	936.70	118	50.66	118	254.15	120	439.25	121	658.00	121	40.2	119
406	337	C	D5201a	N,N-dimethylpropanamide	758-96-3	1.01	298.15	920.32	118	-	-	228.15	120	444.65	121	-	-	(35.30)	-
407	338	C	D6202a	N,N-dimethylbutanamide	760-79-2	1.0	298.15	906.40	120	-	-	233.15	120	459.15	121	-	-	(30.40)	-
408	339	C	D6203a	N,N-diethylacetamide	685-91-6	1.0	290.15	913.00	120	53.70	118	-	-	458.65	121	700.00	121	30.4	122
409	340	V	O7101a	2-methyl-2-propan-2-yloxypropane	17348-59-3	1.0	298.15	736.39	116	34.50	114	184.85	120	378.66	121	549.68	121	(3.78)	-
410	341	V	O7102a	2-ethoxy-2-methylbutane	919-94-8	1.0	298.15	761.80	116	38.20	114	-	-	375.15	121	546.00	121	(3.78)	-
411	342	V	O7103a	2-methyl-2-propoxypropane	29072-93-3	1.0	298.15	746.68	116	37.20	114	-	-	373.15	121	549.68	121	(3.78)	-
412	343	V	O7104a	2-methyl-1-propan-2-yloxypropane	78448-33-6	1.0	298.15	734.90	116	-	-	-	-	371.20	121	549.68	121	(3.78)	-
413	344	V	O7105a	2-propan-2-yloxybutane	18641-81-1	1.0	298.15	739.60	116	-	-	-	-	-	-	549.68	121	(3.78)	-
414	345	V	O7106a	1-ethoxy-3-methylbutane	628-04-6	1.0	298.15	752.10	116	-	-	-	-	385.65	121	549.68	121	3.955	120
415	346	V	O7107a	2-methyl-1-propoxypropane	15268-49-2	1.0	298.15	744.00	116	-	-	-	-	378.15	121	549.68	121	(3.78)	-
416	346	V	O7107b	2-methyl-1-propoxypropane	15268-49-2	0.03	298.15	-	-	38.07	121	-	-	378.15	121	549.68	121	(3.78)	-
417	347	V	O7108a	2-propoxybutane	61962-23-0	1.0	298.15	750.10	116	-	-	-	-	-	-	-	-	(3.78)	-
418	348	V	O7109a	1-propan-2-yloxybutane	1860-27-1	1.0	298.15	746.00	116	-	-	-	-	380.15	120	-	-	(3.78)	-
419	349	V	O7110a	1-methoxyhexane	4747-07-3	1.0	298.15	766.30	116	-	-	-	-	398.15	120	-	-	(3.78)	-
420	350	V	O7111a	1-ethoxypentane	17952-11-3	1.0	298.15	757.20	116	-	-	-	-	391.15	120	-	-	3.6	120
421	351	V	O7112a	1-propoxybutane	3073-92-5	1.0	298.15	754.20	116	-	-	-	-	390.15	120	-	-	(3.78)	-
422	352	V	O8101a	2-methyl-2-[(2-methylpropan-2-yl)oxy]propane	6163-66-2	1.0	298.15	757.80	116	37.60	114	-	-	380.40	121	550.00	121	(3.08)	-
423	353	V	O8102a	2-methyl-2-propan-2-yloxybutane	3249-46-5	1.0	298.0	-	-	41.60	114	-	-	-	-	-	-	(3.08)	-
424	354	V	O8103a	2-methyl-1-[(2-methylpropan-2-yl)oxy]propane	33021-02-2	1.0	298.15	748.00	116	40.10	114	-	-	439.93	121	571.41	121	(3.08)	-
425	355	V	O8104a	2-[(2-methylpropan-2-yl)oxy]butane	32970-45-9	1.0	298.15	757.10	116	-	-	-	-	-	-	-	-	(3.08)	-
426	356	V	O8105a	1-[(2-methylpropan-2-yl)oxy]butane	1000-63-1	1.0	298.15	758.10	116	42.30	114	-	-	-	-	571.41	121	(3.08)	-
427	357	V	O8106a	2-methyl-1-(2-methylpropoxy)propane	628-55-7	1.0	298.15	745.20	116	41.20	114	-	-	395.85	121	571.41	121	(3.08)	-
428	358	V	O8107a	2-(2-methylpropoxy)butane	92097-00-2	1.0	298.15	750.84	116	-	-	-	-	-	-	-	-	(3.08)	-
429	359	V	O8108a	3-methyl-1-propan-2-yloxybutane	92096-99-6	1.0	298.15	754.50	116	-	-	-	-	-	-	-	-	(3.08)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
430	360	V	O8109a	2-butan-2-yloxybutane	6863-58-7	1.0	298.15	758.80	116	-	-	-	-	394.20	121	571.41	121	(3.08)	-
431	360	V	O8109b	2-butan-2-yloxybutane	6863-58-7	0.02	298.15	-	-	39.99	121	-	-	394.20	121	571.41	121	(3.08)	-
432	361	V	O8110a	3-methyl-1-propoxybutane	17071-48-6	1.0	298.15	760.10	116	-	-	-	-	-	-	-	-	(3.08)	-
433	362	V	O8111a	1-(2-methylpropoxy)butane	17071-47-5	1.0	298.15	755.20	116	-	-	-	-	424.15	121	571.41	121	(3.08)	-
434	362	V	O8111b	1-(2-methylpropoxy)butane	17071-47-5	0.01	319.77	-	-	42.85	121	-	-	424.15	121	571.41	121	(3.08)	-
435	363	V	O8112a	1-butan-2-yloxybutane	999-65-5	1.0	298.15	761.10	116	-	-	-	-	-	-	-	-	(3.08)	-
436	364	V	O8113a	1-propan-2-yloxypentane	5756-37-6	1.0	298.15	759.80	116	-	-	-	-	-	-	571.41	121	(3.08)	-
437	365	V	O8114a	1-methoxyheptane	629-32-3	1.0	298.15	775.60	116	46.90	114	-	-	424.15	121	-	-	(3.08)	-
438	366	V	O8115a	1-ethoxyhexane	5756-43-4	1.0	298.15	768.20	116	-	-	-	-	415.15	120	-	-	(3.08)	-
439	367	V	O8116a	1-propoxypentane	18641-82-2	1.0	298.15	765.30	116	-	-	-	-	-	-	571.41	121	(3.08)	-
440	368	V	O8117a	1-butoxybutane	142-96-1	1.0	298.15	764.06	116	44.70	114	177.15	120	413.44	121	584.10	121	3.0830	120
441	369	V	O9101a	2-methoxy-2,4,4-trimethylpentane	62108-41-2	1.01	298.15	792.40	118	-	-	-	-	-	-	-	-	(3.76)	-
442	369	V	O9101b	2-methoxy-2,4,4-trimethylpentane	62108-41-2	1.0	396.0	-	-	38.50	114	-	-	-	-	-	-	(3.76)	-
443	370	V	O9102a	3-methyl-1-[(2-methylpropan-2-yl)oxy]butane	92097-05-7	1.0	298.15	761.60	116	-	-	-	-	-	-	-	-	(3.76)	-
444	371	V	O9103a	1-[(2-methylpropan-2-yl)oxy]pentane	10100-95-5	1.0	298.15	766.40	116	-	-	-	-	-	-	-	-	(3.76)	-
445	372	V	O9104a	3-methyl-1-(2-methylpropoxy)butane	92097-02-4	1.0	298.15	759.40	116	-	-	-	-	-	-	-	-	(3.76)	-
446	373	V	O9105a	1-butan-2-yloxy-3-methylbutane	92097-04-6	1.0	298.15	764.30	116	-	-	-	-	-	-	-	-	(3.76)	-
447	374	V	O9106a	1-butoxy-3-methylbutane	17071-52-2	1.0	298.15	767.60	116	-	-	-	-	-	-	-	-	(3.76)	-
448	375	V	O9107a	1-(2-methylpropoxy)pentane	92097-01-3	1.0	298.15	765.60	116	-	-	-	-	-	-	-	-	(3.76)	-
449	376	V	O9108a	2-methoxyoctane	1541-09-9	1.0	298.15	802.09	116	-	-	-	-	-	-	-	-	(3.76)	-
450	377	V	O9109a	1-butan-2-yloxypentane	92097-03-5	1.0	298.15	768.70	116	-	-	-	-	-	-	-	-	(3.76)	-
451	378	V	O9110a	1-propan-2-yloxyhexane	18636-65-2	1.0	298.15	767.80	116	-	-	-	-	-	-	-	-	(3.76)	-
452	379	V	O9111a	1-methoxyoctane	929-56-6	1.0	298.15	783.00	116	-	-	-	-	-	-	591.55	121	(3.76)	-
453	380	V	O9112a	1-ethoxyheptane	1969-43-3	1.0	298.15	775.30	116	-	-	-	-	-	-	-	-	(3.76)	-
454	381	V	O9113a	1-propoxyhexane	53685-78-2	1.0	298.15	773.00	116	-	-	-	-	-	-	-	-	(3.76)	-
455	382	V	O9114a	1-butoxypentane	18636-66-3	1.0	298.15	772.70	116	-	-	-	-	-	-	-	-	(3.76)	-
456	383	V	O0101a	2-ethoxy-2,4,4-trimethylpentane	187103-12-4	1.0	298.0	-	-	45.30	114	-	-	-	-	-	-	(2.81)	-
457	384	V	O0102a	1-[(2-methylpropan-2-yl)oxy]hexane	69775-79-7	1.0	298.0	-	-	53.20	114	-	-	-	-	-	-	(2.81)	-
458	385	V	O0103a	3-pentan-3-yloxypentane	56761-99-0	1.0	293.15	784.80	116	-	-	-	-	-	-	-	-	(2.81)	-
459	386	V	O0104a	3-methyl-1-(3-methylbutoxy)butane	544-01-4	1.0	298.15	771.50	116	51.40	114	-	-	445.65	121	610.37	121	2.817	120
460	387	V	O0105a	2-pentan-2-yloxypentane	56762-00-6	1.0	293.15	777.80	116	-	-	-	-	-	-	-	-	(2.81)	-
461	388	V	O0106a	1-(3-methylbutoxy)pentane	92097-07-9	1.0	298.15	775.10	116	-	-	-	-	-	-	-	-	(2.81)	-
462	389	V	O0107a	1-(2-methylpropoxy)hexane	92097-06-8	1.0	298.15	771.20	116	-	-	-	-	-	-	-	-	(2.81)	-
463	390	V	O0108a	2-ethoxyoctane	63028-01-3	1.0	298.15	782.14	116	-	-	-	-	-	-	-	-	(2.81)	-
464	391	V	O0109a	2-butoxyhexane	101581-41-3	1.0	293.15	787.40	116	-	-	-	-	-	-	-	-	(2.81)	-
465	392	V	O0110a	1-butan-2-yloxyhexane	65270-00-0	1.0	298.15	775.80	116	-	-	-	-	-	-	-	-	(2.81)	-
466	393	V	O0111a	1-propan-2-yloxyheptane	86724-25-6	1.0	298.15	773.60	116	-	-	-	-	-	-	-	-	(2.81)	-
467	394	V	O0112a	1-methoxynonane	7289-51-2	1.0	298.15	788.60	116	-	-	-	-	-	-	-	-	(2.81)	-
468	395	V	O0113a	1-ethoxyoctane	929-61-3	1.0	298.15	782.30	116	-	-	-	-	-	-	-	-	(2.81)	-
469	396	V	O0114a	1-propoxyheptane	71112-89-5	1.0	298.15	779.80	116	-	-	-	-	-	-	-	-	(2.81)	-
470	397	V	O0115a	1-butoxyhexane	54459-71-1	1.0	298.15	778.80	116	53.20	114	-	-	-	-	-	-	(2.81)	-
471	398	V	O0116a	1-pentoxypentane	693-65-2	1.0	298.15	779.20	116	-	-	203.95	120	460.15	120	-	-	2.798	120
472	398	V	O0116b	1-pentoxypentane	693-65-2	1.0	388.0	-	-	46.20	114	203.95	120	460.15	120	-	-	2.798	120
473	399	V	O7201a	2-(2-methoxyethoxy)-2-methylpropane	66728-50-5	1.0	404.65	-	-	34.80	121	-	-	404.65	121	-	-	(4.09)	-
474	400	V	O7202a	2,2-diethoxypropane	126-84-1	1.0	298.15	868.80	116	43.90	114	-	-	387.15	121	-	-	(4.09)	-
475	401	V	O7203a	2-(propan-2-yloxymethoxy)propane	2568-89-0	1.0	298.15	813.72	116	-	-	-	-	-	-	-	-	(4.09)	-
476	402	V	O7204a	1,1-diethoxypropane	4744-08-5	1.0	293.15	825.00	120	-	-	-	-	396.15	121	-	-	(4.09)	-
477	402	V	O7204b	1,1-diethoxypropane	4744-08-5	1.0	396.15	-	-	34.00	121	-	-	396.15	121	-	-	(4.09)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
478	403	V	O7205a	1,5-dimethoxypentane	111-89-7	1.0	298.15	851.60	116	-	-	-	-	-	-	-	-	(4.09)	-
479	404	V	O7206a	1-(2-methoxyethoxy)butane	13343-98-1	1.0	298.15	840.90	116	47.80	114	-	-	420.08	121	659.33	121	(4.09)	-
480	405	V	O7207a	1-methoxy-3-propoxypropane	89851-49-0	1.0	298.15	840.30	116	-	-	-	-	-	-	-	-	(4.09)	-
481	406	V	O7208a	1,3-diethoxypropane	3459-83-4	1.0	298.15	831.20	116	45.90	114	-	-	-	-	-	-	(4.09)	-
482	407	V	O7209a	1-(propoxymethoxy)propane	505-84-0	1.0	293.15	834.50	120	-	-	175.85	120	413.65	121	-	-	(4.09)	-
483	407	V	O7209b	1-(propoxymethoxy)propane	505-84-0	1.0	413.65	-	-	35.65	121	175.85	120	413.65	121	-	-	(4.09)	-
484	408	V	O7210a	1-(2-ethoxyethoxy)propane	18854-31-4	1.0	298.15	832.70	116	46.80	114	-	-	-	-	-	-	(4.09)	-
485	409	V	O8201a	2,2-dimethoxyhexane	98944-43-5	1.0	298.15	852.70	116	-	-	-	-	-	-	-	-	(4.09)	-
486	410	V	O8202a	2-(2-ethoxyethoxy)-2-methylpropane	51422-54-9	1.0	421.15	-	-	36.36	121	-	-	421.15	121	-	-	(4.09)	-
487	411	V	O8203a	1,1-diethoxybutane	3658-95-5	1.0	416.5	-	-	35.92	121	-	-	416.50	121	-	-	(4.09)	-
488	412	V	O8204a	1-(1-propoxyethoxy)propane	105-82-8	1.0	298.15	825.58	116	-	-	-	-	478.13	121	-	-	(4.09)	-
489	413	V	O8205a	1,6-dimethoxyhexane	13179-98-1	1.0	298.15	851.80	116	-	-	-	-	-	-	-	-	(4.09)	-
490	414	V	O8206a	1-ethoxy-5-methoxypentane	17315-35-4	1.0	298.15	843.30	116	-	-	-	-	-	-	-	-	(4.09)	-
491	415	V	O8207a	1-methoxy-4-propoxybutane	-	1.0	298.15	840.70	116	-	-	-	-	-	-	-	-	(4.09)	-
492	416	V	O8208a	1,4-diethoxybutane	13344-00-8	1.0	298.15	833.50	116	-	-	-	-	-	-	-	-	(4.09)	-
493	417	V	O8209a	1-(2-ethoxyethoxy)butane	4413-13-2	1.0	298.15	833.10	116	50.90	114	-	-	434.03	121	-	-	(4.09)	-
494	418	V	O8210a	1-(2-propoxyethoxy)propane	18854-56-3	1.0	298.15	831.20	120	50.60	114	-	-	478.13	121	-	-	(4.09)	-
495	419	V	O9201a	2-methyl-1-(2-methylpropoxymethoxy)propane	2568-91-4	1.0	298.15	820.27	116	-	-	-	-	438.65	121	-	-	(4.09)	-
496	419	V	O9201b	2-methyl-1-(2-methylpropoxymethoxy)propane	2568-91-4	1.0	438.65	-	-	38.02	121	-	-	438.65	121	-	-	(4.09)	-
497	420	V	O9202a	1,1-diethoxypentane	3658-79-5	1.0	295.15	829.00	120	-	-	-	-	520.68	121	-	-	(4.09)	-
498	421	V	O9203a	1-ethoxy-6-methoxyhexane	93281-63-1	1.0	298.15	844.00	116	-	-	-	-	-	-	-	-	(4.09)	-
499	422	V	O9204a	1,5-diethoxypentane	90724-89-3	1.0	298.15	838.60	116	-	-	-	-	-	-	-	-	(4.09)	-
500	423	V	O9205a	1-butoxy-4-methoxybutane	91391-43-4	1.0	298.15	840.60	116	-	-	-	-	-	-	-	-	(4.09)	-
501	424	V	O9206a	1-(butoxymethoxy)butane	2568-90-3	1.0	298.15	831.53	116	48.10	114	214.15	120	452.35	121	-	-	(4.09)	-
502	425	V	O9207a	1-(2-propoxyethoxy)butane	18854-58-5	1.0	298.0	-	-	54.70	114	-	-	-	-	-	-	(4.09)	-
503	426	V	O0201a	2-methyl-1-[1-(2-methylpropoxy)ethoxy]propane	5669-09-0	1.0	298.15	816.80	116	-	-	-	-	444.45	121	-	-	(4.09)	-
504	426	V	O0201b	2-methyl-1-[1-(2-methylpropoxy)ethoxy]propane	5669-09-0	1.0	351.0	-	-	46.10	114	-	-	444.45	121	-	-	(4.09)	-
505	427	V	O0203a	1-(1-butoxyethoxy)butane	871-22-7	1.0	298.15	829.03	116	57.80	114	-	-	415.43	121	-	-	(4.09)	-
506	428	V	O0204a	1-butoxy-5-methoxypentane	-	1.0	298.15	840.90	116	-	-	-	-	-	-	-	-	(4.09)	-
507	429	V	O0205a	1,4-dipropoxybutane	-	1.0	293.15	840.90	116	-	-	-	-	-	-	-	-	(4.09)	-
508	430	V	O0206a	1-(2-butoxyethoxy)butane	112-48-1	1.0	298.15	833.70	116	58.80	114	204.05	120	476.45	121	715.45	121	(4.09)	-
509	431	V	O7301a	1,3,3-trimethoxybutane	6607-66-5	1.0	426.15	-	-	36.84	121	-	-	426.15	121	-	-	(4.78)	-
510	432	V	O7302a	1,1,1-trimethoxybutane	43083-12-1	1.0	419.15	-	-	36.17	121	-	-	419.15	121	-	-	(4.78)	-
511	433	V	O7303a	1,1,3-trimethoxybutane	10138-89-3	1.0	430.15	-	-	37.22	121	-	-	430.15	121	-	-	(4.78)	-
512	434	V	O7304a	1,1-diethoxy-2-methoxyethane	4819-75-4	1.0	419.15	-	-	36.17	121	-	-	419.15	121	-	-	(4.78)	-
513	435	V	O7305a	diethoxymethoxyethane	122-51-0	1.0	298.15	893.80	116	47.80	114	-	-	416.15	121	-	-	4.779	120
514	436	V	O7306a	1-(2-ethoxyethoxy)-2-methoxyethane	1002-67-1	1.0	293.15	922.90	116	-	-	-	-	416.90	121	-	-	(4.78)	-
515	437	V	O8301a	1,1,1-trimethoxypentane	13820-09-2	1.0	438.15	-	-	37.98	121	-	-	438.15	121	-	-	(6.00)	-
516	438	V	O8302a	1,1,1-triethoxyethane	78-39-7	1.0	298.15	884.70	120	-	-	-	-	418.15	121	-	-	(6.00)	-
517	438	V	O8302b	1,1,1-triethoxyethane	78-39-7	1.0	418.15	-	-	36.08	121	-	-	418.15	121	-	-	(6.00)	-
518	439	V	O8303a	1-ethoxy-2-(2-ethoxyethoxy)ethane	112-36-7	1.0	298.15	903.30	116	56.40	114	228.85	120	462.15	121	624.00	121	(6.00)	-
519	440	V	O9301a	1,1,1-triethoxypropane	115-80-0	1.0	444.15	-	-	38.55	121	-	-	444.15	121	-	-	(6.00)	-
520	441	V	O0301a	2-[di(propan-2-yloxy)methoxy]propane	4447-60-3	1.0	293.15	862.10	120	-	-	-	-	440.15	121	-	-	(6.00)	-
521	441	V	O0301b	2-[di(propan-2-yloxy)methoxy]propane	4447-60-3	1.0	440.15	-	-	38.16	121	-	-	440.15	121	-	-	(6.00)	-
522	442	V	O0303a	1-(dipropoxymethoxy)propane	621-76-1	1.0	467.15	-	-	40.74	121	-	-	467.15	121	-	-	(6.00)	-
523	443	V	O0304a	1-[2-(2-propoxyethoxy)ethoxy]propane	72072-32-3	1.0	288.15	886.90	116	-	-	-	-	-	-	-	-	(6.00)	-
524	444	V	O7401a	1,1,3,3-tetramethoxypropane	102-52-3	1.0	298.15	997.00	120	-	-	-	-	456.15	121	-	-	(5.01)	-
525	445	V	O7402a	ethoxymethoxymethoxymethoxyethane	4431-82-7	1.0	298.0	-	-	53.60	114	-	-	-	-	-	-	(5.01)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
526	446	V	O8401a	1-methoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane	112-49-2	1.0	293.15	986.00	[120]	-	-	229.35	[120]	489.15	[121]	651.00	[121]	7.62	[120]
527	446	V	O8401b	1-methoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane	112-49-2	1.0	489.15	-	-	50.90	[121]	229.35	[120]	489.15	[121]	651.00	[121]	7.62	[120]
528	447	V	O9401a	triethoxymethoxyethane	78-09-1	1.0	293.15	918.60	[120]	52.90	[114]	-	-	432.65	[121]	-	-	(5.01)	-
529	448	V	A7102a	2-ethyl-3-methylbutanal	26254-92-2	1.0	298.15	829.50	[117]	-	-	-	-	-	-	-	-	(9.07)	-
530	449	V	A7104a	3,4-dimethylpentanal	19353-21-0	1.0	298.15	823.10	[117]	-	-	-	-	-	-	-	-	(9.07)	-
531	449	V	A7104b	3,4-dimethylpentanal	19353-21-0	1.0	334.0	-	-	42.40	[114]	-	-	-	-	-	-	(9.07)	-
532	450	V	A7107a	3-methylhexanal	19269-28-4	1.0	298.15	814.33	[117]	-	-	-	-	416.15	[121]	620.41	[121]	(9.07)	-
533	450	V	A7107b	3-methylhexanal	19269-28-4	1.0	329.0	-	-	42.80	[114]	-	-	416.15	[121]	620.41	[121]	(9.07)	-
534	451	V	A7108a	4-methylhexanal	41065-97-8	1.0	298.15	824.00	[117]	-	-	-	-	-	-	620.41	[121]	(9.07)	-
535	452	V	A7109a	5-methylhexanal	1860-39-5	1.0	293.15	820.60	[117]	-	-	-	-	-	-	620.41	[121]	(9.07)	-
536	453	V	A7110a	heptanal	111-71-7	1.0	298.15	813.29	[117]	48.00	[114]	229.21	[120]	425.95	[121]	616.80	[121]	9.07	[120]
537	454	V	A8101a	2-ethyl-4-methylpentanal	10349-95-8	1.0	293.15	847.60	[117]	-	-	-	-	-	-	-	-	(13.51)	-
538	455	V	A8102a	2,4-dimethylhexanal	-	1.0	293.15	847.60	[117]	-	-	-	-	-	-	-	-	(13.51)	-
539	456	V	A8103a	2-propylpentanal	18295-59-5	0.01	329.07	802.38	[121]	-	-	-	-	433.15	[121]	642.39	[121]	(13.51)	-
540	457	V	A8104a	2-ethylhexanal	123-05-7	1.0	298.15	815.16	[117]	-	-	-	-	433.80	[121]	642.39	[121]	(13.51)	-
541	457	V	A8104b	2-ethylhexanal	123-05-7	0.01	329.59	-	-	44.66	[121]	-	-	433.80	[121]	642.39	[121]	(13.51)	-
542	458	V	A8109a	octanal	124-13-0	1.01	298.15	821.07	[118]	51.00	[114]	-	-	447.15	[121]	638.90	[121]	(13.51)	-
543	459	V	A9101a	2-ethyl-2,4-dimethylpentanal	-	1.0	298.15	827.00	[117]	-	-	-	-	-	-	-	-	(13.51)	-
544	460	V	A9102a	3,5,5-trimethylhexanal	5435-64-3	0.01	347.35	778.97	[121]	-	-	-	-	456.62	[121]	662.74	[121]	(13.51)	-
545	461	V	A9103a	2,4,5-trimethylhexanal	-	1.0	291.15	884.30	[117]	-	-	-	-	-	-	-	-	(13.51)	-
546	462	V	A9104a	2-ethyl-4-methylhexanal	-	1.0	293.15	848.30	[117]	-	-	-	-	-	-	-	-	(13.51)	-
547	463	V	A9105a	4-methyl-2-propylpentanal	-	1.0	293.15	842.30	[117]	-	-	-	-	-	-	-	-	(13.51)	-
548	464	V	A9106a	2-methyloctanal	7786-29-0	0.01	347.53	785.37	[121]	-	-	-	-	456.62	[121]	662.74	[121]	(13.51)	-
549	465	V	A9109a	nonanal	124-19-6	1.01	298.15	831.04	[118]	55.30	[114]	-	-	468.15	[121]	662.74	[121]	(13.51)	-
550	466	V	A0101a	4-methyl-2-propylhexanal	85153-29-3	1.0	293.15	843.00	[117]	-	-	-	-	-	-	-	-	(13.51)	-
551	467	V	A0103a	3,7-dimethyloctanal	5988-91-0	1.0	298.15	813.40	[117]	-	-	-	-	403.15	[121]	656.59	[121]	(13.51)	-
552	467	V	A0103b	3,7-dimethyloctanal	5988-91-0	1.0	403.15	-	-	24.28	[121]	-	-	403.15	[121]	656.59	[121]	(13.51)	-
553	468	V	A0107a	decanal	112-31-2	1.0	298.15	824.90	[117]	59.50	[114]	-	-	488.15	[121]	674.20	[121]	(13.51)	-
554	469	V	K7101a	3,3-dimethylpentan-2-one	20669-04-9	1.0	294.15	823.00	[117]	-	-	-	-	403.75	[121]	611.41	[121]	(12.70)	-
555	469	V	K7101b	3,3-dimethylpentan-2-one	20669-04-9	0.01	300.55	-	-	40.69	[121]	-	-	403.75	[121]	611.41	[121]	(12.70)	-
556	470	V	K7102a	2,2-dimethylpentan-3-one	564-04-5	1.0	298.15	808.40	[117]	42.30	[114]	228.15	[120]	398.15	[121]	611.41	[121]	(12.70)	-
557	471	V	K7103a	4,4-dimethylpentan-2-one	590-50-1	1.0	298.15	801.20	[117]	-	-	209.15	[120]	398.15	[121]	611.41	[121]	(12.70)	-
558	471	V	K7103b	4,4-dimethylpentan-2-one	590-50-1	0.02	298.15	-	-	39.71	[121]	209.15	[120]	398.15	[121]	611.41	[121]	(12.70)	-
559	472	V	K7104a	2,4-dimethylpentan-3-one	565-80-0	1.0	298.15	799.73	[117]	41.50	[114]	204.75	[120]	397.55	[121]	611.41	[121]	(12.70)	-
560	473	V	K7105a	3,4-dimethylpentan-2-one	565-78-6	1.0	293.15	827.30	[117]	-	-	-	-	405.15	[121]	611.41	[121]	(12.70)	-
561	473	V	K7105b	3,4-dimethylpentan-2-one	565-78-6	0.01	301.67	-	-	41.38	[121]	-	-	405.15	[121]	611.41	[121]	(12.70)	-
562	474	V	K7106a	4-methylhexan-3-one	17042-16-9	1.0	298.15	824.00	[117]	-	-	-	-	409.15	[121]	611.41	[121]	(12.70)	-
563	475	V	K7107a	2-methylhexan-3-one	7379-12-6	0.01	302.47	809.45	[121]	41.15	[121]	-	-	406.15	[121]	611.41	[121]	(12.70)	-
564	476	V	K7108a	3-ethylpentan-2-one	6137-03-7	1.0	295.15	815.30	[117]	-	-	-	-	411.15	[121]	611.41	[121]	(12.70)	-
565	476	V	K7108b	3-ethylpentan-2-one	6137-03-7	0.01	306.47	-	-	41.70	[121]	-	-	411.15	[121]	611.41	[121]	(12.70)	-
566	477	V	K7109a	3-methylhexan-2-one	2550-21-2	1.0	298.15	828.00	[117]	-	-	-	-	413.15	[121]	611.41	[121]	(12.70)	-
567	477	V	K7109b	3-methylhexan-2-one	2550-21-2	0.01	308.07	-	-	41.81	[121]	-	-	413.15	[121]	611.41	[121]	(12.70)	-
568	478	V	K7110a	5-methylhexan-3-one	623-56-3	1.0	293.15	812.00	[117]	-	-	-	-	409.15	[121]	611.41	[121]	(12.70)	-
569	478	V	K7110b	5-methylhexan-3-one	623-56-3	0.01	304.87	-	-	41.59	[121]	-	-	409.15	[121]	611.41	[121]	(12.70)	-
570	479	V	K7111a	4-methylhexan-2-one	105-42-0	1.0	298.15	808.50	[117]	-	-	-	-	412.15	[121]	611.41	[121]	(12.70)	-
571	479	V	K7111b	4-methylhexan-2-one	105-42-0	0.01	307.27	-	-	42.04	[121]	-	-	412.15	[121]	611.41	[121]	(12.70)	-
572	480	V	K7112a	5-methylhexan-2-one	110-12-3	1.0	293.15	811.60	[117]	-	-	-	-	417.95	[121]	611.41	[121]	13.53	[120]
573	480	V	K7112b	5-methylhexan-2-one	110-12-3	0.01	311.91	-	-	42.18	[121]	-	-	417.95	[121]	611.41	[121]	13.53	[120]

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
574	481	V	K7113a	heptan-4-one	123-19-3	1.0	298.15	811.60	117	-	-	241.05	120	417.15	121	602.00	121	12.60	120
575	481	V	K7113b	heptan-4-one	123-19-3	0.01	311.27	-	-	42.89	121	241.05	120	417.15	121	602.00	121	12.60	120
576	482	V	K7114a	heptan-3-one	106-35-4	1.0	298.15	814.64	117	-	-	235.95	120	420.55	121	606.60	121	12.7	120
577	482	V	K7114b	heptan-3-one	106-35-4	0.01	313.99	-	-	43.20	121	235.95	120	420.55	121	606.60	121	12.7	120
578	483	V	K7115a	heptan-2-one	110-43-0	1.0	298.15	811.64	117	46.10	114	238.45	120	424.05	121	611.40	121	11.95	120
579	484	V	K8101a	3,3,4-trimethylpentan-2-one	5340-47-6	1.0	293.15	839.50	117	-	-	-	-	-	-	-	-	(10.00)	-
580	485	V	K8102a	2,2,4-trimethylpentan-3-one	5857-36-3	1.0	298.15	802.30	117	43.30	114	-	-	408.25	121	633.39	121	(10.00)	-
581	486	V	K8103a	3,4,4-trimethylpentan-2-one	5340-45-4	1.0	293.15	826.00	117	-	-	-	-	-	-	-	-	(10.00)	-
582	487	V	K8104a	3-ethyl-3-methylpentan-2-one	19780-65-5	1.0	293.15	838.90	117	-	-	-	-	426.60	121	633.39	121	(10.00)	-
583	487	V	K8104b	3-ethyl-3-methylpentan-2-one	19780-65-5	0.01	318.83	-	-	43.56	121	-	-	426.60	121	633.39	121	(10.00)	-
584	488	V	K8105a	4,4-dimethylhexan-3-one	19550-14-2	1.0	293.15	829.80	117	-	-	-	-	421.15	121	633.39	121	(10.00)	-
585	488	V	K8105b	4,4-dimethylhexan-3-one	19550-14-2	0.01	314.47	-	-	43.21	121	-	-	421.15	121	633.39	121	(10.00)	-
586	489	V	K8106a	3,3-dimethylhexan-2-one	26118-38-7	1.0	293.15	825.70	117	-	-	-	-	420.15	121	633.39	121	(10.00)	-
587	490	V	K8107a	2,2-dimethylhexan-3-one	5405-79-8	1.0	298.15	810.50	117	-	-	-	-	419.15	121	633.39	121	(10.00)	-
588	490	V	K8107b	2,2-dimethylhexan-3-one	5405-79-8	0.01	312.87	-	-	42.32	121	-	-	419.15	121	633.39	121	(10.00)	-
589	491	V	K8108a	4,4-dimethylhexan-2-one	40239-18-7	1.0	293.15	829.00	117	-	-	-	-	-	-	-	-	(10.00)	-
590	492	V	K8109a	5,5-dimethylhexan-3-one	5340-30-7	1.0	293.15	812.00	117	-	-	-	-	-	-	-	-	(10.00)	-
591	493	V	K8110a	2,4-dimethylhexan-3-one	18641-70-8	1.0	365.0	-	-	42.50	114	-	-	-	-	-	-	(10.00)	-
592	494	V	K8111a	2,5-dimethylhexan-3-one	1888-57-9	1.0	293.15	812.10	117	-	-	-	-	420.65	121	633.39	121	(10.00)	-
593	494	V	K8111b	2,5-dimethylhexan-3-one	1888-57-9	0.01	314.07	-	-	42.57	121	-	-	420.65	121	633.39	121	(10.00)	-
594	495	V	K8112a	3-ethyl-4-methylpentan-2-one	71172-57-1	0.01	319.67	790.97	121	43.48	121	-	-	427.65	121	633.39	121	(10.00)	-
595	496	V	K8113a	3,4-dimethylhexan-2-one	19550-10-8	1.0	295.15	829.50	117	-	-	-	-	431.15	121	633.39	121	(10.00)	-
596	496	V	K8113b	3,4-dimethylhexan-2-one	19550-10-8	0.01	322.47	-	-	44.14	121	-	-	431.15	121	633.39	121	(10.00)	-
597	497	V	K8114a	3-methylheptan-4-one	15726-15-5	1.0	298.15	817.00	117	-	-	-	-	426.15	121	633.39	121	(10.00)	-
598	498	V	K8115a	4-methylheptan-3-one	6137-11-7	1.0	298.15	820.00	117	-	-	-	-	-	-	633.39	121	(10.00)	-
599	499	V	K8116a	2-methylheptan-3-one	13019-20-0	1.0	293.15	817.50	117	-	-	-	-	431.15	121	633.39	121	(10.00)	-
600	499	V	K8116b	2-methylheptan-3-one	13019-20-0	0.01	322.47	-	-	44.14	121	-	-	431.15	121	633.39	121	(10.00)	-
601	500	V	K8117a	3-methylheptan-2-one	2371-19-9	0.01	327.27	794.22	121	43.84	121	-	-	437.15	121	633.39	121	(10.00)	-
602	501	V	K8118a	5-methylheptan-3-one	541-85-5	1.0	297.15	829.00	117	-	-	-	-	435.14	121	633.39	121	(10.00)	-
603	501	V	K8118b	5-methylheptan-3-one	541-85-5	0.01	322.36	-	-	44.44	121	-	-	435.14	121	633.39	121	(10.00)	-
604	502	V	K8119a	2-methylheptan-4-one	626-33-5	1.0	295.15	813.00	120	-	-	-	-	427.15	121	633.39	121	(10.00)	-
605	502	V	K8119b	2-methylheptan-4-one	626-33-5	0.01	319.27	-	-	43.50	121	-	-	427.15	121	633.39	121	(10.00)	-
606	503	V	K8120a	6-methylheptan-3-one	624-42-0	1.0	293.15	830.40	120	-	-	-	-	437.15	121	633.39	121	(10.00)	-
607	504	V	K8122a	5-methylheptan-2-one	18217-12-4	1.0	298.15	811.00	117	-	-	-	-	437.00	121	633.39	121	(10.00)	-
608	504	V	K8122b	5-methylheptan-2-one	18217-12-4	0.01	327.15	-	-	44.24	121	-	-	437.00	121	633.39	121	(10.00)	-
609	505	V	K8123a	6-methylheptan-2-one	928-68-7	1.0	298.15	810.00	117	-	-	-	-	440.15	121	633.39	121	(10.00)	-
610	505	V	K8123b	6-methylheptan-2-one	928-68-7	0.01	329.67	-	-	46.31	121	-	-	440.15	121	633.39	121	(10.00)	-
611	506	V	K8124a	octan-4-one	589-63-9	1.0	298.15	814.72	117	-	-	-	-	436.15	121	633.39	121	(10.00)	-
612	506	V	K8124b	octan-4-one	589-63-9	0.01	326.47	-	-	45.47	121	-	-	436.15	121	633.39	121	(10.00)	-
613	507	V	K8125a	octan-3-one	106-68-3	1.0	298.15	822.00	120	-	-	-	-	440.65	121	633.39	121	10.50	120
614	507	V	K8125b	octan-3-one	106-68-3	1.0	308.0	-	-	43.80	114	-	-	440.65	121	633.39	121	10.50	120
615	508	V	K8126a	octan-2-one	111-13-7	1.0	298.15	815.25	117	51.80	114	252.84	120	445.75	121	632.70	121	9.51	120
616	509	V	K9101a	2,2,4,4-tetramethylpentan-3-one	815-24-7	1.0	298.15	820.20	117	45.40	114	247.95	120	425.15	121	653.74	121	10.0	120
617	510	V	K9102a	2,2,5-trimethylhexan-3-one	14705-50-1	1.0	296.15	812.00	117	-	-	-	-	-	-	-	-	(9.91)	-
618	511	V	K9103a	2,2-dimethylheptan-3-one	19078-97-8	1.0	293.15	816.80	117	-	-	-	-	-	-	-	-	(9.91)	-
619	512	V	K9104a	2,2-dimethylheptan-4-one	1762-19-2	1.0	298.15	809.00	117	-	-	-	-	-	-	-	-	(9.91)	-
620	513	V	K9105a	3,5-dimethylheptan-4-one	19549-84-9	1.0	287.15	826.00	117	-	-	-	-	435.15	121	653.74	121	(9.91)	-
621	513	V	K9105b	3,5-dimethylheptan-4-one	19549-84-9	0.01	325.67	-	-	44.19	121	-	-	435.15	121	653.74	121	(9.91)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
622	514	V	K9106a	2,6-dimethylheptan-3-one	19549-83-8	1.0	298.15	813.50	117	-	-	-	-	445.00	121	653.74	121	(9.91)	-
623	514	V	K9106b	2,6-dimethylheptan-3-one	19549-83-8	0.01	333.55	-	-	45.65	121	-	-	445.00	121	653.74	121	(9.91)	-
624	515	V	K9107a	2,6-dimethylheptan-4-one	108-83-8	1.0	298.15	802.43	117	50.90	114	227.15	120	441.41	121	653.74	121	9.91	120
625	516	V	K9108a	5,6-dimethylheptan-2-one	2867-76-7	1.0	293.15	833.50	117	-	-	-	-	-	-	-	-	(9.91)	-
626	517	V	K9109a	4,6-dimethylheptan-2-one	19549-80-5	1.0	298.15	817.00	117	-	-	-	-	-	-	-	-	(9.91)	-
627	518	V	K9110a	3-methyloctan-4-one	20754-04-5	1.0	287.15	829.00	117	-	-	-	-	447.15	121	653.74	121	(9.91)	-
628	518	V	K9110b	3-methyloctan-4-one	20754-04-5	0.01	335.27	-	-	45.95	121	-	-	447.15	121	653.74	121	(9.91)	-
629	519	V	K9111a	4-methyloctan-3-one	6137-15-1	1.0	298.15	820.00	117	-	-	-	-	456.62	121	653.74	121	(9.91)	-
630	520	V	K9112a	2-methyloctan-3-one	923-28-4	1.0	293.15	821.20	117	-	-	-	-	456.00	121	653.74	121	(9.91)	-
631	520	V	K9112b	2-methyloctan-3-one	923-28-4	0.01	342.35	-	-	47.36	121	-	-	456.00	121	653.74	121	(9.91)	-
632	521	V	K9113a	3-ethylheptan-2-one	6137-09-3	1.0	293.15	824.60	117	-	-	-	-	-	-	-	-	(9.91)	-
633	522	V	K9114a	3-methyloctan-2-one	6137-08-2	1.0	300.15	832.00	117	-	-	-	-	456.62	121	653.74	121	(9.91)	-
634	523	V	K9115a	2-methyloctan-4-one	7492-38-8	1.0	298.15	815.00	117	-	-	-	-	-	-	653.74	121	(9.91)	-
635	524	V	K9116a	7-methyloctan-4-one	20809-46-5	1.0	293.15	823.90	117	-	-	-	-	451.15	121	653.74	121	(9.91)	-
636	524	V	K9116b	7-methyloctan-4-one	20809-46-5	0.01	338.47	-	-	46.57	121	-	-	451.15	121	653.74	121	(9.91)	-
637	525	V	K9120a	6-methyloctan-2-one	925-69-9	1.0	298.15	822.00	117	-	-	-	-	-	-	653.74	121	(9.91)	-
638	526	V	K9121a	nonan-5-one	502-56-7	1.0	298.15	817.77	117	53.30	114	269.31	120	461.60	121	640.00	121	10.6	120
639	527	V	K9122a	nonan-4-one	4485-09-0	1.0	298.15	819.68	117	-	-	-	-	460.65	121	653.74	121	(9.91)	-
640	527	V	K9122b	nonan-4-one	4485-09-0	0.01	346.07	-	-	48.12	121	-	-	460.65	121	653.74	121	(9.91)	-
641	528	V	K9123a	nonan-3-one	925-78-0	1.0	298.15	820.44	117	55.60	114	265.15	120	463.15	121	653.74	121	(9.91)	-
642	529	V	K9124a	nonan-2-one	821-55-6	1.0	298.15	817.78	117	-	-	265.75	120	467.15	121	652.50	121	9.14	120
643	529	V	K9124b	nonan-2-one	821-55-6	0.01	351.27	-	-	49.41	121	265.75	120	467.15	121	652.50	121	9.14	120
644	530	V	K0101a	2,2,5,5-tetramethylhexan-3-one	868-91-7	1.0	298.15	816.90	117	48.80	114	-	-	-	-	-	-	(8.30)	-
645	531	V	K0102a	4-ethyl-2,2-dimethylhexan-3-one	40239-63-2	1.0	298.15	825.20	117	-	-	-	-	-	-	-	-	(8.30)	-
646	532	V	K0103a	4,6,6-trimethylheptan-2-one	40239-01-8	1.0	288.65	825.20	117	-	-	-	-	-	-	-	-	(8.30)	-
647	533	V	K0104a	2,2-dimethyloctan-3-one	5340-64-7	1.0	293.15	832.00	117	-	-	-	-	-	-	-	-	(8.30)	-
648	534	V	K0105a	2,2-dimethyloctan-4-one	22319-52-4	1.0	293.15	814.30	117	-	-	-	-	-	-	-	-	(8.30)	-
649	535	V	K0106a	2-methylnonan-3-one	5445-31-8	1.0	293.15	822.60	117	-	-	-	-	473.00	121	672.74	121	(8.30)	-
650	535	V	K0106b	2-methylnonan-3-one	5445-31-8	0.01	355.95	-	-	49.44	121	-	-	473.00	121	672.74	121	(8.30)	-
651	536	V	K0107a	2-methylnonan-4-one	6627-76-5	1.0	298.15	818.00	117	-	-	-	-	-	-	-	-	(8.30)	-
652	537	V	K0108a	2-methylnonan-5-one	22287-02-1	1.0	293.15	821.30	117	-	-	-	-	476.65	121	672.74	121	(8.30)	-
653	537	V	K0108b	2-methylnonan-5-one	22287-02-1	0.01	358.87	-	-	50.05	121	-	-	476.65	121	672.74	121	(8.30)	-
654	538	V	K0109a	6-methylnonan-2-one	104092-42-4	1.0	293.15	838.40	117	-	-	-	-	-	-	-	-	(8.30)	-
655	539	V	K0110a	decan-5-one	820-29-1	1.0	298.15	820.55	117	-	-	-	-	477.05	121	672.74	121	(8.30)	-
656	539	V	K0110b	decan-5-one	820-29-1	0.01	359.19	-	-	50.09	121	-	-	477.05	121	672.74	121	(8.30)	-
657	540	V	K0111a	decan-4-one	624-16-8	1.0	293.65	822.00	117	-	-	264.15	120	479.65	121	672.74	121	(8.30)	-
658	540	V	K0111b	decan-4-one	624-16-8	0.01	361.27	-	-	50.54	121	264.15	120	479.65	121	672.74	121	(8.30)	-
659	541	V	K0112a	decan-3-one	928-80-3	1.0	298.15	821.92	117	-	-	275.15	120	476.15	121	672.74	121	(8.30)	-
660	541	V	K0112b	decan-3-one	928-80-3	0.01	358.47	-	-	50.28	121	275.15	120	476.15	121	672.74	121	(8.30)	-
661	542	V	K0113a	decan-2-one	693-54-9	1.0	298.15	820.10	117	60.90	114	287.15	120	483.35	121	672.74	121	8.3	120
662	543	V	K7201a	3,3-dimethylpentane-2,4-dione	3142-58-3	0.01	333.97	923.27	121	-	-	-	-	446.15	121	645.00	121	(15.28)	-
663	544	V	K7202a	5-methylhexane-2,3-dione	13706-86-0	1.0	295.15	908.00	120	-	-	-	-	411.15	121	645.00	121	(15.28)	-
664	545	V	K7203a	3-ethylpentane-2,4-dione	1540-34-7	1.0	292.15	953.10	120	-	-	-	-	451.65	121	645.00	121	(15.28)	-
665	546	V	K7204a	3-methylhexane-2,5-dione	4437-50-7	0.01	352.37	902.85	121	-	-	-	-	469.15	121	645.00	121	(15.28)	-
666	547	V	K7205a	heptane-2,3-dione	96-04-8	1.0	291.15	919.00	120	-	-	-	-	417.15	121	645.00	121	(15.28)	-
667	548	V	K7206a	heptane-3,5-dione	7424-54-6	1.0	293.15	945.00	120	-	-	-	-	449.15	121	645.00	121	(15.28)	-
668	549	V	K7207a	heptane-2,4-dione	7307-02-0	1.0	447.2	-	-	38.84	121	-	-	447.20	121	-	-	(15.28)	-
669	550	V	K7208a	heptane-2,6-dione	13505-34-5	0.01	373.17	885.33	121	-	-	-	-	495.15	121	645.00	121	(15.28)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
670	551	V	K8202a	2,5-dimethylhexane-3,4-dione	4388-87-8	0.01	311.17	909.01	121	41.82	121	-	-	417.65	121	648.00	121	(15.28)	-
671	552	V	K8206a	octane-4,5-dione	5455-24-3	0.01	329.97	907.83	121	45.27	121	-	-	441.15	121	648.00	121	(15.28)	-
672	553	V	K8207a	octane-2,4-dione	14090-87-0	0.01	350.77	882.20	121	-	-	-	-	467.15	121	648.00	121	(15.28)	-
673	554	V	K9201a	2,6-dimethylheptane-3,5-dione	18362-64-6	1.0	298.0	-	-	56.10	114	-	-	339.15	121	-	-	(15.28)	-
674	555	V	K9202a	nonane-2,4-dione	6175-23-1	0.01	351.39	893.69	121	-	-	-	-	467.93	121	680.91	121	(15.28)	-
675	556	V	K0201a	2,2,5,5-tetramethylhexane-3,4-dione	4388-88-9	1.0	442.15	-	-	38.35	121	-	-	442.15	121	-	-	(15.28)	-
676	557	V	K0202a	2,2,6-trimethylheptane-3,5-dione	7333-23-5	1.0	298.0	-	-	57.70	114	-	-	-	-	-	-	(15.28)	-
677	558	V	K7301a	3-acetylpentane-2,4-dione	815-68-9	1.0	384.0	-	-	54.90	114	-	-	476.65	121	-	-	(15.0)	-
678	559	V	K7302a	heptane-2,4,6-trione	626-53-9	1.0	313.15	1059.90	120	-	-	322.15	120	455.78	121	-	-	(15.0)	-
679	559	V	K7302b	heptane-2,4,6-trione	626-53-9	1.0	455.78	-	-	39.65	121	322.15	120	455.78	121	-	-	(15.0)	-
680	560	V	E7201a	ethyl 2,2-dimethylpropanoate	3938-95-2	1.0	298.15	849.50	116	41.30	114	183.65	120	391.55	121	-	-	(4.67)	-
681	561	V	E7202a	methyl 3,3-dimethylbutanoate	10250-48-3	1.0	293.15	870.00	116	43.90	114	-	-	-	-	-	-	(4.67)	-
682	562	V	E7203a	2,2-dimethylpropyl acetate	926-41-0	1.0	298.15	853.90	116	-	-	-	-	-	-	586.34	121	(4.67)	-
683	562	V	E7203b	2,2-dimethylpropyl acetate	926-41-0	0.01	300.07	-	-	43.46	121	-	-	-	-	586.34	121	(4.67)	-
684	563	V	E7204a	2-methylbutan-2-yl acetate	625-16-1	1.0	297.85	872.50	116	40.30	114	-	-	-	-	-	-	(4.67)	-
685	564	V	E7205a	tert-butyl propanoate	20487-40-5	1.0	293.15	864.70	116	-	-	-	-	414.55	121	-	-	(4.67)	-
686	564	V	E7205b	tert-butyl propanoate	20487-40-5	1.0	414.55	-	-	41.09	121	-	-	414.55	121	-	-	(4.67)	-
687	565	V	E7206a	propan-2-yl 2-methylpropanoate	617-50-5	1.0	294.5	846.74	116	-	-	-	-	396.15	120	-	-	(4.67)	-
688	565	V	E7206b	propan-2-yl 2-methylpropanoate	617-50-5	1.0	272.0	-	-	43.30	114	-	-	396.15	120	-	-	(4.67)	-
689	566	V	E7207a	3-methylbutan-2-yl acetate	5343-96-4	1.0	298.15	866.00	116	-	-	-	-	401.65	121	586.34	121	(4.67)	-
690	567	V	E7208a	methyl 2-ethylbutanoate	816-11-5	1.0	293.15	879.70	116	-	-	-	-	409.15	121	586.34	121	(4.67)	-
691	568	V	E7209a	methyl 2-methylpentanoate	2177-77-7	1.0	293.15	876.50	116	-	-	-	-	-	-	-	-	(4.67)	-
692	569	V	E7210a	ethyl 2-methylbutanoate	7452-79-1	1.0	293.15	867.80	116	44.70	114	-	-	-	-	-	-	(4.67)	-
693	570	V	E7211a	propyl 2-methylpropanoate	644-49-5	1.0	298.15	859.46	116	-	-	-	-	407.15	120	-	-	(4.67)	-
694	570	V	E7211b	propyl 2-methylpropanoate	644-49-5	1.0	282.0	-	-	50.50	114	-	-	407.15	120	-	-	(4.67)	-
695	571	V	E7212a	ethyl 3-methylbutanoate	108-64-5	1.0	298.15	861.23	116	-	-	173.85	120	408.15	120	-	-	4.71	120
696	571	V	E7212b	ethyl 3-methylbutanoate	108-64-5	1.0	282.0	-	-	44.50	114	173.85	120	408.15	120	-	-	4.71	120
697	572	V	E7213a	2-methylpropyl propanoate	540-42-1	1.0	298.15	867.52	116	-	-	201.75	120	409.15	120	592.00	121	(4.67)	-
698	572	V	E7213b	2-methylpropyl propanoate	540-42-1	1.0	286.0	-	-	44.90	114	201.75	120	409.15	120	592.00	121	(4.67)	-
699	573	V	E7214a	butan-2-yl propanoate	591-34-4	1.0	298.15	861.25	116	-	-	-	-	406.15	120	-	-	(4.67)	-
700	574	V	E7215a	propan-2-yl butanoate	638-11-9	1.0	298.15	853.92	116	-	-	-	-	402.15	120	-	-	(4.67)	-
701	575	V	E7216a	2-methylbutyl acetate	624-41-9	1.0	293.15	867.80	116	-	-	-	-	413.15	121	586.34	121	(4.67)	-
702	575	V	E7216b	2-methylbutyl acetate	624-41-9	0.01	309.67	-	-	42.89	121	-	-	413.15	121	586.34	121	(4.67)	-
703	576	V	E7217a	pentan-3-yl acetate	620-11-1	0.01	303.27	861.47	121	41.83	121	-	-	405.15	121	586.34	121	(4.67)	-
704	577	V	E7218a	3-methylbutyl acetate	123-92-2	1.0	298.75	864.80	116	46.40	114	194.65	120	414.75	120	586.10	121	4.72	120
705	578	V	E7219a	pentan-2-yl acetate	626-38-0	1.0	298.15	863.07	116	-	-	-	-	406.15	121	586.34	121	(4.67)	-
706	578	V	E7219b	pentan-2-yl acetate	626-38-0	0.01	304.07	-	-	41.99	121	-	-	406.15	121	586.34	121	(4.67)	-
707	579	V	E7220a	methyl hexanoate	106-70-7	1.0	298.15	880.40	116	47.70	114	203.15	120	422.65	121	586.34	121	4.615	120
708	580	V	E7221a	ethyl pentanoate	539-82-2	1.01	298.15	869.42	118	47.00	114	181.95	120	419.25	121	586.34	121	4.71	120
709	581	V	E7222a	propyl butanoate	105-66-8	1.0	298.15	868.23	116	-	-	177.95	120	416.45	121	593.70	121	4.3	120
710	581	V	E7222b	propyl butanoate	105-66-8	1.0	286.0	-	-	44.30	114	177.95	120	416.45	121	593.70	121	4.3	120
711	582	V	E7223a	butyl propanoate	590-01-2	1.0	298.15	871.54	116	48.50	114	183.65	120	419.75	121	594.60	121	4.838	120
712	583	V	E7224a	pentyl acetate	628-63-7	1.0	298.15	872.23	116	48.60	114	202.25	120	422.15	121	599.90	121	4.79	120
713	584	V	E8201a	propan-2-yl 2,2-dimethylpropanoate	5129-36-2	1.0	293.15	830.00	116	-	-	-	-	-	-	-	-	(4.48)	-
714	585	V	E8202a	methyl 2,3,3-trimethylbutanoate	19910-30-6	1.0	298.15	874.90	116	-	-	-	-	-	-	-	-	(4.48)	-
715	586	V	E8203a	tert-butyl 2-methylpropanoate	16889-72-8	1.0	399.85	-	-	30.47	121	-	-	399.85	121	-	-	(4.48)	-
716	587	V	E8204a	ethyl 2,2-dimethylbutanoate	5129-40-8	1.0	277.15	883.00	116	-	-	-	-	-	-	-	-	(4.48)	-
717	588	V	E8205a	3-methylpentan-3-yl acetate	10250-47-2	0.01	316.07	860.15	121	-	-	-	-	421.15	121	606.49	121	(4.48)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
718	589	V	E8206a	ethyl 3,3-dimethylbutanoate	5340-78-3	1.0	293.15	860.40	[116]	-	-	-	-	-	-	-	-	(4.48)	-
719	590	V	E8208a	3,3-dimethylbutyl acetate	1421-87-0	1.0	293.15	867.90	[116]	-	-	-	-	-	-	-	-	(4.48)	-
720	591	V	E8209b	2-methylbutan-2-yl propanoate	34949-22-9	1.0	298.0	-	-	45.70	[114]	-	-	437.43	[121]	606.49	[121]	(4.48)	-
721	592	V	E8210b	2-methylpentan-2-yl acetate	34859-98-8	1.0	298.0	-	-	45.60	[114]	-	-	426.15	[121]	606.49	[121]	(4.48)	-
722	593	V	E8211a	tert-butyl butanoate	2308-38-5	1.0	409.15	-	-	36.39	[121]	-	-	409.15	[121]	-	-	(4.48)	-
723	594	V	E8212a	ethyl 2,3-dimethylbutanoate	54004-42-1	1.0	298.15	866.00	[116]	-	-	-	-	-	-	-	-	(4.48)	-
724	595	V	E8213a	2-methylpropyl 2-methylpropanoate	97-85-8	1.0	293.15	847.00	[116]	48.50	[114]	192.55	[120]	421.15	[120]	-	-	(4.48)	-
725	596	V	E8214a	butan-2-yl 2-methylpropanoate	23412-21-7	1.0	289.15	870.00	[116]	-	-	-	-	-	-	606.49	[121]	(4.48)	-
726	597	V	E8216a	propan-2-yl 3-methylbutanoate	32665-23-9	1.0	298.15	846.10	[116]	-	-	-	-	420.15	[120]	-	-	(4.48)	-
727	598	V	E8217a	2-methylpentan-3-yl acetate	35897-16-6	0.01	316.87	846.63	[121]	-	-	-	-	422.15	[121]	606.49	[121]	(4.48)	-
728	599	V	E8218a	4-methylpentan-2-yl acetate	108-84-9	1.0	298.15	880.50	[120]	-	-	-	-	420.65	[120]	-	-	(4.48)	-
729	600	V	E8219a	methyl 2-ethylpentanoate	816-16-0	1.0	293.15	875.00	[116]	-	-	-	-	-	-	-	-	(4.48)	-
730	601	V	E8220a	ethyl 2-ethylbutanoate	2983-38-2	1.0	293.15	863.30	[116]	-	-	-	-	-	-	-	-	(4.48)	-
731	602	V	E8221a	ethyl 2-methylpentanoate	39255-32-8	1.0	293.15	876.50	[116]	48.40	[114]	-	-	428.3	[118]	-	-	(4.48)	-
732	602	V	E8221b	ethyl 2-methylpentanoate	39255-32-8	1.0	298.15	-	-	48.40	[118]	-	-	428.3	[118]	-	-	(4.48)	-
733	603	V	E8222a	propyl 2-methylbutanoate	37064-20-3	1.0	293.15	869.70	[116]	-	-	-	-	-	-	-	-	(4.48)	-
734	604	V	E8223a	butyl 2-methylpropanoate	97-87-0	1.0	298.15	857.37	[116]	-	-	-	-	-	-	-	-	(4.48)	-
735	605	V	E8224a	ethyl 3-methylpentanoate	5870-68-8	1.0	293.15	878.00	[116]	-	-	-	-	-	-	-	-	(4.48)	-
736	606	V	E8225a	propyl 3-methylbutanoate	557-00-6	1.0	298.15	857.48	[116]	44.30	[114]	-	-	429.05	[121]	-	-	(4.48)	-
737	607	V	E8227a	ethyl 4-methylpentanoate	25415-67-2	1.0	293.15	870.50	[120]	-	-	-	-	436.15	[121]	606.49	[121]	(4.48)	-
738	607	V	E8227b	ethyl 4-methylpentanoate	25415-67-2	1.0	299.0	-	-	45.40	[114]	-	-	436.15	[121]	606.49	[121]	(4.48)	-
739	608	V	E8228a	2-methylpropyl butanoate	539-90-2	1.0	298.15	860.60	[116]	-	-	-	-	430.15	[120]	611.00	[121]	(4.48)	-
740	608	V	E8228b	2-methylpropyl butanoate	539-90-2	1.0	292.0	-	-	41.70	[114]	-	-	430.15	[120]	611.00	[121]	(4.48)	-
741	609	V	E8229a	3-methylbutyl propanoate	105-68-0	1.0	298.15	865.00	[116]	44.10	[114]	-	-	446.15	[120]	606.49	[121]	5.21	[120]
742	610	V	E8230a	butan-2-yl butanoate	819-97-6	1.0	298.15	863.24	[116]	-	-	-	-	-	-	-	-	(4.48)	-
743	611	V	E8231a	pentan-2-yl propanoate	54004-43-2	1.0	298.15	861.28	[116]	-	-	-	-	440.22	[121]	606.49	[121]	(4.48)	-
744	612	V	E8232a	propan-2-yl pentanoate	18362-97-5	1.0	293.15	857.90	[120]	-	-	-	-	436.35	[121]	606.49	[121]	(4.48)	-
745	613	V	E8233a	2-ethylbutyl acetate	10031-87-5	1.0	293.15	879.00	[120]	-	-	-	-	435.65	[121]	606.49	[121]	(4.48)	-
746	613	V	E8233b	2-ethylbutyl acetate	10031-87-5	0.01	327.67	-	-	44.88	[121]	-	-	435.65	[121]	606.49	[121]	(4.48)	-
747	614	V	E8235a	2-methylpentyl acetate	7789-99-3	1.0	298.15	869.10	[116]	-	-	-	-	436.15	[120]	606.49	[121]	(4.48)	-
748	614	V	E8235b	2-methylpentyl acetate	7789-99-3	0.01	328.07	-	-	45.70	[121]	-	-	436.15	[120]	606.49	[121]	(4.48)	-
749	615	V	E8236a	hexan-2-yl acetate	5953-49-1	1.0	298.15	859.91	[116]	-	-	-	-	-	-	606.49	[121]	(4.48)	-
750	616	V	E8237a	methyl heptanoate	106-73-0	1.01	298.15	875.88	[118]	51.60	[114]	217.45	[120]	447.15	[121]	606.49	[121]	4.355	[120]
751	617	V	E8238a	ethyl hexanoate	123-66-0	1.0	298.15	866.69	[116]	50.60	[114]	205.55	[120]	440.15	[121]	606.49	[121]	4.45	[120]
752	618	V	E8239a	propyl pentanoate	141-06-0	1.0	298.15	865.78	[116]	-	-	202.45	[120]	440.65	[121]	606.49	[121]	4.0	[120]
753	618	V	E8239b	propyl pentanoate	141-06-0	0.01	329.57	-	-	46.64	[121]	202.45	[120]	440.65	[121]	606.49	[121]	4.0	[120]
754	619	V	E8240a	butyl butanoate	109-21-7	1.01	298.15	869.14	[118]	-	-	181.65	[120]	438.15	[121]	606.49	[121]	4.39	[120]
755	619	V	E8240b	butyl butanoate	109-21-7	0.01	327.57	-	-	46.39	[121]	181.65	[120]	438.15	[121]	606.49	[121]	4.39	[120]
756	620	V	E8241a	pentyl propanoate	624-54-4	1.0	298.15	868.10	[116]	52.20	[114]	200.05	[120]	441.90	[121]	606.49	[121]	4.552	[120]
757	621	V	E8242a	hexyl acetate	142-92-7	1.0	298.15	868.60	[116]	51.90	[114]	212.15	[120]	444.65	[121]	606.49	[121]	4.42	[120]
758	622	V	E9201a	methyl 2,4,4-trimethylpentanoate	-	1.0	298.0	-	-	48.40	[114]	-	-	-	-	-	-	(4.04)	-
759	623	V	E9202a	2-methylbutan-2-yl 2-methylpropanoate	194784-93-5	1.0	298.0	-	-	47.80	[114]	-	-	-	-	-	-	(4.04)	-
760	624	V	E9203a	butyl 2,2-dimethylpropanoate	5129-37-3	1.0	298.0	-	-	50.40	[114]	-	-	-	-	-	-	(4.04)	-
761	625	V	E9205b	2-methylbutan-2-yl butanoate	2050-00-2	1.0	298.0	-	-	50.30	[114]	-	-	460.31	[121]	625.31	[121]	(4.04)	-
762	626	V	E9207a	ethyl 2,4-dimethylpentanoate	172103-12-7	1.0	301.15	855.00	[116]	-	-	-	-	-	-	-	-	(4.04)	-
763	627	V	E9209a	3-methylbutyl 2-methylpropanoate	2050-01-3	1.0	293.15	862.70	[120]	51.70	[114]	-	-	442.15	[120]	-	-	(4.04)	-
764	628	V	E9210a	ethyl 3,4-dimethylpentanoate	6570-83-8	1.0	298.15	869.00	[116]	-	-	-	-	-	-	-	-	(4.04)	-
765	629	V	E9212a	2-methylpropyl 3-methylbutanoate	589-59-3	1.0	298.15	861.70	[116]	-	-	-	-	442.15	[120]	-	-	(4.04)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
766	629	V	E9212b	2-methylpropyl 3-methylbutanoate	589-59-3	1.0	304.0	-	-	47.30	[114]	-	-	442.15	[120]	-	-	(4.04)	-
767	630	V	E9213a	butan-2-yl 3-methylbutanoate	2051-38-9	1.0	293.15	848.20	[116]	-	-	-	-	-	-	-	-	(4.04)	-
768	631	V	E9214a	methyl 2-propylpentanoate	22632-59-3	1.0	293.15	871.00	[116]	-	-	-	-	-	-	-	-	(4.04)	-
769	632	V	E9215a	ethyl 2-ethylpentanoate	43164-26-7	1.0	293.15	857.20	[116]	-	-	-	-	-	-	-	-	(4.04)	-
770	633	V	E9216a	propyl 2-ethylbutanoate	5129-46-4	1.0	293.15	868.80	[116]	-	-	-	-	-	-	-	-	(4.04)	-
771	634	V	E9217a	propyl 2-methylpentanoate	6639-14-1	1.0	293.15	866.90	[116]	-	-	-	-	-	-	-	-	(4.04)	-
772	635	V	E9218a	butyl 2-methylbutanoate	15706-73-7	1.0	293.15	862.00	[120]	50.60	[114]	-	-	452.15	[121]	-	-	(4.04)	-
773	636	V	E9219a	pentyl 2-methylpropanoate	2445-72-9	1.0	293.15	872.10	[116]	-	-	-	-	-	-	625.31	[121]	(4.04)	-
774	637	V	E9220a	ethyl 3-methylhexanoate	41692-47-1	1.0	293.15	867.90	[116]	-	-	-	-	450.15	[121]	625.31	[121]	(4.04)	-
775	638	V	E9221a	butyl 3-methylbutanoate	109-19-3	1.0	298.15	856.69	[116]	-	-	-	-	456.91	[121]	-	-	(4.04)	-
776	638	V	E9221b	butyl 3-methylbutanoate	109-19-3	1.0	456.91	-	-	39.76	[121]	-	-	456.91	[121]	-	-	(4.04)	-
777	639	V	E9222a	ethyl 4-methylhexanoate	1561-10-0	1.0	293.15	870.80	[120]	-	-	-	-	453.15	[121]	625.31	[121]	(4.04)	-
778	640	V	E9223a	2-methylbutyl butanoate	51115-64-1	0.01	336.57	-	-	49.17	[121]	-	-	452.15	[121]	620.00	[121]	(4.04)	-
779	641	V	E9225a	3-methylbutyl butanoate	106-27-4	1.0	298.15	860.30	[116]	-	-	-	-	452.15	[121]	625.31	[121]	4.0	[120]
780	641	V	E9225b	3-methylbutyl butanoate	106-27-4	1.0	309.0	-	-	47.40	[114]	-	-	452.15	[121]	625.31	[121]	4.0	[120]
781	642	V	E9226a	2-methylpropyl pentanoate	10588-10-0	1.0	298.15	853.57	[116]	-	-	-	-	456.15	[120]	625.31	[121]	3.8	[120]
782	642	V	E9226b	2-methylpropyl pentanoate	10588-10-0	0.01	338.77	-	-	48.78	[121]	-	-	456.15	[120]	625.31	[121]	3.8	[120]
783	643	V	E9227a	pentan-2-yl butanoate	60415-61-4	1.0	298.15	864.72	[116]	-	-	-	-	455.15	[121]	625.31	[121]	(4.04)	-
784	644	V	E9228a	butan-2-yl pentanoate	23361-74-2	1.0	298.15	854.87	[116]	-	-	-	-	-	-	-	-	(4.04)	-
785	645	V	E9229a	propan-2-yl hexanoate	2311-46-8	1.0	298.15	852.50	[116]	-	-	-	-	-	-	-	-	(4.04)	-
786	645	V	E9229b	propan-2-yl hexanoate	2311-46-8	1.0	322.0	-	-	51.60	[114]	-	-	-	-	-	-	(4.04)	-
787	646	V	E9232a	heptan-3-yl acetate	5921-83-5	0.01	346.57	818.20	[121]	-	-	-	-	-	-	625.31	[121]	(4.04)	-
788	647	V	E9234a	heptan-2-yl acetate	5921-82-4	1.0	298.15	857.03	[116]	-	-	-	-	-	-	625.31	[121]	(4.04)	-
789	648	V	E9235a	methyl octanoate	111-11-5	1.0	298.15	873.12	[116]	56.40	[114]	236.25	[120]	466.05	[121]	625.31	[121]	4.101	[120]
790	649	V	E9236a	ethyl heptanoate	106-30-9	1.0	298.15	864.71	[116]	-	-	206.95	[120]	460.15	[121]	625.31	[121]	(4.04)	-
791	650	V	E9237a	propyl hexanoate	626-77-7	1.0	298.15	863.02	[116]	-	-	199.15	[120]	460.15	[121]	625.31	[121]	(4.04)	-
792	650	V	E9237b	propyl hexanoate	626-77-7	1.0	330.0	-	-	52.10	[114]	199.15	[120]	460.15	[121]	625.31	[121]	(4.04)	-
793	651	V	E9238a	butyl pentanoate	591-68-4	1.0	298.15	863.37	[116]	-	-	189.38	[120]	459.15	[120]	625.31	[121]	(4.04)	-
794	651	V	E9238b	butyl pentanoate	591-68-4	0.01	344.77	-	-	49.19	[121]	189.38	[120]	459.15	[120]	625.31	[121]	(4.04)	-
795	652	V	E9239a	pentyl butanoate	540-18-1	1.0	298.15	861.89	[116]	53.60	[114]	200.49	[120]	458.15	[121]	625.31	[121]	4.08	[120]
796	653	V	E9240a	hexyl propanoate	2445-76-3	1.0	298.15	865.42	[116]	57.10	[114]	215.65	[120]	463.15	[121]	625.31	[121]	(4.04)	-
797	654	V	E9241a	heptyl acetate	112-06-1	1.0	298.15	866.43	[116]	56.90	[114]	222.85	[120]	465.55	[121]	625.31	[121]	4.2	[120]
798	655	V	E0201a	2,2-dimethylpropyl 2,2-dimethylpropanoate	5340-26-1	1.0	293.15	843.10	[116]	48.90	[114]	-	-	-	-	-	-	(4.04)	-
799	656	V	E0202a	2-methylbutan-2-yl 2,2-dimethylpropanoate	89397-96-6	1.0	298.0	-	-	48.00	[114]	-	-	-	-	-	-	(4.04)	-
800	657	V	E0203a	2-methylbutan-2-yl 3-methylbutanoate	542-37-0	1.0	273.15	872.90	[120]	-	-	-	-	461.15	[120]	-	-	(4.04)	-
801	658	V	E0204a	ethyl 2,2-diethylbutanoate	34666-17-6	1.0	289.15	883.70	[116]	-	-	-	-	-	-	-	-	(4.04)	-
802	659	V	E0205a	butyl 3,3-dimethylbutanoate	85204-26-8	1.0	293.15	856.80	[116]	-	-	-	-	-	-	-	-	(4.04)	-
803	660	V	E0209a	3-methylbutyl 3-methylbutanoate	659-70-1	1.0	298.15	854.10	[116]	-	-	-	-	463.15	[120]	-	-	4.39	[120]
804	660	V	E0209b	3-methylbutyl 3-methylbutanoate	659-70-1	1.0	315.0	-	-	47.20	[114]	-	-	463.15	[120]	-	-	4.39	[120]
805	661	V	E0210a	2-methylpropyl 4-methylpentanoate	25415-70-7	0.01	333.17	819.40	[121]	-	-	-	-	445.15	[121]	643.00	[121]	(4.04)	-
806	662	V	E0212a	6-methylheptan-3-yl acetate	32764-34-4	0.01	345.27	810.29	[121]	-	-	-	-	457.65	[121]	643.00	[121]	(4.04)	-
807	663	V	E0213a	6-methylheptan-2-yl acetate	67952-57-2	1.0	293.15	847.40	[120]	-	-	-	-	460.15	[120]	-	-	(4.04)	-
808	664	V	E0214a	ethyl 2-propylpentanoate	17022-31-0	1.0	293.15	865.90	[116]	-	-	-	-	-	-	-	-	(4.04)	-
809	665	V	E0215a	methyl 2-ethylheptanoate	816-63-7	1.0	298.15	864.40	[116]	-	-	-	-	-	-	-	-	(4.04)	-
810	666	V	E0216a	ethyl 2-ethylhexanoate	2983-37-1	1.0	298.15	858.60	[120]	-	-	-	-	473.73	[121]	643.00	[121]	(4.04)	-
811	667	V	E0217a	methyl 2-methyloctanoate	2177-86-8	1.0	277.15	875.90	[116]	-	-	-	-	-	-	-	-	(4.04)	-
812	668	V	E0218a	hexyl 2-methylpropanoate	2349-07-7	1.0	293.15	870.00	[116]	-	-	-	-	-	-	-	-	(4.04)	-
813	669	V	E0219a	2-ethylbutyl butanoate	74398-53-1	1.0	292.95	872.60	[116]	-	-	-	-	-	-	643.00	[121]	(4.04)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
814	670	V	E0220a	3-methylpentyl butanoate	84254-83-1	0.01	354.97	826.08	[121]	51.33	[121]	-	-	-	-	643.00	[121]	(4.04)	-
815	671	V	E0222a	3-methylbutyl pentanoate	2050-09-1	1.0	293.15	858.00	[116]	-	-	-	-	466.15	[120]	643.00	[121]	3.6	[120]
816	672	V	E0223a	2-methylpropyl hexanoate	105-79-3	0.01	318.69	-	-	53.05	[121]	-	-	427.05	[121]	643.00	[121]	(4.04)	-
817	673	V	E0224a	butan-2-yl hexanoate	820-00-8	1.0	298.15	857.49	[116]	-	-	-	-	-	-	-	-	(4.04)	-
818	674	V	E0225a	2-ethylhexyl acetate	103-09-3	1.0	298.15	868.80	[116]	-	-	193.15	[120]	471.75	[121]	642.40	[121]	(4.04)	-
819	674	V	E0225b	2-ethylhexyl acetate	103-09-3	1.0	348.0	-	-	50.10	[114]	193.15	[120]	471.75	[121]	642.40	[121]	(4.04)	-
820	675	V	E0227a	2-methylheptyl acetate	-	0.01	353.67	805.44	[121]	-	-	-	-	-	-	643.00	[121]	(4.04)	-
821	676	V	E0228a	octan-3-yl acetate	4864-61-3	0.01	348.17	814.17	[121]	-	-	-	-	-	-	643.00	[121]	(4.04)	-
822	677	V	E0230a	octan-2-yl acetate	2051-50-5	1.0	298.15	858.09	[116]	-	-	-	-	-	-	643.00	[121]	(4.04)	-
823	678	V	E0231a	methyl nonanoate	1731-84-6	1.0	298.15	870.87	[116]	61.60	[114]	-	-	486.65	[121]	643.00	[121]	3.943	[120]
824	679	V	E0232a	ethyl octanoate	106-32-1	1.0	298.15	862.92	[116]	59.50	[114]	228.45	[120]	481.65	[121]	643.00	[121]	(4.04)	-
825	680	V	E0233a	propyl heptanoate	7778-87-2	1.0	298.15	861.59	[116]	-	-	-	-	481.15	[121]	643.00	[121]	(4.04)	-
826	680	V	E0233b	propyl heptanoate	7778-87-2	0.01	361.97	-	-	52.12	[121]	-	-	481.15	[121]	643.00	[121]	(4.04)	-
827	681	V	E0234a	butyl hexanoate	626-82-4	1.0	298.15	862.30	[116]	-	-	223.15	[120]	481.15	[121]	643.00	[121]	(4.04)	-
828	681	V	E0234b	butyl hexanoate	626-82-4	0.01	361.97	-	-	52.07	[121]	223.15	[120]	481.15	[121]	643.00	[121]	(4.04)	-
829	682	V	E0235a	pentyl pentanoate	2173-56-0	1.0	298.15	860.20	[116]	-	-	194.35	[120]	476.85	[121]	643.00	[121]	4.076	[120]
830	682	V	E0235b	pentyl pentanoate	2173-56-0	0.01	358.53	-	-	51.86	[121]	194.35	[120]	476.85	[121]	643.00	[121]	4.076	[120]
831	683	V	E0236a	hexyl butanoate	2639-63-6	1.01	298.15	851.00	[118]	-	-	195.15	[120]	479.15	[121]	643.00	[121]	(4.04)	-
832	683	V	E0236b	hexyl butanoate	2639-63-6	0.01	361.97	-	-	51.44	[121]	195.15	[120]	479.15	[121]	643.00	[121]	(4.04)	-
833	684	V	E0237a	heptyl propanoate	2216-81-1	1.0	298.15	863.97	[116]	-	-	-	-	483.15	[121]	643.00	[121]	(4.04)	-
834	684	V	E0237b	heptyl propanoate	2216-81-1	0.01	364.47	-	-	52.45	[121]	-	-	483.15	[121]	643.00	[121]	(4.04)	-
835	685	V	E0238a	octyl acetate	112-14-1	1.0	298.15	864.30	[116]	60.70	[114]	235.15	[120]	484.45	[121]	643.00	[121]	4.18	[120]
836	686	V	E7401a	dimethyl 2,2-dimethylpropanedioate	6065-54-9	1.0	293.0	-	-	55.60	[114]	-	-	-	-	-	-	(7.71)	-
837	687	V	E7403a	dimethyl 2-ethylpropanedioate	26717-67-9	1.0	298.15	1061.39	[116]	-	-	-	-	-	-	-	-	(7.71)	-
838	688	V	E7404a	dimethyl 2-methylbutanedioate	1604-11-1	1.0	298.15	1076.00	[120]	-	-	-	-	469.15	[121]	-	-	(7.71)	-
839	688	V	E7404b	dimethyl 2-methylbutanedioate	1604-11-1	1.0	469.15	-	-	40.93	[121]	-	-	469.15	[121]	-	-	(7.71)	-
840	689	V	E7405a	ethyl 2-acetyloxypropanoate	2985-28-6	1.0	328.0	-	-	57.90	[114]	-	-	-	-	-	-	(7.71)	-
841	690	V	E7406a	2-acetyloxypropyl acetate	623-84-7	1.0	293.15	1059.00	[120]	-	-	-	-	463.65	[121]	-	-	(7.71)	-
842	690	V	E7406b	2-acetyloxypropyl acetate	623-84-7	1.0	323.0	-	-	54.90	[114]	-	-	463.65	[121]	-	-	(7.71)	-
843	691	V	E7407a	diethyl propanedioate	105-53-3	1.0	298.15	1049.80	[116]	58.70	[114]	223.15	[120]	472.05	[121]	653.00	[121]	7.550	[120]
844	692	V	E7408a	4-O-ethyl 1-O-methyl butanedioate	627-73-6	1.0	293.15	1076.00	[116]	-	-	-	-	481.35	[121]	-	-	(7.71)	-
845	692	V	E7408b	4-O-ethyl 1-O-methyl butanedioate	627-73-6	1.0	481.35	-	-	42.09	[121]	-	-	481.35	[121]	-	-	(7.71)	-
846	693	V	E7409a	dimethyl pentanedioate	1119-40-0	1.01	293.15	1087.67	[118]	65.70	[114]	230.65	[120]	487.15	[121]	-	-	7.87	[120]
847	694	V	E7411a	ethyl 3-acetyloxypropanoate	40326-37-2	1.0	358.0	-	-	72.10	[114]	-	-	-	-	-	-	(7.71)	-
848	695	V	E7412a	3-acetyloxypropyl acetate	628-66-0	1.0	293.15	1054.70	[116]	-	-	-	-	482.65	[121]	-	-	(7.71)	-
849	695	V	E7412b	3-acetyloxypropyl acetate	628-66-0	1.0	482.65	-	-	42.22	[121]	-	-	482.65	[121]	-	-	(7.71)	-
850	696	V	E8402a	dipropan-2-yl oxalate	615-81-6	1.0	298.15	989.19	[116]	60.20	[114]	-	-	463.15	[121]	-	-	6.403	[120]
851	697	V	E8403a	dimethyl 2-propylpropanedioate	14035-96-2	1.0	298.15	1036.93	[116]	-	-	-	-	-	-	-	-	(6.45)	-
852	698	V	E8404a	diethyl 2-methylpropanedioate	609-08-5	1.0	298.15	1017.38	[116]	-	-	-	-	474.15	[121]	-	-	(6.45)	-
853	698	V	E8404b	diethyl 2-methylpropanedioate	609-08-5	1.0	327.0	-	-	52.50	[114]	-	-	474.15	[121]	-	-	(6.45)	-
854	699	V	E8407a	dipropyl oxalate	615-98-5	1.0	298.15	1013.98	[116]	-	-	228.85	[120]	484.15	[121]	-	-	(6.45)	-
855	699	V	E8407b	dipropyl oxalate	615-98-5	1.0	341.0	-	-	57.80	[114]	228.85	[120]	484.15	[121]	-	-	(6.45)	-
856	700	V	E8408a	diethyl butanedioate	123-25-1	1.0	298.15	1035.30	[116]	64.50	[114]	251.55	[120]	489.65	[121]	663.00	[121]	6.098	[120]
857	701	V	E8409a	dimethyl hexanedioate	627-93-0	1.0	298.15	1057.57	[116]	69.00	[114]	283.45	[120]	495.09	[121]	-	-	6.84	[120]
858	702	V	E8410a	2-propanoyloxyethyl propanoate	123-80-8	1.0	293.15	1042.00	[116]	67.60	[114]	-	-	484.15	[121]	-	-	(6.45)	-
859	703	V	E8411a	propyl 3-acetyloxypropanoate	200867-13-6	1.0	367.0	-	-	74.70	[114]	-	-	-	-	-	-	(6.45)	-
860	704	V	E8412a	4-acetyloxybutyl acetate	628-67-1	1.0	293.15	1046.00	[116]	-	-	285.15	[120]	502.15	[121]	-	-	(6.45)	-
861	704	V	E8412b	4-acetyloxybutyl acetate	628-67-1	1.0	502.15	-	-	44.09	[121]	285.15	[120]	502.15	[121]	-	-	(6.45)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
862	705	V	E9402a	diethyl 2,2-dimethylpropanedioate	1619-62-1	1.0	470.15	-	-	41.02	121	-	-	470.15	121	-	-	(6.66)	-
863	706	V	E9406a	dipropan-2-yl propanedioate	13195-64-7	1.0	298.0	-	-	63.90	114	-	-	509.23	121	-	-	(6.66)	-
864	707	V	E9407a	diethyl 2-ethylpropanedioate	133-13-1	1.0	298.15	1000.71	116	-	-	-	-	481.15	121	-	-	(6.66)	-
865	707	V	E9407b	diethyl 2-ethylpropanedioate	133-13-1	1.0	338.0	-	-	55.30	114	-	-	481.15	121	-	-	(6.66)	-
866	708	V	E9408a	diethyl 2-methylbutanedioate	4676-51-1	1.0	490.65	-	-	42.99	121	-	-	490.65	121	-	-	(6.66)	-
867	709	V	E9409a	butyl 2-acetyloxypropanoate	5422-69-5	1.0	340.0	-	-	63.20	114	-	-	-	-	-	-	(6.66)	-
868	710	V	E9410a	dipropyl propanedioate	1117-19-7	1.0	298.0	-	-	66.20	114	-	-	502.15	121	-	-	(6.66)	-
869	711	V	E9411a	diethyl pentanedioate	818-38-2	1.0	293.15	1022.00	120	67.00	114	249.05	120	509.65	121	-	-	6.659	120
870	712	V	E9412a	dimethyl heptanedioate	1732-08-7	1.0	293.15	1039.10	116	73.50	114	252.15	120	509.23	121	-	-	(6.66)	-
871	713	V	E9413a	butyl 3-acetyloxypropanoate	40326-38-3	1.0	382.0	-	-	75.40	114	-	-	-	-	-	-	(6.66)	-
872	714	V	E9414a	5-acetyloxypentyl acetate	6963-44-6	1.0	293.15	1029.60	120	-	-	275.15	120	514.15	121	-	-	(6.66)	-
873	714	V	E9414b	5-acetyloxypentyl acetate	6963-44-6	1.0	514.15	-	-	45.24	121	275.15	120	514.15	121	-	-	(6.66)	-
874	715	V	E0401a	ditert-butyl oxalate	691-64-5	1.0	298.0	-	-	63.50	114	-	-	-	-	-	-	(6.11)	-
875	716	V	E0403a	diethyl 2-ethyl-2-methylpropanedioate	2049-70-9	1.0	332.0	-	-	53.20	114	-	-	-	-	-	-	(6.11)	-
876	717	V	E0404a	bis(2-methylpropyl) oxalate	2050-61-5	1.0	351.0	-	-	55.50	114	-	-	502.15	121	-	-	(6.11)	-
877	718	V	E0405a	diethyl 2-propan-2-ylpropanedioate	759-36-4	1.0	293.15	996.10	120	-	-	-	-	488.15	121	-	-	(6.11)	-
878	718	V	E0405b	diethyl 2-propan-2-ylpropanedioate	759-36-4	1.0	488.15	-	-	42.75	121	-	-	488.15	121	-	-	(6.11)	-
879	719	V	E0406a	dipropan-2-yl butanedioate	924-88-9	1.0	298.15	980.26	116	70.80	114	-	-	-	-	-	-	(6.11)	-
880	720	V	E0407a	diethyl 2-propylpropanedioate	2163-48-6	1.0	298.15	982.75	116	-	-	-	-	494.15	121	-	-	(6.11)	-
881	720	V	E0407b	diethyl 2-propylpropanedioate	2163-48-6	1.0	494.15	-	-	43.32	121	-	-	494.15	121	-	-	(6.11)	-
882	721	V	E0408a	dibutyl oxalate	2050-60-4	1.0	298.15	983.33	116	71.40	114	242.65	120	514.15	121	-	-	(6.11)	-
883	722	V	E0409a	dipropyl butanedioate	925-15-5	1.0	298.15	997.36	116	71.00	114	267.25	120	523.95	121	-	-	(6.11)	-
884	723	V	E0410a	diethyl hexanedioate	141-28-6	1.0	298.15	1003.70	116	73.00	114	253.15	120	518.15	121	-	-	6.109	120
885	724	V	E0411a	dimethyl octanedioate	1732-09-8	1.0	298.15	1019.17	116	78.10	114	279.15	120	541.15	121	-	-	(6.11)	-
886	725	V	E0412a	2-butanoyloxyethyl butanoate	105-72-6	1.0	298.15	995.30	116	73.20	114	-	-	513.15	121	-	-	(6.11)	-
887	726	V	F7202a	hexyl formate	629-33-4	1.0	298.15	874.61	116	50.00	114	210.55	120	428.65	121	586.34	121	(6.91)	-
888	727	V	F8201a	heptyl formate	112-23-2	1.0	302.25	869.00	116	53.80	114	-	-	451.25	121	606.49	121	(6.91)	-
889	728	V	F9201a	octyl formate	112-32-3	1.0	298.15	871.00	116	58.20	114	234.05	120	471.95	121	625.31	121	(6.91)	-
890	729	V	F0203a	nonyl formate	5451-92-3	1.0	293.15	867.00	116	-	-	240.15	120	485.72	121	643.00	121	(6.91)	-
891	730	V	L7101a	2,3,3-trimethylbutan-2-ol	594-83-2	1.0	298.15	833.50	115	-	-	290.15	120	404.15	121	619.68	121	(6.16)	-
892	730	V	L7101b	2,3,3-trimethylbutan-2-ol	594-83-2	1.0	313.0	-	-	48.70	114	290.15	120	404.15	121	619.68	121	(6.16)	-
893	731	V	L7102a	2,2,3-trimethylbutan-1-ol	55505-23-2	1.0	293.15	846.60	115	-	-	-	-	430.15	121	619.68	121	(6.16)	-
894	732	V	L7103a	3,3-dimethylpentan-2-ol	19781-24-9	1.0	293.15	827.00	115	-	-	-	-	420.15	121	619.68	121	(6.16)	-
895	733	V	L7104a	2,3-dimethylpentan-3-ol	595-41-5	1.0	298.15	837.27	115	-	-	-	-	413.15	121	619.68	121	(6.16)	-
896	733	V	L7104b	2,3-dimethylpentan-3-ol	595-41-5	1.0	333.0	-	-	53.20	114	-	-	413.15	121	619.68	121	(6.16)	-
897	734	V	L7105a	2,3,3-trimethylbutan-1-ol	36794-64-6	1.0	298.15	823.80	115	-	-	-	-	433.15	121	619.68	121	(6.16)	-
898	735	V	L7106a	2,2-dimethylpentan-3-ol	3970-62-5	1.0	298.15	822.40	115	-	-	282.45	120	409.15	121	619.68	121	(6.16)	-
899	735	V	L7106b	2,2-dimethylpentan-3-ol	3970-62-5	1.0	333.0	-	-	51.40	114	282.45	120	409.15	121	619.68	121	(6.16)	-
900	736	V	L7107a	2,3-dimethylpentan-2-ol	4911-70-0	1.0	298.15	828.50	115	-	-	-	-	412.15	121	619.68	121	(6.16)	-
901	737	V	L7108a	4,4-dimethylpentan-2-ol	6144-93-0	1.0	293.15	811.90	115	-	-	-	-	411.15	121	619.68	121	(6.16)	-
902	738	V	L7109a	2,4-dimethylpentan-2-ol	625-06-9	1.0	298.15	810.00	115	-	-	-	-	406.15	121	619.68	121	(6.16)	-
903	738	V	L7109b	2,4-dimethylpentan-2-ol	625-06-9	1.0	343.0	-	-	49.70	114	-	-	406.15	121	619.68	121	(6.16)	-
904	739	V	L7110a	3,4-dimethylpentan-2-ol	64502-86-9	1.0	294.15	836.00	115	-	-	-	-	426.15	121	619.68	121	(6.16)	-
905	740	V	L7111a	2,4-dimethylpentan-3-ol	600-36-2	1.0	298.15	824.94	115	-	-	-	-	411.95	121	619.68	121	(6.16)	-
906	740	V	L7111b	2,4-dimethylpentan-3-ol	600-36-2	1.0	322.0	-	-	53.60	114	-	-	411.95	121	619.68	121	(6.16)	-
907	741	V	L7112a	2-ethyl-2-methylbutan-1-ol	18371-13-6	1.0	293.15	828.20	115	-	-	-	-	430.15	121	619.68	121	(6.16)	-
908	741	V	L7112b	2-ethyl-2-methylbutan-1-ol	18371-13-6	1.0	373.0	-	-	55.70	114	-	-	430.15	121	619.68	121	(6.16)	-
909	742	V	L7113a	3-ethylpentan-3-ol	597-49-9	1.0	298.15	839.56	115	57.30	114	260.15	120	415.65	121	619.68	121	3.158	120

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
910	743	V	L7114a	3,3-dimethylpentan-1-ol	19264-94-9	1.0	293.15	832.00	115	-	-	-	-	438.15	121	619.68	121	(6.16)	-
911	744	V	L7115a	2,2-dimethylpentan-1-ol	2370-12-9	1.0	293.15	837.90	115	-	-	-	-	426.15	121	619.68	121	6.020	120
912	745	V	L7116a	3-methylhexan-3-ol	597-96-6	1.0	298.15	820.18	115	-	-	-	-	415.95	121	619.68	121	3.248	120
913	745	V	L7116b	3-methylhexan-3-ol	597-96-6	1.0	338.0	-	-	53.60	114	-	-	415.95	121	619.68	121	3.248	120
914	746	V	L7117a	4,4-dimethylpentan-1-ol	3121-79-7	1.0	293.15	815.10	115	-	-	-	-	433.15	121	619.68	121	(6.16)	-
915	747	V	L7118a	2-methylhexan-2-ol	625-23-0	1.0	298.15	809.80	115	58.60	114	-	-	415.95	121	619.68	121	3.257	120
916	748	V	L7119a	2-ethyl-3-methylbutan-1-ol	32444-34-1	1.0	298.15	832.70	115	-	-	-	-	435.15	121	619.68	121	(6.16)	-
917	749	V	L7120a	3-ethylpentan-2-ol	609-27-8	1.0	298.15	833.30	115	-	-	-	-	425.15	121	619.68	121	(6.16)	-
918	750	V	L7121a	2,3-dimethylpentan-1-ol	10143-23-4	1.0	296.15	836.00	115	-	-	-	-	437.15	121	619.68	121	(6.16)	-
919	751	V	L7122a	4-methylhexan-3-ol	615-29-2	0.01	314.89	805.69	121	-	-	-	-	422.15	121	619.68	121	(6.16)	-
920	752	V	L7123a	3,4-dimethylpentan-1-ol	6570-87-2	1.0	297.15	819.00	115	-	-	-	-	438.15	121	619.68	121	(6.16)	-
921	753	V	L7124a	3-methylhexan-2-ol	2313-65-7	1.0	298.15	822.00	120	-	-	-	-	425.15	121	619.68	121	4.990	120
922	754	V	L7125a	2-methylhexan-3-ol	617-29-8	1.0	293.15	823.90	115	-	-	-	-	418.15	121	619.68	121	(6.16)	-
923	754	V	L7125b	2-methylhexan-3-ol	617-29-8	1.0	338.0	-	-	55.70	114	-	-	418.15	121	619.68	121	(6.16)	-
924	755	V	L7126a	2,4-dimethylpentan-1-ol	6305-71-1	1.0	298.15	816.00	115	-	-	-	-	432.15	121	619.68	121	(6.16)	-
925	756	V	L7127a	4-methylhexan-2-ol	2313-61-3	1.0	298.15	817.70	115	-	-	-	-	424.15	121	619.68	121	(6.16)	-
926	757	V	L7128a	5-methylhexan-3-ol	623-55-2	1.0	293.15	833.10	115	59.80	114	-	-	421.15	121	619.68	121	(6.16)	-
927	758	V	L7129a	5-methylhexan-2-ol	627-59-8	1.0	293.15	813.10	115	-	-	-	-	424.15	121	619.68	121	(6.16)	-
928	759	V	L7130a	3-ethylpentan-1-ol	66225-51-2	0.01	328.67	803.52	121	-	-	-	-	439.15	121	619.68	121	(6.16)	-
929	760	V	L7131a	2-ethylpentan-1-ol	27522-11-8	1.0	298.15	828.80	115	-	-	-	-	439.15	121	619.68	121	(6.16)	-
930	761	V	L7132a	3-methylhexan-1-ol	13231-81-7	1.0	298.15	824.50	115	-	-	-	-	445.15	121	619.68	121	(6.16)	-
931	762	V	L7133a	4-methylhexan-1-ol	818-49-5	1.0	297.15	821.00	115	-	-	-	-	446.15	121	619.68	121	(6.16)	-
932	762	V	L7133b	4-methylhexan-1-ol	818-49-5	1.0	363.0	-	-	62.60	114	-	-	446.15	121	619.68	121	(6.16)	-
933	763	V	L7134a	2-methylhexan-1-ol	624-22-6	1.0	293.15	827.00	115	-	-	-	-	436.15	121	619.68	121	10.65	122
934	764	V	L7135a	heptan-4-ol	589-55-9	1.0	298.15	815.60	115	62.40	114	231.95	120	427.85	121	619.68	121	6.18	120
935	765	V	L7136a	heptan-3-ol	589-82-2	1.0	298.15	816.50	115	-	-	-	-	429.85	121	619.68	121	(6.16)	-
936	765	V	L7136b	heptan-3-ol	589-82-2	1.0	364.0	-	-	53.10	114	-	-	429.85	121	619.68	121	(6.16)	-
937	766	V	L7137a	5-methylhexan-1-ol	627-98-5	1.0	298.15	819.20	115	-	-	-	-	445.15	121	619.68	121	(6.16)	-
938	767	V	L7138a	heptan-2-ol	543-49-7	1.0	298.15	813.38	115	62.10	114	-	-	432.35	121	608.32	121	(6.16)	-
939	768	V	L7139a	heptan-1-ol	111-70-6	1.0	298.15	819.17	115	66.50	114	239.95	120	449.45	121	632.60	121	11.75	120
940	769	V	L8102a	2,3,3-trimethylpentan-2-ol	23171-85-9	1.0	298.15	815.10	115	-	-	-	-	433.15	121	641.41	121	(5.46)	-
941	770	V	L8103a	2,2,3-trimethylpentan-3-ol	7294-05-5	1.0	298.15	842.91	115	-	-	-	-	425.15	121	641.41	121	(5.46)	-
942	770	V	L8103b	2,2,3-trimethylpentan-3-ol	7294-05-5	1.0	333.0	-	-	47.30	114	-	-	425.15	121	641.41	121	(5.46)	-
943	771	V	L8104a	2,4,4-trimethylpentan-2-ol	690-37-9	1.0	293.15	823.70	115	-	-	253.15	120	419.55	121	641.41	121	(5.46)	-
944	772	V	L8105a	3,3,4-trimethylpentan-2-ol	19411-41-7	1.0	293.15	855.70	115	-	-	-	-	438.15	121	641.41	121	(5.46)	-
945	773	V	L8106a	2,3,4-trimethylpentan-3-ol	3054-92-0	1.0	293.15	849.20	115	-	-	-	-	430.15	121	641.41	121	(5.46)	-
946	774	V	L8107a	3,4,4-trimethylpentan-2-ol	10575-56-1	1.0	293.15	840.80	115	-	-	-	-	431.15	121	641.41	121	(5.46)	-
947	775	V	L8108a	2,2,4-trimethylpentan-3-ol	5162-48-1	1.0	293.15	832.40	115	-	-	260.15	120	424.15	121	641.41	121	(5.46)	-
948	775	V	L8108b	2,2,4-trimethylpentan-3-ol	5162-48-1	1.0	343.0	-	-	57.10	114	260.15	120	424.15	121	641.41	121	(5.46)	-
949	776	V	L8109a	2,3,4-trimethylpentan-2-ol	66576-26-9	1.0	293.15	808.00	115	-	-	-	-	431.15	121	641.41	121	(5.46)	-
950	777	V	L8110a	3-ethyl-3-methylpentan-2-ol	66576-22-5	1.0	293.15	857.60	115	-	-	-	-	433.00	121	641.41	121	(5.46)	-
951	778	V	L8111a	3-ethyl-2-methylpentan-3-ol	597-05-7	1.0	293.15	829.50	115	-	-	-	-	433.15	121	641.41	121	(5.46)	-
952	779	V	L8112a	4,4-dimethylhexan-3-ol	19550-09-5	1.0	293.15	834.10	115	-	-	-	-	432.15	121	641.41	121	(5.46)	-
953	780	V	L8113a	3,3-dimethylhexan-2-ol	22025-20-3	1.0	293.15	845.70	115	-	-	-	-	433.00	121	641.41	121	(5.46)	-
954	781	V	L8114a	3,4-dimethylhexan-3-ol	19550-08-4	1.0	298.15	834.50	115	-	-	-	-	425.15	121	641.41	121	(5.46)	-
955	782	V	L8115a	2,3-dimethylhexan-3-ol	4166-46-5	1.0	293.15	837.10	115	-	-	-	-	431.35	121	641.41	121	(5.46)	-
956	783	V	L8116a	2-ethyl-3,3-dimethylbutan-1-ol	66576-56-5	1.0	298.15	842.50	115	-	-	-	-	446.00	121	641.41	121	(5.46)	-
957	784	V	L8118a	2,2-dimethylhexan-3-ol	4209-90-9	1.0	293.15	834.20	115	-	-	-	-	429.25	121	641.41	121	(5.46)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
958	785	V	L8119a	3-ethyl-2-methylpentan-2-ol	19780-63-3	1.0	298.15	834.60	[115]	-	-	-	-	430.95	[121]	641.41	[121]	(5.46)	-
959	786	V	L8120a	2,3-dimethylhexan-2-ol	19550-03-9	1.0	298.15	831.00	[115]	-	-	-	-	433.25	[121]	641.41	[121]	(5.46)	-
960	787	V	L8121a	2,2,4-trimethylpentan-1-ol	123-44-4	1.0	293.15	838.40	[115]	-	-	-	-	441.45	[121]	641.41	[121]	(5.46)	-
961	787	V	L8121b	2,2,4-trimethylpentan-1-ol	123-44-4	1.0	348.0	-	-	54.70	[114]	-	-	441.45	[121]	641.41	[121]	(5.46)	-
962	788	V	L8122a	3,5-dimethylhexan-3-ol	4209-91-0	1.0	298.15	827.00	[115]	-	-	-	-	425.15	[121]	641.41	[121]	(5.46)	-
963	789	V	L8123a	2,4,4-trimethylpentan-1-ol	16325-63-6	1.0	293.15	833.00	[115]	-	-	-	-	444.15	[121]	641.41	[121]	(5.46)	-
964	790	V	L8124a	5,5-dimethylhexan-3-ol	66576-31-6	1.0	293.15	833.90	[115]	-	-	-	-	426.15	[121]	641.41	[121]	(5.46)	-
965	791	V	L8126a	2,4-dimethylhexan-2-ol	42328-76-7	1.0	301.15	806.50	[115]	-	-	-	-	423.85	[121]	641.41	[121]	(5.46)	-
966	792	V	L8127a	2,5-dimethylhexan-2-ol	3730-60-7	1.0	298.15	811.51	[115]	-	-	-	-	425.65	[121]	641.41	[121]	(5.46)	-
967	793	V	L8128a	3-methyl-2-propan-2-ylbutan-1-ol	18593-92-5	1.0	298.15	842.50	[115]	-	-	-	-	446.15	[121]	641.41	[121]	(5.46)	-
968	794	V	L8130a	2,3,4-trimethylpentan-1-ol	6570-88-3	1.0	293.15	849.80	[115]	-	-	-	-	456.15	[121]	641.41	[121]	(5.46)	-
969	795	V	L8131a	3,4-dimethylhexan-2-ol	19550-05-1	0.01	331.02	805.00	[121]	-	-	-	-	444.15	[121]	641.41	[121]	(5.46)	-
970	796	V	L8134a	2,5-dimethylhexan-3-ol	19550-07-3	1.0	298.15	813.53	[115]	-	-	-	-	432.15	[121]	641.41	[121]	(5.46)	-
971	796	V	L8134b	2,5-dimethylhexan-3-ol	19550-07-3	1.0	352.0	-	-	55.00	[114]	-	-	432.15	[121]	641.41	[121]	(5.46)	-
972	797	V	L8137a	3-ethylhexan-3-ol	597-76-2	1.0	298.15	834.20	[115]	-	-	-	-	432.15	[121]	641.41	[121]	(5.46)	-
973	797	V	L8137b	3-ethylhexan-3-ol	597-76-2	1.0	345.0	-	-	49.20	[114]	-	-	432.15	[121]	641.41	[121]	(5.46)	-
974	798	V	L8138a	3,3-dimethylhexan-1-ol	10524-70-6	1.0	293.15	839.00	[115]	-	-	-	-	454.00	[121]	641.41	[121]	(5.46)	-
975	799	V	L8140a	2,2-dimethylhexan-1-ol	2370-13-0	1.0	293.15	826.50	[115]	-	-	-	-	445.65	[121]	641.41	[121]	4.50	[120]
976	800	V	L8141a	4-methylheptan-4-ol	598-01-6	1.0	298.15	820.20	[115]	-	-	191.15	[120]	434.25	[121]	641.41	[121]	2.902	[120]
977	800	V	L8141b	4-methylheptan-4-ol	598-01-6	1.0	345.0	-	-	54.80	[114]	191.15	[120]	434.25	[121]	641.41	[121]	2.902	[120]
978	801	V	L8142a	3-methylheptan-3-ol	5582-82-1	1.0	298.15	824.90	[115]	-	-	190.15	[120]	434.15	[121]	641.41	[121]	3.013	[120]
979	801	V	L8142b	3-methylheptan-3-ol	5582-82-1	1.0	353.0	-	-	54.70	[114]	190.15	[120]	434.15	[121]	641.41	[121]	3.013	[120]
980	802	V	L8144a	2-methylheptan-2-ol	625-25-2	1.0	298.15	805.00	[115]	-	-	222.75	[120]	429.85	[121]	641.41	[121]	3.43	[120]
981	802	V	L8144b	2-methylheptan-2-ol	625-25-2	1.0	358.0	-	-	53.10	[114]	222.75	[120]	429.85	[121]	641.41	[121]	3.43	[120]
982	803	V	L8145a	4-ethylhexan-3-ol	19780-44-0	0.01	332.39	812.92	[121]	-	-	-	-	437.15	[121]	641.41	[121]	(5.46)	-
983	804	V	L8146a	4-methylheptan-3-ol	14979-39-6	1.0	298.15	794.16	[115]	-	-	150.15	[120]	428.55	[121]	641.41	[121]	3.312	[120]
984	804	V	L8146b	4-methylheptan-3-ol	14979-39-6	0.01	318.66	-	-	43.54	[121]	150.15	[120]	428.55	[121]	641.41	[121]	3.312	[120]
985	805	V	L8147a	3-methylheptan-4-ol	1838-73-9	1.0	298.15	833.50	[115]	-	-	-	-	437.85	[121]	641.41	[121]	7.46	[120]
986	805	V	L8147b	3-methylheptan-4-ol	1838-73-9	1.0	355.0	-	-	48.00	[114]	-	-	437.85	[121]	641.41	[121]	7.46	[120]
987	806	V	L8148a	3-methylheptan-2-ol	31367-46-1	1.0	298.15	817.63	[115]	-	-	-	-	439.25	[121]	641.41	[121]	7.47	[120]
988	806	V	L8148b	3-methylheptan-2-ol	31367-46-1	1.0	356.0	-	-	48.00	[114]	-	-	439.25	[121]	641.41	[121]	7.47	[120]
989	807	V	L8149a	2-methylheptan-3-ol	18720-62-2	1.0	298.15	821.00	[115]	-	-	-	-	440.75	[121]	641.41	[121]	(5.46)	-
990	807	V	L8149b	2-methylheptan-3-ol	18720-62-2	1.0	364.0	-	-	54.80	[114]	-	-	440.75	[121]	641.41	[121]	(5.46)	-
991	808	V	L8150a	2-ethyl-4-methylpentan-1-ol	106-67-2	1.0	293.15	827.30	[115]	-	-	-	-	449.65	[121]	641.41	[121]	(5.46)	-
992	808	V	L8150b	2-ethyl-4-methylpentan-1-ol	106-67-2	1.0	365.0	-	-	53.30	[114]	-	-	449.65	[121]	641.41	[121]	(5.46)	-
993	809	V	L8152a	5-methylheptan-3-ol	18720-65-5	1.0	298.15	814.14	[115]	-	-	181.95	[120]	426.75	[121]	641.41	[121]	3.832	[120]
994	810	V	L8153a	3,5-dimethylhexan-1-ol	13501-73-0	1.0	293.15	828.20	[115]	-	-	-	-	456.15	[121]	641.41	[121]	(5.46)	-
995	811	V	L8154a	4-methylheptan-2-ol	56298-90-9	1.0	298.15	799.00	[115]	-	-	171.15	[120]	444.75	[121]	641.41	[121]	3.59	[120]
996	811	V	L8154b	4-methylheptan-2-ol	56298-90-9	1.0	366.0	-	-	54.20	[114]	171.15	[120]	444.75	[121]	641.41	[121]	3.59	[120]
997	812	V	L8155a	2,5-dimethylhexan-1-ol	6886-16-4	1.0	298.15	824.54	[115]	-	-	-	-	452.15	[121]	641.41	[121]	(5.46)	-
998	813	V	L8156a	5-methylheptan-2-ol	54630-50-1	1.0	298.15	810.00	[115]	-	-	212.15	[120]	445.05	[121]	641.41	[121]	7.5	[120]
999	813	V	L8156b	5-methylheptan-2-ol	54630-50-1	1.0	363.0	-	-	47.20	[114]	212.15	[120]	445.05	[121]	641.41	[121]	7.5	[120]
1000	814	V	L8157a	2-methylheptan-4-ol	21570-35-4	1.0	298.15	809.80	[115]	-	-	192.15	[120]	439.25	[121]	641.41	[121]	3.338	[120]
1001	814	V	L8157b	2-methylheptan-4-ol	21570-35-4	1.0	363.0	-	-	54.80	[114]	192.15	[120]	439.25	[121]	641.41	[121]	3.338	[120]
1002	815	V	L8158a	6-methylheptan-3-ol	18720-66-6	1.0	298.15	776.60	[115]	-	-	-	-	433.00	[121]	641.41	[121]	(5.46)	-
1003	816	V	L8159a	6-methylheptan-2-ol	4730-22-7	1.0	298.15	803.40	[115]	-	-	168.15	[120]	445.05	[121]	641.41	[121]	6.41	[120]
1004	816	V	L8159b	6-methylheptan-2-ol	4730-22-7	1.0	369.0	-	-	55.20	[114]	168.15	[120]	445.05	[121]	641.41	[121]	6.41	[120]
1005	817	V	L8160a	3-ethylhexan-1-ol	41065-95-6	1.0	301.15	829.00	[115]	-	-	-	-	453.00	[121]	641.41	[121]	(5.46)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1006	818	V	L8161a	2-propylpentan-1-ol	58175-57-8	1.0	294.15	900.00	115	-	-	-	-	452.15	121	641.41	121	(5.46)	-
1007	819	V	L8162a	2-ethylhexan-1-ol	104-76-7	1.0	298.15	828.70	115	68.50	114	203.15	120	457.75	121	640.60	121	7.58	120
1008	820	V	L8163a	4-methylheptan-1-ol	817-91-4	1.0	298.15	806.02	115	-	-	-	-	456.35	121	641.41	121	4.63	120
1009	820	V	L8163b	4-methylheptan-1-ol	817-91-4	1.0	372.0	-	-	55.90	114	-	-	456.35	121	641.41	121	4.63	120
1010	821	V	L8164a	3-methylheptan-1-ol	1070-32-2	1.0	298.15	784.50	115	-	-	183.15	120	459.15	121	641.41	121	2.884	120
1011	821	V	L8164b	3-methylheptan-1-ol	1070-32-2	1.0	375.0	-	-	53.40	114	183.15	120	459.15	121	641.41	121	2.884	120
1012	822	V	L8165a	5-methylheptan-1-ol	7212-53-5	1.0	298.15	815.20	115	-	-	-	-	459.75	121	641.41	121	(5.46)	-
1013	822	V	L8165b	5-methylheptan-1-ol	7212-53-5	1.0	379.0	-	-	57.60	114	-	-	459.75	121	641.41	121	(5.46)	-
1014	823	V	L8166a	2-methylheptan-1-ol	60435-70-3	1.0	298.15	798.70	115	-	-	-	-	448.75	121	641.41	121	(5.46)	-
1015	824	V	L8167a	octan-4-ol	589-62-8	1.0	298.15	815.90	115	67.20	114	-	-	449.75	121	641.41	121	(5.46)	-
1016	825	V	L8168a	octan-3-ol	589-98-0	1.0	298.15	817.01	115	-	-	228.15	120	447.85	121	641.41	121	5.55	120
1017	826	V	L8169a	6-methylheptan-1-ol	1653-40-3	1.0	298.15	817.56	115	-	-	167.15	120	460.85	121	641.41	121	10.54	120
1018	826	V	L8169b	6-methylheptan-1-ol	1653-40-3	1.0	383.0	-	-	61.00	114	167.15	120	460.85	121	641.41	121	10.54	120
1019	827	V	L8170a	octan-2-ol	123-96-6	1.0	298.15	817.00	115	67.90	114	-	-	452.95	121	629.60	121	(5.46)	-
1020	828	V	L8171a	octan-1-ol	111-87-5	1.0	298.15	821.79	115	70.10	114	258.45	120	468.35	121	652.50	121	10.30	120
1021	829	V	L9103a	2,2,3,4-tetramethylpentan-3-ol	62185-29-9	0.01	344.93	813.97	121	-	-	-	-	447.35	121	661.55	121	(6.19)	-
1022	830	V	L9107a	3-ethyl-2,2-dimethylpentan-3-ol	66793-96-2	1.0	298.15	852.60	115	-	-	-	-	447.15	121	661.55	121	(6.19)	-
1023	831	V	L9108a	3,4,4-trimethylhexan-3-ol	66793-74-6	1.0	294.15	832.30	115	-	-	-	-	439.15	121	661.55	121	(6.19)	-
1024	832	V	L9109a	2,2,3-trimethylhexan-3-ol	5340-41-0	1.0	293.15	846.20	115	-	-	-	-	446.25	121	661.55	121	(6.19)	-
1025	832	V	L9109b	2,2,3-trimethylhexan-3-ol	5340-41-0	1.0	358.0	-	-	55.10	114	-	-	446.25	121	661.55	121	(6.19)	-
1026	833	V	L9110a	2,4,4-trimethylhexan-2-ol	66793-91-7	1.0	293.15	847.50	115	-	-	-	-	466.00	121	661.55	121	(6.19)	-
1027	834	V	L9111a	3,5,5-trimethylhexan-3-ol	66810-87-5	1.0	293.15	835.00	115	-	-	-	-	439.00	121	661.55	121	(6.19)	-
1028	835	V	L9113a	3-ethyl-2,4-dimethylpentan-3-ol	3970-59-0	1.0	298.15	854.92	115	-	-	-	-	451.05	121	661.55	121	(6.19)	-
1029	835	V	L9113b	3-ethyl-2,4-dimethylpentan-3-ol	3970-59-0	1.0	384.0	-	-	50.00	114	-	-	451.05	121	661.55	121	(6.19)	-
1030	836	V	L9115a	2,4,4-trimethylhexan-3-ol	66793-92-8	1.0	293.15	848.80	115	-	-	-	-	444.15	121	661.55	121	(6.19)	-
1031	837	V	L9116a	2,3,5-trimethylhexan-3-ol	65927-60-8	1.0	293.15	825.60	115	-	-	-	-	439.00	121	661.55	121	(6.19)	-
1032	838	V	L9119a	2,2,5-trimethylhexan-3-ol	3970-60-3	0.01	333.57	758.13	121	-	-	-	-	433.15	121	661.55	121	(6.19)	-
1033	839	V	L9120a	2,3,4-trimethylhexan-2-ol	21102-13-6	1.0	288.15	835.30	115	-	-	-	-	466.00	121	661.55	121	(6.19)	-
1034	840	V	L9121a	2,5,5-trimethylhexan-3-ol	66793-72-4	1.0	293.15	825.00	115	-	-	-	-	442.00	121	661.55	121	(6.19)	-
1035	841	V	L9122a	2,4,5-trimethylhexan-2-ol	66793-93-9	0.01	359.85	778.46	121	-	-	-	-	466.00	121	661.55	121	(6.19)	-
1036	842	V	L9124a	3-ethyl-4-methylhexan-3-ol	51200-80-7	1.0	288.15	861.00	115	-	-	-	-	452.00	121	661.55	121	(6.19)	-
1037	843	V	L9125a	3-ethyl-2-methylhexan-3-ol	66794-03-4	1.0	298.15	844.50	115	-	-	-	-	457.25	121	661.55	121	(6.19)	-
1038	844	V	L9128a	4-ethyl-3-methylhexan-3-ol	66794-05-6	1.0	298.15	899.40	115	-	-	-	-	452.00	121	661.55	121	(6.19)	-
1039	845	V	L9129a	2,3-dimethylheptan-3-ol	19549-71-4	1.0	294.15	838.30	115	-	-	-	-	447.15	121	661.55	121	(6.19)	-
1040	846	V	L9130a	4,5,5-trimethylhexan-1-ol	66793-75-7	1.0	293.15	846.00	115	-	-	-	-	475.15	121	661.55	121	(6.19)	-
1041	847	V	L9131a	2,2-dimethylheptan-3-ol	19549-70-3	1.0	298.15	823.74	115	-	-	-	-	451.00	121	661.55	121	(6.19)	-
1042	848	V	L9132a	3-ethyl-2-methylhexan-2-ol	66794-02-3	1.0	298.15	833.40	115	-	-	-	-	451.15	121	661.55	121	(6.19)	-
1043	849	V	L9133a	2-ethyl-2,4-dimethylpentan-1-ol	66793-98-4	1.0	298.15	837.00	115	-	-	-	-	461.15	121	661.55	121	(6.19)	-
1044	850	V	L9134a	3-ethyl-5-methylhexan-3-ol	597-77-3	1.0	295.15	839.60	115	-	-	-	-	445.15	121	661.55	121	(6.19)	-
1045	851	V	L9136a	3,5-dimethylheptan-3-ol	19549-74-7	1.0	298.15	821.83	115	-	-	-	-	450.00	121	661.55	121	(6.19)	-
1046	852	V	L9137a	2,4-dimethylheptan-4-ol	19549-77-0	1.0	293.15	824.20	115	-	-	-	-	444.55	121	661.55	121	(6.19)	-
1047	853	V	L9138a	3,6-dimethylheptan-3-ol	1573-28-0	1.0	289.15	828.50	115	-	-	-	-	446.15	121	661.55	121	(6.19)	-
1048	854	V	L9139a	3,5,5-trimethylhexan-1-ol	3452-97-9	1.0	298.15	823.60	120	67.90	114	-	-	466.15	121	661.55	121	(6.19)	-
1049	855	V	L9141a	2,4-dimethylheptan-2-ol	65822-93-7	1.0	298.15	828.00	115	-	-	-	-	455.00	121	661.55	121	(6.19)	-
1050	856	V	L9142a	2,5-dimethylheptan-2-ol	1561-18-8	1.0	295.15	830.00	115	-	-	-	-	-	-	-	-	(6.19)	-
1051	857	V	L9143a	2,6-dimethylheptan-2-ol	13254-34-7	1.0	293.15	818.60	120	-	-	-	-	444.15	121	661.55	121	(6.19)	-
1052	858	V	L9144a	4-ethyl-2-methylhexan-3-ol	33943-21-4	1.0	293.15	827.50	115	-	-	-	-	452.00	121	661.55	121	(6.19)	-
1053	859	V	L9145a	3,5-dimethylheptan-4-ol	19549-79-2	1.0	293.15	859.20	115	-	-	-	-	460.15	121	661.55	121	(6.19)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1054	860	V	L9147a	2,6-dimethylheptan-3-ol	19549-73-6	1.0	293.15	814.80	115	-	-	-	-	448.15	121	661.55	121	(6.19)	-
1055	861	V	L9148a	4,6-dimethylheptan-2-ol	51079-52-8	1.0	273.15	878.70	115	-	-	-	-	467.15	121	661.55	121	(6.19)	-
1056	862	V	L9149a	2,6-dimethylheptan-4-ol	108-82-7	1.0	298.15	806.43	115	65.20	114	-	-	451.00	121	661.55	121	(6.19)	-
1057	863	V	L9150a	4-ethylheptan-4-ol	597-90-0	1.0	298.15	829.90	115	-	-	-	-	452.15	121	661.55	121	(6.19)	-
1058	864	V	L9151a	3-ethylheptan-3-ol	19780-41-7	1.0	298.15	829.90	115	-	-	-	-	455.35	121	661.55	121	(6.19)	-
1059	865	V	L9153a	4-methyloctan-4-ol	23418-37-3	1.0	298.15	824.56	115	-	-	-	-	454.15	121	661.55	121	(6.19)	-
1060	866	V	L9154a	3-methyloctan-3-ol	5340-36-3	1.0	298.15	827.50	115	-	-	-	-	-	-	-	-	(6.19)	-
1061	866	V	L9154b	3-methyloctan-3-ol	5340-36-3	1.0	368.0	-	-	53.20	114	-	-	-	-	-	-	(6.19)	-
1062	867	V	L9155a	6,6-dimethylheptan-1-ol	65769-10-0	1.0	293.15	843.90	115	-	-	-	-	455.00	121	661.55	121	(6.19)	-
1063	868	V	L9156a	2-methyloctan-2-ol	628-44-4	1.0	298.15	813.40	115	-	-	-	-	451.15	121	661.55	121	(6.19)	-
1064	868	V	L9156b	2-methyloctan-2-ol	628-44-4	1.0	353.0	-	-	64.60	114	-	-	451.15	121	661.55	121	(6.19)	-
1065	869	V	L9157a	2-ethyl-3-methylhexan-1-ol	66794-04-5	1.0	298.15	835.80	115	-	-	-	-	466.15	121	661.55	121	(6.19)	-
1066	870	V	L9159a	5-methyloctan-4-ol	59734-23-5	1.0	298.15	815.60	115	-	-	-	-	455.00	121	661.55	121	(6.19)	-
1067	871	V	L9160a	4-methyloctan-3-ol	66793-80-4	1.0	298.15	843.70	115	-	-	-	-	459.00	121	661.55	121	(6.19)	-
1068	872	V	L9161a	3-methyloctan-4-ol	26533-35-7	1.0	291.15	834.00	115	-	-	-	-	453.15	121	661.55	121	(6.19)	-
1069	873	V	L9162a	3-methyloctan-2-ol	27644-49-1	1.0	300.15	831.00	115	-	-	-	-	454.00	121	661.55	121	(6.19)	-
1070	874	V	L9163a	2-methyloctan-3-ol	26533-34-6	1.0	293.15	827.00	115	-	-	-	-	457.15	121	661.55	121	(6.19)	-
1071	874	V	L9163b	2-methyloctan-3-ol	26533-34-6	1.0	403.0	-	-	49.50	114	-	-	457.15	121	661.55	121	(6.19)	-
1072	875	V	L9164a	2-ethyl-4-methylhexan-1-ol	66794-06-7	1.0	293.15	828.80	115	-	-	-	-	468.15	121	661.55	121	(6.19)	-
1073	876	V	L9165a	4-methyl-2-propylpentan-1-ol	54004-41-0	1.0	293.15	825.60	115	-	-	-	-	465.15	121	661.55	121	(6.19)	-
1074	877	V	L9166a	2-ethyl-5-methylhexan-1-ol	66794-07-8	1.0	298.15	820.80	115	-	-	-	-	466.00	121	661.55	121	(6.19)	-
1075	878	V	L9167a	6-methyloctan-4-ol	66793-82-6	1.0	296.15	822.00	115	-	-	-	-	455.00	121	661.55	121	(6.19)	-
1076	879	V	L9169a	6-methyloctan-3-ol	40225-75-0	1.0	301.15	832.00	115	-	-	-	-	459.00	121	661.55	121	(6.19)	-
1077	880	V	L9170a	3,6-dimethylheptan-1-ol	1573-33-7	1.0	300.15	823.00	115	-	-	-	-	-	-	-	-	(6.19)	-
1078	881	V	L9171a	5-methyloctan-2-ol	66793-81-5	1.0	298.15	821.00	115	-	-	-	-	454.00	121	661.55	121	(6.19)	-
1079	882	V	L9172a	2-methyloctan-4-ol	40575-41-5	1.0	298.15	815.00	115	-	-	-	-	457.15	121	661.55	121	(6.19)	-
1080	883	V	L9173a	7-methyloctan-4-ol	33933-77-6	1.0	293.15	813.60	115	-	-	-	-	455.00	121	661.55	121	(6.19)	-
1081	884	V	L9174a	7-methyloctan-3-ol	66793-84-8	1.0	285.15	840.20	115	-	-	-	-	459.00	121	661.55	121	(6.19)	-
1082	885	V	L9177a	3-ethylheptan-1-ol	3525-25-5	1.0	296.15	834.00	115	-	-	-	-	480.15	121	661.55	121	(6.19)	-
1083	886	V	L9179a	5-ethylheptan-1-ol	998-65-2	1.0	298.15	848.00	115	-	-	-	-	472.00	121	661.55	121	(6.19)	-
1084	887	V	L9181a	4-methyloctan-1-ol	38514-03-3	1.0	300.65	820.00	115	-	-	-	-	473.00	121	661.55	121	(6.19)	-
1085	888	V	L9182a	5-methyloctan-1-ol	38514-04-4	1.0	297.15	828.00	115	-	-	-	-	473.00	121	661.55	121	(6.19)	-
1086	889	V	L9183a	3-methyloctan-1-ol	38514-02-2	1.0	297.15	827.00	115	-	-	-	-	473.00	121	661.55	121	(6.19)	-
1087	890	V	L9184a	6-methyloctan-1-ol	38514-05-5	0.01	370.37	770.37	121	-	-	-	-	479.15	121	661.55	121	(6.19)	-
1088	891	V	L9185a	2-methyloctan-1-ol	818-81-5	1.0	277.15	841.80	115	-	-	-	-	473.00	121	661.55	121	(6.19)	-
1089	892	V	L9186a	nonan-5-ol	623-93-8	1.0	298.15	818.30	115	71.40	114	278.75	120	468.25	121	661.55	121	3.54	120
1090	893	V	L9187a	nonan-4-ol	5932-79-6	1.0	293.15	826.30	115	71.50	114	-	-	466.15	121	661.55	121	(6.19)	-
1091	894	V	L9188a	nonan-3-ol	624-51-1	1.0	298.15	823.55	115	70.90	114	-	-	467.85	121	661.55	121	(6.19)	-
1092	895	V	L9189a	7-methyloctan-1-ol	2430-22-0	1.0	298.15	826.00	115	-	-	-	-	479.15	121	661.55	121	(6.19)	-
1093	896	V	L9190a	nonan-2-ol	628-99-9	1.0	298.15	819.35	115	72.90	114	-	-	471.65	121	649.60	121	(6.19)	-
1094	897	V	L9191a	nonan-1-ol	143-08-8	1.0	298.15	824.60	115	72.20	114	268.15	120	486.25	121	670.70	121	8.83	120
1095	898	V	L0103a	3-ethyl-2,2,4-trimethylpentan-3-ol	66256-41-5	1.0	293.15	862.40	115	-	-	-	-	464.15	121	680.37	121	(5.30)	-
1096	899	V	L0104a	3,4,4,5-tetramethylhexan-3-ol	66256-39-1	1.0	293.15	874.20	115	-	-	-	-	475.15	121	680.37	121	(5.30)	-
1097	900	V	L0105a	2,3,4,4-tetramethylhexan-3-ol	66256-67-5	1.0	293.15	874.50	115	-	-	-	-	474.15	121	680.37	121	(5.30)	-
1098	901	V	L0106a	2,2,3,4-tetramethylhexan-3-ol	66256-63-1	1.0	293.15	858.40	115	-	-	-	-	465.15	121	680.37	121	(5.30)	-
1099	902	V	L0107a	2,2,3,5-tetramethylhexan-3-ol	66256-64-2	1.0	293.15	839.30	115	-	-	-	-	513.48	121	680.37	121	(5.30)	-
1100	903	V	L0108a	2,2,4,4-tetramethylhexan-3-ol	66256-65-3	1.0	293.15	854.90	115	-	-	-	-	463.15	121	680.37	121	(5.30)	-
1101	904	V	L0111a	3,4,5,5-tetramethylhexan-3-ol	66256-40-4	1.0	293.15	862.30	115	-	-	-	-	468.15	121	680.37	121	(5.30)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1102	905	V	L0112a	2,3,5,5-tetramethylhexan-3-ol	5396-09-8	1.0	293.15	837.80	115	-	-	-	-	475.00	121	680.37	121	(5.30)	-
1103	906	V	L0115a	2,4-dimethyl-3-propan-2-ylpentan-3-ol	51200-83-0	1.0	298.15	859.10	115	-	-	-	-	467.65	121	680.37	121	(5.30)	-
1104	907	V	L0117a	2,2,3-trimethylheptan-3-ol	29772-40-5	1.0	293.15	848.70	115	-	-	-	-	459.15	121	680.37	121	(5.30)	-
1105	908	V	L0118a	3-ethyl-5,5-dimethylhexan-3-ol	5340-62-5	1.0	293.15	842.80	115	-	-	-	-	460.00	121	680.37	121	(5.30)	-
1106	909	V	L0119a	3,5,5-trimethylheptan-3-ol	66256-50-6	1.0	293.15	854.30	115	-	-	-	-	468.75	121	680.37	121	(5.30)	-
1107	910	V	L011aa	decan-2-ol	1120-06-5	1.0	293.15	825.20	115	-	-	-	-	490.15	121	680.37	121	(5.30)	-
1108	911	V	L011ba	decan-1-ol	112-30-1	1.0	298.15	826.53	115	80.90	114	280.15	120	503.35	121	687.30	121	7.93	120
1109	912	V	L0120a	2,2,4-trimethylheptan-4-ol	57233-31-5	1.0	293.15	833.00	115	-	-	-	-	454.15	121	680.37	121	(5.30)	-
1110	913	V	L0121a	2-methyl-3-propan-2-ylhexan-3-ol	51200-81-8	1.0	293.15	853.70	115	-	-	-	-	465.15	121	680.37	121	(5.30)	-
1111	914	V	L0122a	4-ethyl-2,4-dimethylhexan-3-ol	66719-48-0	1.0	293.15	860.60	115	-	-	-	-	460.00	121	680.37	121	(5.30)	-
1112	915	V	L0124a	2,3,6-trimethylheptan-3-ol	58046-40-5	1.0	293.15	839.80	115	-	-	-	-	463.00	121	680.37	121	(5.30)	-
1113	916	V	L0126a	4-ethyl-2,2-dimethylhexan-3-ol	66719-47-9	1.0	293.15	833.90	115	-	-	-	-	460.15	121	680.37	121	(5.30)	-
1114	917	V	L0127a	2,2,6-trimethylheptan-3-ol	66256-43-7	1.0	293.15	823.60	115	-	-	-	-	463.00	121	680.37	121	(5.30)	-
1115	918	V	L0128a	2,4,6-trimethylheptan-4-ol	60836-07-9	1.0	294.15	823.00	115	-	-	-	-	455.15	121	680.37	121	(5.30)	-
1116	919	V	L0129a	2,2,5-trimethylheptan-4-ol	66256-42-6	1.0	289.15	751.30	115	-	-	-	-	455.00	121	680.37	121	(5.30)	-
1117	920	V	L0130a	4,6,6-trimethylheptan-2-ol	51079-79-9	1.0	293.15	826.50	115	-	-	-	-	466.00	121	680.37	121	(5.30)	-
1118	921	V	L0132a	2,5,6-trimethylheptan-2-ol	66256-48-2	1.0	291.15	833.00	115	-	-	-	-	466.15	121	680.37	121	(5.30)	-
1119	922	V	L0134a	4-propan-2-ylheptan-4-ol	51200-82-9	1.0	298.15	841.34	115	-	-	-	-	463.15	121	680.37	121	(5.30)	-
1120	923	V	L0135a	3-ethyl-2-methylheptan-3-ol	66719-37-7	1.0	293.15	845.50	115	-	-	-	-	466.15	121	680.37	121	(5.30)	-
1121	924	V	L0137a	2,3-dimethyloctan-3-ol	19781-10-3	1.0	298.15	824.90	115	-	-	-	-	462.25	121	680.37	121	(5.30)	-
1122	925	V	L0139a	4,6-dimethyloctan-4-ol	56065-43-1	1.0	301.15	825.80	115	-	-	-	-	464.00	121	680.37	121	(5.30)	-
1123	926	V	L0140a	3,5-dimethyloctan-3-ol	56065-42-0	1.0	298.15	837.00	115	-	-	-	-	466.00	121	680.37	121	(5.30)	-
1124	927	V	L0141a	2,4-dimethyloctan-4-ol	33933-79-8	1.0	293.15	823.20	115	-	-	-	-	464.00	121	680.37	121	(5.30)	-
1125	928	V	L0142a	3,6-dimethyloctan-3-ol	151-19-9	1.0	295.15	834.70	120	-	-	205.65	120	465.15	121	680.37	121	(5.30)	-
1126	929	V	L0143a	4,7-dimethyloctan-4-ol	19781-13-6	1.0	273.15	842.10	115	-	-	-	-	465.15	121	680.37	121	(5.30)	-
1127	930	V	L0144a	3,7-dimethyloctan-3-ol	78-69-3	1.0	298.15	826.00	120	-	-	-	-	469.15	121	680.37	121	(5.30)	-
1128	931	V	L0145a	2,2-dimethyloctan-4-ol	66719-52-6	1.0	293.15	821.20	115	-	-	-	-	463.15	121	680.37	121	(5.30)	-
1129	932	V	L0146a	2,4-dimethyloctan-2-ol	18675-20-2	1.0	293.15	825.70	115	-	-	-	-	485.00	121	680.37	121	(5.30)	-
1130	933	V	L0147a	2,6-dimethyloctan-2-ol	18479-57-7	1.0	293.15	827.30	115	-	-	-	-	485.00	121	680.37	121	(5.30)	-
1131	934	V	L0148a	2,7-dimethyloctan-2-ol	42007-73-8	1.0	298.15	821.10	115	-	-	-	-	485.00	121	680.37	121	(5.30)	-
1132	935	V	L0149a	5-ethyl-4-methylheptan-3-ol	66731-94-0	1.0	290.15	865.00	115	-	-	-	-	466.00	121	680.37	121	(5.30)	-
1133	936	V	L0151a	5-methyl-2-propan-2-ylhexan-1-ol	2051-33-4	1.0	293.15	832.20	115	-	-	-	-	486.15	121	680.37	121	(5.30)	-
1134	937	V	L0152a	3,6-dimethyloctan-4-ol	66719-31-1	0.01	358.25	786.10	121	-	-	-	-	464.00	121	680.37	121	(5.30)	-
1135	938	V	L0153a	2,5-dimethyloctan-4-ol	66719-53-7	1.0	298.15	821.50	115	-	-	-	-	464.00	121	680.37	121	(5.30)	-
1136	939	V	L0154a	3,7-dimethyloctan-2-ol	15340-96-2	1.0	293.15	829.10	115	-	-	-	-	485.00	121	680.37	121	(5.30)	-
1137	940	V	L0155a	2,7-dimethyloctan-3-ol	66719-55-9	1.0	293.15	815.20	115	-	-	-	-	467.15	121	680.37	121	(5.30)	-
1138	941	V	L0156a	4-methyl-2-(2-methylpropyl)pentan-1-ol	22417-45-4	1.0	277.15	846.00	115	-	-	-	-	477.15	121	680.37	121	(5.30)	-
1139	942	V	L0157a	2,6-dimethyloctan-4-ol	66719-54-8	0.01	361.57	759.68	121	-	-	-	-	468.15	121	680.37	121	(5.30)	-
1140	943	V	L0158a	2,7-dimethyloctan-4-ol	19781-11-4	1.0	293.15	814.00	115	-	-	-	-	475.15	121	680.37	121	(5.30)	-
1141	944	V	L0159a	4-propylheptan-4-ol	2198-72-3	1.0	298.15	828.30	115	-	-	-	-	467.15	121	680.37	121	(5.30)	-
1142	945	V	L0160a	4-ethyloctan-4-ol	38395-42-5	1.0	298.15	826.80	115	-	-	-	-	466.00	121	680.37	121	(5.30)	-
1143	946	V	L0161a	3-ethyloctan-3-ol	2051-32-3	1.0	298.15	836.10	115	-	-	-	-	472.15	121	680.37	121	(5.30)	-
1144	947	V	L0162a	2,2-dimethyloctan-1-ol	2370-14-1	1.0	293.15	830.00	115	-	-	-	-	481.15	121	680.37	121	7.86	120
1145	948	V	L0163a	5-methylnonan-5-ol	33933-78-7	1.0	298.15	825.38	115	-	-	-	-	475.15	121	680.37	121	(5.30)	-
1146	949	V	L0164a	4-methylnonan-4-ol	23418-38-4	1.0	298.15	827.10	115	-	-	-	-	482.00	121	680.37	121	(5.30)	-
1147	950	V	L0165a	3-methylnonan-3-ol	21078-72-8	1.0	298.15	826.45	115	-	-	-	-	482.00	121	680.37	121	(5.30)	-
1148	951	V	L0166a	2-methylnonan-2-ol	10297-57-1	1.0	298.15	807.80	115	-	-	-	-	487.00	121	680.37	121	(5.30)	-
1149	952	V	L0167a	3-propan-2-ylheptan-1-ol	38514-15-7	1.0	303.15	834.10	115	-	-	-	-	488.35	121	680.37	121	(5.30)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1150	953	V	L0169a	5-methylnonan-4-ol	66719-44-6	1.0	300.15	826.00	[115]	-	-	-	-	482.00	[121]	680.37	[121]	(5.30)	-
1151	954	V	L0170a	3-methylnonan-2-ol	60671-32-1	1.0	295.15	845.00	[115]	-	-	-	-	487.00	[121]	680.37	[121]	(5.30)	-
1152	955	V	L0171a	2-methylnonan-3-ol	26533-33-5	1.0	298.15	824.50	[115]	-	-	-	-	481.55	[121]	680.37	[121]	(5.30)	-
1153	956	V	L0172a	4-methyl-2-propylhexan-1-ol	66256-62-0	1.0	293.15	828.60	[115]	-	-	-	-	481.15	[121]	680.37	[121]	(5.30)	-
1154	957	V	L0173a	6-ethyloctan-3-ol	19781-27-2	1.0	297.65	839.60	[115]	-	-	-	-	472.00	[121]	680.37	[121]	(5.30)	-
1155	958	V	L0176a	2,6-dimethyloctan-1-ol	62417-08-7	1.0	291.15	830.00	[115]	-	-	-	-	483.00	[121]	680.37	[121]	(5.30)	-
1156	959	V	L0179a	3,7-dimethyloctan-1-ol	106-21-8	1.0	298.15	832.00	[120]	-	-	-	-	485.15	[121]	680.37	[121]	(5.30)	-
1157	959	V	L0179b	3,7-dimethyloctan-1-ol	106-21-8	1.0	356.0	-	-	79.10	[114]	-	-	485.15	[121]	680.37	[121]	(5.30)	-
1158	960	V	L0180a	2,7-dimethyloctan-1-ol	15250-22-3	1.0	288.15	830.30	[115]	-	-	-	-	-	-	-	-	(5.30)	-
1159	961	V	L0182a	6-methylnonan-2-ol	66256-60-8	1.0	293.15	833.20	[115]	-	-	-	-	487.00	[121]	680.37	[121]	(5.30)	-
1160	962	V	L0184a	2-methylnonan-4-ol	26533-31-3	1.0	298.15	820.00	[115]	-	-	-	-	482.00	[121]	680.37	[121]	(5.30)	-
1161	963	V	L0185a	2-methylnonan-5-ol	29843-62-7	1.0	293.15	821.50	[115]	-	-	-	-	482.00	[121]	680.37	[121]	(5.30)	-
1162	964	V	L0186a	8-methylnonan-2-ol	14779-92-1	0.01	376.65	760.15	[121]	-	-	-	-	487.00	[121]	680.37	[121]	(5.30)	-
1163	965	V	L0187a	3-ethyloctan-1-ol	66719-36-6	0.01	372.65	763.39	[121]	-	-	-	-	482.00	[121]	680.37	[121]	(5.30)	-
1164	966	V	L0188a	2-butylhexan-1-ol	2768-15-2	1.0	289.15	836.00	[115]	-	-	-	-	-	-	-	-	(5.30)	-
1165	967	V	L0189a	2-propylheptan-1-ol	10042-59-8	1.0	293.15	832.20	[115]	-	-	-	-	491.05	[121]	680.37	[121]	(5.30)	-
1166	968	V	L0191a	5-methylnonan-1-ol	2768-16-3	1.0	297.15	831.00	[115]	-	-	-	-	487.00	[121]	680.37	[121]	(5.30)	-
1167	969	V	L0192a	4-methylnonan-1-ol	1489-47-0	1.0	300.15	826.00	[115]	-	-	-	-	489.15	[121]	680.37	[121]	(5.30)	-
1168	970	V	L0193a	3-methylnonan-1-ol	22663-64-5	1.0	296.15	837.00	[115]	-	-	-	-	487.00	[121]	680.37	[121]	(5.30)	-
1169	971	V	L0194a	7-methylnonan-1-ol	33234-93-4	1.0	298.15	828.20	[115]	-	-	-	-	487.00	[121]	680.37	[121]	(5.30)	-
1170	972	V	L0195a	2-methylnonan-1-ol	40589-14-8	1.0	288.15	833.65	[115]	-	-	-	-	495.15	[121]	680.37	[121]	(5.30)	-
1171	973	V	L0196a	decan-5-ol	5205-34-5	1.0	298.15	820.60	[115]	-	-	281.85	[120]	474.15	[121]	680.37	[121]	3.24	[120]
1172	974	V	L0197a	decan-4-ol	2051-31-2	1.0	293.15	825.00	[115]	-	-	262.15	[120]	483.15	[121]	680.37	[121]	3.42	[120]
1173	975	V	L0198a	decan-3-ol	1565-81-7	1.0	298.15	822.90	[115]	-	-	265.65	[120]	483.00	[121]	680.37	[121]	4.05	[120]
1174	976	V	L0199a	8-methylnonan-1-ol	25339-17-7	0.01	381.45	771.13	[121]	-	-	-	-	493.00	[121]	680.37	[121]	(5.30)	-
1175	977	V	L7201a	2,3-dimethylpentane-2,3-diol	6931-70-0	1.0	293.15	961.30	[115]	-	-	-	-	525.85	[121]	799.33	[121]	(26.35)	-
1176	978	V	L7202a	2,4-dimethylpentane-2,4-diol	24892-49-7	1.0	293.15	920.60	[115]	-	-	-	-	470.00	[121]	799.33	[121]	(26.35)	-
1177	979	V	L7204a	3-ethylpentane-2,3-diol	-	1.0	298.15	961.20	[115]	-	-	-	-	-	-	-	-	(26.35)	-
1178	980	V	L7206a	3,4-dimethylpentane-1,4-diol	63521-36-8	1.0	293.15	952.80	[115]	-	-	-	-	517.03	[121]	799.33	[121]	(26.35)	-
1179	981	V	L7207a	4-methylhexane-2,4-diol	38836-25-8	1.0	293.15	929.60	[115]	-	-	-	-	517.03	[121]	799.33	[121]	(26.35)	-
1180	982	V	L7208a	2-methylhexane-2,4-diol	66225-35-2	1.0	291.15	932.10	[115]	-	-	-	-	517.03	[121]	799.33	[121]	(26.35)	-
1181	983	V	L7212a	2,2-diethylpropane-1,3-diol	115-76-4	1.0	334.45	949.00	[115]	-	-	334.45	[120]	507.15	[121]	799.33	[121]	(26.35)	-
1182	984	V	L7217a	5-methylhexane-1,5-diol	1462-11-9	1.0	295.15	967.00	[115]	-	-	-	-	494.25	[121]	799.33	[121]	(26.35)	-
1183	985	V	L7220a	2-propan-2-ylbutane-1,4-diol	39497-66-0	1.0	293.15	967.20	[115]	-	-	-	-	508.21	[121]	799.33	[121]	(26.35)	-
1184	986	V	L7221a	heptane-3,4-diol	62593-33-3	1.0	295.15	943.00	[115]	-	-	-	-	-	-	-	-	(26.35)	-
1185	987	V	L7224a	heptane-2,4-diol	20748-86-1	1.0	298.15	926.00	[115]	-	-	-	-	508.21	[121]	799.33	[121]	(26.35)	-
1186	988	V	L7226a	2-propylbutane-1,4-diol	62946-68-3	1.0	293.15	962.50	[115]	-	-	-	-	485.43	[121]	799.33	[121]	(26.35)	-
1187	989	V	L7227a	2-ethylpentane-1,5-diol	14189-13-0	1.0	293.15	967.90	[115]	-	-	-	-	485.43	[121]	799.33	[121]	(26.35)	-
1188	990	V	L7228a	2-butylpropane-1,3-diol	2612-26-2	1.0	298.15	946.10	[115]	-	-	-	-	-	-	-	-	(26.35)	-
1189	991	V	L7230a	heptane-1,4-diol	40646-07-9	1.0	298.15	950.40	[115]	-	-	-	-	515.15	[121]	799.33	[121]	(26.35)	-
1190	992	V	L7232a	heptane-1,5-diol	60096-09-5	1.0	293.15	970.50	[115]	-	-	-	-	489.79	[121]	799.33	[121]	(26.35)	-
1191	993	V	L7234a	heptane-1,6-diol	13175-27-4	1.0	298.15	962.00	[115]	-	-	-	-	485.43	[121]	799.33	[121]	(26.35)	-
1192	994	V	L7235a	heptane-1,7-diol	629-30-1	1.0	298.15	952.25	[115]	96.50	[114]	295.05	[120]	535.15	[121]	799.33	[121]	(26.35)	-
1193	995	V	L8202a	2,4-dimethylhexane-2,4-diol	29649-22-7	1.0	293.35	922.90	[115]	-	-	-	-	-	-	-	-	(18.73)	-
1194	996	V	L8203a	2,5-dimethylhexane-2,5-diol	110-03-2	0.01	362.0	852.16	[121]	-	-	364.15	[120]	487.15	[121]	819.27	[121]	(18.73)	-
1195	997	V	L8204a	2,2,4-trimethylpentane-1,3-diol	144-19-4	0.01	391.21	865.06	[121]	-	-	328.35	[120]	508.15	[121]	819.27	[121]	(18.73)	-
1196	997	V	L8204b	2,2,4-trimethylpentane-1,3-diol	144-19-4	1.0	428.0	-	-	58.50	[114]	328.35	[120]	508.15	[121]	819.27	[121]	(18.73)	-
1197	998	V	L8205a	3,5-dimethylhexane-2,3-diol	99799-29-8	1.0	298.15	928.50	[115]	-	-	-	-	-	-	-	-	(18.73)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1198	999	V	L8206a	2,5-dimethylhexane-2,4-diol	3899-89-6	1.0	293.15	917.20	115	-	-	-	-	-	-	-	-	(18.73)	-
1199	1000	V	L8207a	2-methylheptane-2,3-diol	1068-81-1	1.0	298.15	929.00	115	-	-	-	-	-	-	-	-	(18.73)	-
1200	1001	V	L8208a	3-methylheptane-2,4-diol	6964-04-1	0.01	369.56	875.70	121	-	-	-	-	478.13	121	819.27	121	(18.73)	-
1201	1002	V	L8209a	2-butyl-2-methylpropane-1,3-diol	3121-83-3	0.01	415.17	844.98	121	-	-	-	-	535.15	121	819.27	121	(18.73)	-
1202	1003	V	L8210a	4-ethylhexane-1,4-diol	1113-00-4	1.0	292.15	970.40	115	-	-	-	-	-	-	-	-	(18.73)	-
1203	1004	V	L8211a	6-methylheptane-1,6-diol	5392-57-4	1.0	298.15	959.00	115	-	-	-	-	-	-	-	-	(18.73)	-
1204	1005	V	L8212a	2-ethylhexane-1,3-diol	94-96-2	1.0	295.15	932.50	120	79.50	114	233.15	120	517.15	121	819.27	121	18.73	120
1205	1006	V	L8213a	octane-2,4-diol	90162-24-6	1.0	298.15	918.00	115	-	-	-	-	478.13	121	819.27	121	(18.73)	-
1206	1007	V	L8215a	octane-1,5-diol	2736-67-6	1.0	298.15	949.00	115	-	-	-	-	-	-	-	-	(18.73)	-
1207	1008	V	L8217a	octane-1,6-diol	4066-76-6	1.0	298.15	954.00	115	-	-	-	-	-	-	-	-	(18.73)	-
1208	1009	V	L8219a	octane-1,7-diol	13175-32-1	1.0	298.15	943.00	115	-	-	-	-	-	-	-	-	(18.73)	-
1209	1010	V	L8220b	octane-1,8-diol	629-41-4	1.0	356.0	-	-	101.00	114	332.75	120	544.15	121	819.27	121	(18.73)	-
1210	1011	V	L9201a	2,4,5-trimethylhexane-2,4-diol	36587-81-2	1.0	301.35	920.70	115	-	-	-	-	-	-	-	-	(26.35)	-
1211	1012	V	L9202a	2,4-dimethylheptane-2,4-diol	59194-83-1	1.0	290.35	913.80	115	-	-	-	-	-	-	-	-	(26.35)	-
1212	1013	V	L9203a	2,6-dimethylheptane-2,4-diol	73264-93-4	1.0	291.15	902.00	115	-	-	-	-	-	-	-	-	(26.35)	-
1213	1014	V	L9204a	2,2,4-trimethylhexane-1,6-diol	3089-24-5	1.0	434.0	-	-	68.00	114	-	-	-	-	-	-	(26.35)	-
1214	1015	V	L9205a	2-butyl-2-ethylpropane-1,3-diol	115-84-4	1.0	323.15	929.00	115	-	-	316.15	120	535.15	121	837.92	121	(26.35)	-
1215	1015	V	L9205b	2-butyl-2-ethylpropane-1,3-diol	115-84-4	1.0	460.0	-	-	67.20	114	316.15	120	535.15	121	837.92	121	(26.35)	-
1216	1016	V	L9206a	5-ethylheptane-1,5-diol	57740-06-4	1.0	291.15	958.00	115	-	-	-	-	-	-	-	-	(26.35)	-
1217	1017	V	L9207a	2-(2-methylpropyl)pentane-1,5-diol	57740-10-0	1.0	293.15	941.60	115	-	-	-	-	-	-	-	-	(26.35)	-
1218	1018	V	L9208a	nonane-1,5-diol	13686-96-9	1.0	293.15	937.00	115	-	-	-	-	-	-	-	-	(26.35)	-
1219	1019	V	L9209a	nonane-1,4-diol	2430-73-1	1.0	293.15	929.50	115	-	-	-	-	571.15	121	837.92	121	(26.35)	-
1220	1020	V	L9211a	nonane-1,7-diol	4469-84-5	1.0	298.15	944.00	115	-	-	-	-	-	-	-	-	(26.35)	-
1221	1021	V	L9213b	nonane-1,9-diol	3937-56-2	1.0	323.0	-	-	110.00	114	319.55	120	558.15	121	837.92	121	(26.35)	-
1222	1022	V	L0201a	2,4,6-trimethylheptane-2,4-diol	33070-42-7	1.0	288.15	910.24	115	-	-	-	-	-	-	-	-	(26.35)	-
1223	1023	V	L0202a	3,4-diethylhexane-3,4-diol	6931-71-1	1.0	298.15	943.50	115	-	-	-	-	503.15	121	855.45	121	(26.35)	-
1224	1023	V	L0202b	3,4-diethylhexane-3,4-diol	6931-71-1	0.01	389.57	-	-	54.99	121	-	-	503.15	121	855.45	121	(26.35)	-
1225	1024	V	L0203a	3,7-dimethyloctane-3,5-diol	56548-45-9	1.0	285.15	911.80	115	-	-	-	-	-	-	-	-	(26.35)	-
1226	1025	V	L0204a	2-butyl-2-ethylbutane-1,3-diol	2050-83-1	1.0	353.0	-	-	63.40	114	-	-	-	-	-	-	(26.35)	-
1227	1026	V	L0205a	3,7-dimethyloctane-1,3-diol	102880-60-4	1.0	293.15	916.50	115	-	-	-	-	-	-	-	-	(26.35)	-
1228	1027	V	L0206a	3,7-dimethyloctane-1,7-diol	107-74-4	1.0	293.15	926.00	115	-	-	-	-	538.15	121	855.45	121	(26.35)	-
1229	1028	V	L0207a	3,7-dimethyloctane-1,6-diol	53067-10-0	1.0	293.15	948.10	115	-	-	-	-	-	-	-	-	(26.35)	-
1230	1029	V	L0208a	2,3-dipropylbutane-1,4-diol	74854-17-4	1.0	293.15	936.20	115	-	-	-	-	-	-	-	-	(26.35)	-
1231	1030	V	L0209a	2-propylheptane-1,3-diol	6628-65-5	1.0	301.15	915.50	115	-	-	-	-	-	-	-	-	(26.35)	-
1232	1031	V	L0210a	2,5-diethylhexane-1,6-diol	91241-30-4	1.0	298.15	930.70	115	-	-	-	-	-	-	-	-	(26.35)	-
1233	1032	V	L0213a	decane-1,10-diol	112-47-0	1.0	353.15	883.00	115	-	-	345.55	120	572.15	121	855.45	121	(26.35)	-
1234	1032	V	L0213b	decane-1,10-diol	112-47-0	1.0	364.0	-	-	112.40	114	345.55	120	572.15	121	855.45	121	(26.35)	-
1235	1033	V	L7302a	heptane-1,4,7-triol	3920-53-4	1.0	291.0	1075.00	115	-	-	-	-	416.90	121	-	-	(39.02)	-
1236	1034	V	C7202a	2,2-dimethylpentanoic acid	1185-39-3	1.0	293.15	885.60	117	-	-	-	-	-	-	676.34	121	(3.04)	-
1237	1035	V	C7203a	3,3-dimethylpentanoic acid	3177-74-0	1.0	298.15	934.80	117	-	-	-	-	-	-	-	-	(3.04)	-
1238	1036	V	C7205a	2,4-dimethylpentanoic acid	5868-33-7	1.0	298.15	910.00	117	-	-	-	-	-	-	-	-	(3.04)	-
1239	1037	V	C7206a	3,4-dimethylpentanoic acid	3302-06-5	1.0	298.15	923.90	117	-	-	-	-	-	-	-	-	(3.04)	-
1240	1038	V	C7207a	2-ethylpentanoic acid	20225-24-5	1.0	298.15	909.80	117	-	-	-	-	-	-	676.34	121	(3.04)	-
1241	1039	V	C7208a	2-methylhexanoic acid	4536-23-6	1.0	298.15	909.00	117	-	-	-	-	482.65	121	-	-	(3.04)	-
1242	1040	V	C7210a	3-methylhexanoic acid	3780-58-3	1.0	293.15	918.70	117	-	-	-	-	486.15	121	676.34	121	(3.04)	-
1243	1041	V	C7211a	5-methylhexanoic acid	628-46-6	1.0	293.15	916.30	117	-	-	-	-	489.15	121	676.34	121	(3.04)	-
1244	1042	V	C7212a	heptanoic acid	111-14-8	1.0	298.15	913.50	118	72.90	114	265.98	120	496.15	121	677.30	121	3.04	120
1245	1043	V	C8201a	3,4,4-trimethylpentanoic acid	75177-71-8	1.0	298.15	919.90	117	-	-	-	-	-	-	-	-	(2.75)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1246	1044	V	C8202a	2,3,4-trimethylpentanoic acid	90435-18-0	1.0	293.15	929.00	[117]	-	-	-	-	-	-	-	-	(2.75)	-
1247	1045	V	C8203a	2,2-dimethylhexanoic acid	813-72-9	0.01	374.97	849.15	[121]	-	-	-	-	-	-	696.49	[121]	(2.75)	-
1248	1046	V	C8204a	3,3-dimethylhexanoic acid	90808-83-6	1.0	298.15	900.90	[117]	-	-	-	-	-	-	-	-	(2.75)	-
1249	1047	V	C8206a	3,5-dimethylhexanoic acid	60308-87-4	1.0	298.15	902.00	[117]	-	-	-	-	-	-	-	-	(2.75)	-
1250	1048	V	C8207a	2-propylpentanoic acid	99-66-1	1.0	298.15	904.00	[120]	74.80	[114]	-	-	494.15	[121]	696.49	[121]	(2.75)	-
1251	1049	V	C8208a	2-ethylhexanoic acid	149-57-5	1.0	298.15	903.03	[117]	75.60	[114]	-	-	501.15	[121]	673.20	[121]	2.64	[120]
1252	1050	V	C8212a	5-methylheptanoic acid	1070-68-4	1.0	293.15	910.50	[117]	-	-	-	-	-	-	-	-	(2.75)	-
1253	1051	V	C8214a	octanoic acid	124-07-2	1.01	298.15	906.02	[118]	81.20	[114]	289.66	[120]	513.05	[121]	694.26	[121]	2.85	[120]
1254	1052	V	C9201a	3,5,5-trimethylhexanoic acid	3302-10-1	0.01	385.37	839.70	[121]	-	-	-	-	456.91	[121]	715.31	[121]	(2.28)	-
1255	1053	V	C9202a	3-ethyl-3-methylhexanoic acid	50902-82-4	0.01	385.37	849.66	[121]	-	-	-	-	456.91	[121]	715.31	[121]	(2.28)	-
1256	1054	V	C9203a	3,3-dimethylheptanoic acid	67061-30-7	1.0	298.15	910.20	[117]	-	-	-	-	-	-	-	-	(2.28)	-
1257	1055	V	C9207a	2-ethylheptanoic acid	3274-29-1	1.0	298.15	893.50	[117]	-	-	-	-	456.91	[121]	715.31	[121]	1.98	[120]
1258	1055	V	C9207b	2-ethylheptanoic acid	3274-29-1	1.0	401.0	-	-	63.40	[114]	-	-	456.91	[121]	715.31	[121]	1.98	[120]
1259	1056	V	C9208a	2-methyloctanoic acid	3004-93-1	1.0	277.15	909.70	[117]	-	-	-	-	456.91	[121]	715.31	[121]	2.39	[120]
1260	1057	V	C9210a	3-methyloctanoic acid	6061-10-5	1.0	296.15	899.00	[117]	-	-	-	-	456.91	[121]	715.31	[121]	(2.28)	-
1261	1058	V	C9211a	4-methyloctanoic acid	54947-74-9	0.01	395.77	830.88	[121]	-	-	-	-	-	-	715.31	[121]	(2.28)	-
1262	1059	V	C9214a	nonanoic acid	112-05-0	1.0	298.15	901.63	[117]	-	-	285.53	[120]	528.75	[121]	710.70	[121]	2.475	[120]
1263	1059	V	C9214b	nonanoic acid	112-05-0	1.0	304.0	-	-	85.30	[114]	285.53	[120]	528.75	[121]	710.70	[121]	2.475	[120]
1264	1060	V	C0201a	2,2-dimethyloctanoic acid	29662-90-6	1.0	293.15	902.20	[117]	-	-	-	-	473.73	[121]	733.00	[121]	2.8	[120]
1265	1061	V	C0202a	3,3-dimethyloctanoic acid	14352-59-1	1.0	298.15	912.90	[117]	-	-	-	-	-	-	-	-	(2.80)	-
1266	1062	V	C0203a	3,7-dimethyloctanoic acid	5698-27-1	1.0	291.15	897.00	[117]	-	-	-	-	-	-	-	-	(2.80)	-
1267	1063	V	C0204a	2-butylhexanoic acid	3115-28-4	1.0	291.55	897.80	[117]	-	-	-	-	-	-	-	-	(2.80)	-
1268	1064	V	C0206a	2-ethyloctanoic acid	25234-25-7	1.0	293.15	848.10	[117]	-	-	-	-	-	-	733.00	[121]	(2.80)	-
1269	1065	V	C0207a	2-methylnonanoic acid	24323-21-5	1.0	298.15	893.00	[117]	-	-	-	-	-	-	733.00	[121]	(2.80)	-
1270	1066	V	C0208a	3-methylnonanoic acid	35205-79-9	1.0	293.15	898.30	[117]	-	-	-	-	473.73	[121]	733.00	[121]	(2.80)	-
1271	1067	V	C0209a	4-ethyloctanoic acid	16493-80-4	1.0	293.15	908.60	[117]	-	-	-	-	-	-	733.00	[121]	(2.80)	-
1272	1068	V	C0212a	decanoic acid	334-48-5	1.0	313.15	881.70	[117]	88.60	[114]	304.54	[120]	543.15	[121]	722.10	[121]	(2.80)	-
1273	1069	V	C7403a	3,3-dimethylpentanedioic acid	4839-46-7	0.01	479.85	1198.77	[121]	-	-	376.65	[120]	464.16	[121]	809.00	[121]	(3.0)	-
1274	1070	V	C7409a	heptanedioic acid	111-16-0	0.01	486.25	1100.09	[121]	-	-	377.55	[120]	464.16	[121]	805.00	[121]	(3.0)	-
1275	1070	V	C7409b	heptanedioic acid	111-16-0	1.0	451.0	-	-	88.60	[114]	377.55	[120]	464.16	[121]	805.00	[121]	(3.0)	-
1276	1071	V	C8401a	2,2,3,3-tetramethylbutanedioic acid	630-51-3	0.01	480.65	1089.79	[121]	-	-	-	-	495.09	[121]	809.00	[121]	(3.0)	-
1277	1072	V	C8403b	octanedioic acid	505-48-6	1.0	460.0	-	-	91.40	[114]	415.45	[120]	495.09	[121]	809.00	[121]	(3.0)	-
1278	1073	V	C9401a	nonanedioic acid	123-99-9	0.01	501.5	999.70	[121]	-	-	379.65	[120]	633.36	[121]	811.00	[121]	(3.0)	-
1279	1073	V	C9401b	nonanedioic acid	123-99-9	1.0	466.0	-	-	89.30	[114]	379.65	[120]	633.36	[121]	811.00	[121]	(3.0)	-
1280	1074	V	C0403a	decanedioic acid	111-20-6	0.01	507.79	1026.10	[121]	-	-	404.15	[120]	642.09	[121]	815.00	[121]	(3.0)	-
1281	1074	V	C0403b	decanedioic acid	111-20-6	1.0	471.0	-	-	85.90	[114]	404.15	[120]	642.09	[121]	815.00	[121]	(3.0)	-
1282	1075	V	M7101a	2,2-dimethylpentan-3-amine	73153-81-8	1.0	298.15	761.50	[117]	-	-	-	-	-	-	-	-	(3.81)	-
1283	1076	V	M7102a	2,4-dimethylpentan-2-amine	64379-30-2	0.01	298.15	768.20	[121]	-	-	-	-	395.15	[121]	617.70	[121]	(3.81)	-
1284	1077	V	M7103a	2,4-dimethylpentan-3-amine	4083-57-2	1.0	293.15	788.20	[117]	-	-	-	-	-	-	-	-	(3.81)	-
1285	1078	V	M7104a	4-methylhexan-2-amine	105-41-9	0.01	306.57	755.49	[121]	-	-	-	-	405.65	[121]	617.70	[121]	(3.81)	-
1286	1079	V	M7106a	heptan-4-amine	16751-59-0	0.01	312.17	752.73	[121]	-	-	-	-	412.65	[121]	617.70	[121]	(3.81)	-
1287	1080	V	M7107a	heptan-3-amine	28292-42-4	0.01	313.37	-	-	41.78	[121]	-	-	414.15	[121]	617.70	[121]	(3.81)	-
1288	1081	V	M7108a	3-methylhexan-1-amine	65530-93-0	0.01	319.77	756.11	[121]	-	-	-	-	422.15	[121]	617.70	[121]	(3.81)	-
1289	1082	V	M7109a	4-methylhexan-1-amine	34263-68-8	0.01	322.97	757.35	[121]	-	-	-	-	426.15	[121]	617.70	[121]	(3.81)	-
1290	1083	V	M7110a	heptan-2-amine	123-82-0	1.0	293.15	762.90	[117]	-	-	-	-	415.15	[121]	617.70	[121]	(3.81)	-
1291	1084	V	M7111a	heptan-1-amine	111-68-2	1.0	298.15	771.31	[117]	49.90	[114]	250.15	[120]	430.05	[121]	617.70	[121]	3.81	[120]
1292	1085	V	M8101a	2,4,4-trimethylpentan-2-amine	107-45-9	0.01	312.57	794.37	[121]	41.04	[121]	-	-	413.15	[121]	643.92	[121]	(3.58)	-
1293	1086	V	M8102a	6-methylheptan-2-amine	543-82-8	0.002	298.15	767.00	[121]	44.49	[121]	-	-	428.15	[121]	643.92	[121]	(3.58)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1294	1087	V	M8103a	2-ethylhexan-1-amine	104-75-6	0.01	335.93	-	-	45.26	[121]	-	-	442.35	[121]	643.92	[121]	(3.58)	-
1295	1088	V	M8104a	octan-2-amine	693-16-3	1.0	293.15	772.00	[118]	-	-	-	-	438.15	[121]	643.92	[121]	(3.58)	-
1296	1088	V	M8104b	octan-2-amine	693-16-3	0.01	332.57	-	-	44.66	[121]	-	-	438.15	[121]	643.92	[121]	(3.58)	-
1297	1089	V	M8105a	octan-1-amine	111-86-4	1.01	298.15	779.95	[118]	55.10	[114]	273.15	[120]	452.75	[121]	643.92	[121]	3.58	[120]
1298	1090	V	M9101a	2,6-dimethylheptan-4-amine	65530-92-9	1.0	293.15	771.90	[117]	-	-	-	-	-	-	-	-	(3.42)	-
1299	1091	V	M9102a	2-propylhexan-1-amine	857818-18-9	1.0	298.15	789.20	[117]	-	-	-	-	-	-	-	-	(3.42)	-
1300	1092	V	M9103a	nonan-1-amine	112-20-9	1.0	293.15	788.60	[120]	-	-	272.15	[120]	475.35	[121]	668.22	[121]	3.42	[120]
1301	1092	V	M9103b	nonan-1-amine	112-20-9	0.01	362.33	-	-	49.47	[121]	272.15	[120]	475.35	[121]	668.22	[121]	3.42	[120]
1302	1093	V	M0101a	decan-1-amine	2016-57-1	1.0	298.15	789.00	[117]	64.90	[114]	288.15	[120]	493.65	[121]	690.90	[121]	3.31	[120]
1303	1094	V	N7101a	2-methyl-N-propan-2-ylpropan-2-amine	7515-80-2	0.03	298.15	726.91	[121]	-	-	-	-	371.15	[121]	577.70	[121]	(3.12)	-
1304	1094	V	N7101b	2-methyl-N-propan-2-ylpropan-2-amine	7515-80-2	1.0	287.0	-	-	35.70	[114]	-	-	371.15	[121]	577.70	[121]	(3.12)	-
1305	1095	V	N7102a	N-propan-2-ylbutan-1-amine	39099-23-5	1.0	298.0	-	-	42.10	[114]	-	-	-	-	-	-	(3.12)	-
1306	1096	V	N7103a	N-propylbutan-1-amine	20193-21-9	0.01	307.37	737.22	[121]	-	-	-	-	406.65	[121]	577.70	[121]	(3.12)	-
1307	1097	V	N7104a	N-ethylpentan-1-amine	17839-26-8	0.01	307.77	739.62	[121]	-	-	-	-	407.15	[121]	577.70	[121]	(3.12)	-
1308	1098	V	N7105a	N-methylhexan-1-amine	35161-70-7	1.0	293.15	778.70	[117]	-	-	-	-	415.15	[121]	577.70	[121]	(3.12)	-
1309	1098	V	N7105b	N-methylhexan-1-amine	35161-70-7	0.01	314.17	-	-	42.98	[121]	-	-	415.15	[121]	577.70	[121]	(3.12)	-
1310	1099	V	N8101a	N-butan-2-ylbutan-2-amine	626-23-3	1.0	298.15	749.02	[117]	41.3	[114]	-	-	407.15	[121]	603.92	[121]	(2.77)	-
1311	1100	V	N8102a	2-methyl-N-(2-methylpropyl)propan-1-amine	110-96-3	1.0	298.15	740.74	[117]	-	-	199.65	[120]	412.25	[121]	603.92	[121]	(2.77)	-
1312	1100	V	N8102b	2-methyl-N-(2-methylpropyl)propan-1-amine	110-96-3	0.01	311.85	-	-	41.82	[121]	199.65	[120]	412.25	[121]	603.92	[121]	(2.77)	-
1313	1101	V	N8104a	N-(2-methylpropyl)butan-1-amine	20810-06-4	1.0	328.0	-	-	41.20	[114]	-	-	-	-	-	-	(2.77)	-
1314	1102	V	N8105a	N-butylbutan-1-amine	111-92-2	1.0	298.15	755.72	[117]	49.40	[114]	211.35	[120]	432.00	[121]	602.30	[121]	2.765	[120]
1315	1103	V	N8106a	N-ethylhexan-1-amine	20352-67-4	0.01	326.97	735.33	[121]	-	-	-	-	431.15	[121]	603.92	[121]	(2.77)	-
1316	1104	V	N8107a	N-methylheptan-1-amine	36343-05-2	1.0	273.15	771.20	[117]	-	-	-	-	438.15	[121]	603.92	[121]	(2.77)	-
1317	1105	V	N9101a	N- tert-butyl-2-methylbutan-2-amine	2085-66-7	0.01	315.77	756.44	[121]	-	-	-	-	417.15	[121]	628.22	[121]	(3.12)	-
1318	1106	V	N9102a	N-ethylheptan-1-amine	66793-76-8	1.0	298.15	767.52	[117]	-	-	-	-	453.85	[121]	628.22	[121]	(3.12)	-
1319	1107	V	N9103a	N-methyloctan-1-amine	2439-54-5	1.0	293.15	782.40	[117]	-	-	-	-	459.85	[121]	628.22	[121]	(3.12)	-
1320	1107	V	N9103b	N-methyloctan-1-amine	2439-54-5	1.0	380.0	-	-	49.20	[114]	-	-	459.85	[121]	628.22	[121]	(3.12)	-
1321	1108	V	N0101a	3-methyl-N-(3-methylbutyl)butan-1-amine	544-00-3	1.0	298.15	766.88	[117]	-	-	229.15	[120]	461.15	[121]	650.90	[121]	(3.12)	-
1322	1108	V	N0101b	3-methyl-N-(3-methylbutyl)butan-1-amine	544-00-3	0.01	350.97	-	-	48.03	[121]	229.15	[120]	461.15	[121]	650.90	[121]	(3.12)	-
1323	1109	V	N0102a	N-pentylpentan-1-amine	2050-92-2	1.0	298.15	773.25	[117]	61.20	[114]	-	-	476.15	[121]	650.90	[121]	(3.12)	-
1324	1110	V	N0103a	N-ethyloctan-1-amine	4088-36-2	1.0	298.15	774.30	[117]	-	-	-	-	475.15	[121]	650.90	[121]	(3.12)	-
1325	1111	V	N0104a	N-methylnonan-1-amine	39093-27-1	1.0	292.15	784.00	[117]	-	-	-	-	480.15	[121]	650.90	[121]	(3.12)	-
1326	1112	V	R7101a	N,N,2-trimethylbutan-2-amine	57757-60-5	0.02	298.15	732.10	[121]	-	-	-	-	391.15	[121]	577.70	[121]	(2.41)	-
1327	1113	V	R7102a	N-ethyl-N,2-dimethylpropan-2-amine	52841-28-8	0.02	298.15	744.51	[121]	37.78	[121]	-	-	383.15	[121]	577.70	[121]	(2.41)	-
1328	1114	V	R7103a	N,N,2,2-tetramethylpropan-1-amine	10076-31-0	0.02	298.15	732.21	[121]	-	-	-	-	390.50	[121]	577.70	[121]	(2.41)	-
1329	1115	V	R7104a	N-methyl-N-propan-2-ylpropan-2-amine	10342-97-9	0.02	298.15	749.49	[121]	-	-	-	-	385.15	[121]	577.70	[121]	(2.41)	-
1330	1116	V	R7105a	N,N,3-trimethylbutan-2-amine	66225-38-5	0.02	298.15	732.10	[121]	-	-	-	-	390.50	[121]	577.70	[121]	(2.41)	-
1331	1117	V	R7106a	N,N-dimethylpentan-3-amine	18636-94-7	0.02	298.15	750.75	[121]	38.98	[121]	-	-	389.15	[121]	577.70	[121]	(2.41)	-
1332	1118	V	R7107a	N-ethyl-N-methylbutan-2-amine	66225-41-0	0.03	298.15	715.35	[121]	-	-	-	-	376.15	[121]	577.70	[121]	(2.41)	-
1333	1119	V	R7108a	N,N-dimethylpentan-2-amine	57303-85-2	0.02	298.15	717.08	[121]	-	-	-	-	382.15	[121]	577.70	[121]	(2.41)	-
1334	1120	V	R7109a	N,N-diethylpropan-2-amine	6006-15-1	0.03	298.15	738.97	[121]	37.51	[121]	-	-	381.65	[121]	577.70	[121]	(2.41)	-
1335	1121	V	R7110a	N-methyl-N-propan-2-ylpropan-1-amine	66225-42-1	0.02	298.15	749.97	[121]	-	-	-	-	386.00	[121]	577.70	[121]	(2.41)	-
1336	1122	V	R7111a	N,N,2-trimethylbutan-1-amine	66225-39-6	0.02	298.15	752.10	[121]	-	-	-	-	388.00	[121]	577.70	[121]	(2.41)	-
1337	1123	V	R7112a	N-ethyl-N,2-dimethylpropan-1-amine	60247-14-5	0.03	298.15	729.47	[121]	-	-	-	-	380.15	[121]	577.70	[121]	(2.41)	-
1338	1124	V	R7113a	N,N,3-trimethylbutan-1-amine	2315-43-7	0.02	298.15	751.97	[121]	38.42	[121]	-	-	386.65	[121]	577.70	[121]	(2.41)	-
1339	1125	V	R7114a	N,N-diethylpropan-1-amine	4458-31-5	0.02	298.15	737.98	[121]	38.16	[121]	-	-	385.15	[121]	577.70	[121]	(2.41)	-
1340	1126	V	R7115a	N-methyl-N-propylpropan-1-amine	3405-42-3	0.02	298.15	750.10	[121]	38.42	[121]	-	-	387.25	[121]	577.70	[121]	(2.41)	-
1341	1127	V	R7116a	N-ethyl-N-methylbutan-1-amine	66225-40-9	0.02	298.15	731.93	[121]	39.08	[121]	-	-	390.15	[121]	577.70	[121]	(2.41)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1342	1128	V	R7117a	N,N-dimethylpentan-1-amine	26153-88-8	0.01	298.15	731.80	121	40.03	121	-	-	395.15	121	577.70	121	(2.41)	-
1343	1129	V	R8101a	N,2-dimethyl-N-propan-2-ylpropan-2-amine	85523-00-8	0.01	302.17	763.81	121	-	-	-	-	400.15	121	603.92	121	(2.41)	-
1344	1130	V	R8102a	N-ethyl-N-propan-2-ylpropan-2-amine	7087-68-5	1.0	313.15	749.00	117	-	-	-	-	399.65	121	603.92	121	(2.41)	-
1345	1130	V	R8102b	N-ethyl-N-propan-2-ylpropan-2-amine	7087-68-5	0.01	301.77	-	-	40.02	121	-	-	399.65	121	603.92	121	(2.41)	-
1346	1131	V	R8103a	N-ethyl-N-propylpropan-1-amine	20634-92-8	0.01	310.97	795.50	121	40.37	121	-	-	411.15	121	603.92	121	(2.41)	-
1347	1132	V	R8104a	N,N-diethylbutan-1-amine	4444-68-2	1.0	293.15	742.00	117	-	-	-	-	409.15	121	603.92	121	(2.41)	-
1348	1132	V	R8104b	N,N-diethylbutan-1-amine	4444-68-2	0.01	309.37	-	-	41.40	121	-	-	409.15	121	603.92	121	(2.41)	-
1349	1133	V	R8105a	N-methyl-N-propylbutan-1-amine	24551-99-3	1.0	298.15	742.00	117	-	-	-	-	-	-	-	-	(2.41)	-
1350	1134	V	R8106a	N,N-dimethylhexan-1-amine	4385-04-0	0.01	316.57	729.49	121	43.38	121	-	-	418.15	121	603.92	121	(2.41)	-
1351	1135	V	R9101a	N,N-dipropylpropan-1-amine	102-69-2	1.0	298.15	752.88	117	46.20	114	172.65	120	429.65	121	628.22	121	2.380	120
1352	1136	V	R9102a	N,N-diethylpentan-1-amine	2162-91-6	1.0	293.15	766.30	117	-	-	-	-	429.15	121	628.22	121	(2.38)	-
1353	1136	V	R9102b	N,N-diethylpentan-1-amine	2162-91-6	0.01	325.37	-	-	43.83	121	-	-	429.15	121	628.22	121	(2.38)	-
1354	1137	V	R9103a	N-butyl-N-methylbutan-1-amine	3405-45-6	1.0	293.15	759.30	117	-	-	-	-	432.75	121	628.22	121	(2.38)	-
1355	1138	V	R9104a	N,N-dimethylheptan-1-amine	5277-11-2	1.0	293.15	758.00	117	-	-	-	-	445.15	121	628.22	121	(2.38)	-
1356	1138	V	R9104b	N,N-dimethylheptan-1-amine	5277-11-2	0.01	338.17	-	-	45.82	121	-	-	445.15	121	628.22	121	(2.38)	-
1357	1139	V	R0101a	2-methyl-N,N-di(propan-2-yl)propan-1-amine	44976-81-0	0.01	338.05	737.61	121	-	-	-	-	445.00	121	650.90	121	(2.41)	-
1358	1140	V	R0102a	2-ethyl-N,N-dimethylhexan-1-amine	28056-87-3	1.0	293.15	768.60	117	-	-	-	-	-	-	-	-	(2.41)	-
1359	1141	V	R0103a	N,N-diethylhexan-1-amine	44979-90-0	0.01	343.77	732.26	121	46.69	121	-	-	452.15	121	650.90	121	(2.41)	-
1360	1142	V	R0104a	N,N-dimethyloctan-1-amine	7378-99-6	1.0	293.15	768.70	117	-	-	-	-	464.15	121	650.90	121	(2.41)	-
1361	1142	V	R0104b	N,N-dimethyloctan-1-amine	7378-99-6	1.0	303.0	-	-	54.00	114	-	-	464.15	121	650.90	121	(2.41)	-
1362	1143	V	N7201a	N,N,N',N'-tetramethylpropane-1,3-diamine	110-95-2	1.0	291.15	783.70	120	-	-	-	-	417.15	121	-	-	(13.82)	-
1363	1143	V	N7201b	N,N,N',N'-tetramethylpropane-1,3-diamine	110-95-2	1.0	298.0	-	-	45.30	114	-	-	417.15	121	-	-	(13.82)	-
1364	1144	V	N7202a	N',N',2,2-tetramethylpropane-1,3-diamine	53369-71-4	1.0	429.65	-	-	37.17	121	-	-	429.65	121	-	-	(13.82)	-
1365	1145	V	N7203a	N',N'-diethyl-N-methylethane-1,2-diamine	104-79-0	1.0	431.65	-	-	37.36	121	-	-	431.65	121	-	-	(13.82)	-
1366	1146	V	N7205a	N',N'-diethylpropane-1,3-diamine	104-78-9	1.0	293.15	822.00	120	52.40	114	-	-	441.65	121	-	-	(13.82)	-
1367	1147	V	N7206a	heptane-1,7-diamine	646-19-5	1.0	298.0	-	-	67.10	114	298.45	120	497.15	121	-	-	(13.82)	-
1368	1148	V	N8201a	1-N,1-N,3-N,3-N-tetramethylbutane-1,3-diamine	97-84-7	1.0	298.0	-	-	47.90	114	-	-	437.70	121	-	-	(13.82)	-
1369	1149	V	N8202a	N,N,N',N'-tetramethylbutane-1,4-diamine	111-51-3	1.0	288.15	794.20	120	-	-	-	-	441.15	121	-	-	(13.82)	-
1370	1149	V	N8202b	N,N,N',N'-tetramethylbutane-1,4-diamine	111-51-3	1.0	441.15	-	-	38.26	121	-	-	441.15	121	-	-	(13.82)	-
1371	1150	V	N8204a	N',N'-di(propan-2-yl)ethane-1,2-diamine	121-05-1	1.0	394.15	-	-	33.81	121	-	-	394.15	121	-	-	(13.82)	-
1372	1151	V	N8205a	N,N'-di(propan-2-yl)ethane-1,2-diamine	4013-94-9	1.0	443.15	-	-	38.45	121	-	-	443.15	121	-	-	(13.82)	-
1373	1152	V	N8206a	2,5-dimethylhexane-2,5-diamine	23578-35-0	1.0	288.15	848.50	120	-	-	-	-	457.15	121	-	-	(13.82)	-
1374	1152	V	N8206b	2,5-dimethylhexane-2,5-diamine	23578-35-0	1.0	457.15	-	-	39.78	121	-	-	457.15	121	-	-	(13.82)	-
1375	1153	V	N8207a	N,N',N'-triethylethane-1,2-diamine	105-04-4	1.0	327.65	-	-	27.61	121	-	-	327.65	121	-	-	(13.82)	-
1376	1154	V	N8210a	octane-1,8-diamine	373-44-4	1.0	498.15	-	-	43.71	121	324.85	120	498.15	121	-	-	(13.82)	-
1377	1155	V	N9201a	N,N,N',N'-tetraethylmethanediamine	102-53-4	1.0	293.15	800.00	120	-	-	-	-	438.95	121	-	-	(13.82)	-
1378	1155	V	N9201b	N,N,N',N'-tetraethylmethanediamine	102-53-4	1.0	438.95	-	-	38.05	121	-	-	438.95	121	-	-	(13.82)	-
1379	1156	V	N9203a	1-N,1-N-diethylpentane-1,4-diamine	140-80-7	1.0	293.15	814.00	120	-	-	-	-	474.15	121	-	-	(13.82)	-
1380	1156	V	N9203b	1-N,1-N-diethylpentane-1,4-diamine	140-80-7	1.0	474.15	-	-	41.41	121	-	-	474.15	121	-	-	(13.82)	-
1381	1157	V	N9204a	nonane-1,9-diamine	646-24-2	1.0	298.0	-	-	75.50	114	-	-	531.65	121	-	-	(13.82)	-
1382	1158	V	N0201a	N,N'-di tert-butylethane-1,2-diamine	4062-60-6	1.0	326.5	775.74	121	-	-	326.45	120	470.15	121	625.00	121	(13.82)	-
1383	1159	V	N0202a	N,N,N',N'-tetraethylethane-1,2-diamine	150-77-6	1.0	298.15	808.00	120	-	-	-	-	465.15	121	-	-	(13.82)	-
1384	1159	V	N0202b	N,N,N',N'-tetraethylethane-1,2-diamine	150-77-6	1.0	465.15	-	-	40.55	121	-	-	465.15	121	-	-	(13.82)	-
1385	1160	V	N0203a	N,N,N',N'-tetramethylhexane-1,6-diamine	111-18-2	1.0	298.15	806.00	120	-	-	-	-	482.65	121	-	-	(13.82)	-
1386	1160	V	N0203b	N,N,N',N'-tetramethylhexane-1,6-diamine	111-18-2	1.0	482.65	-	-	42.22	121	-	-	482.65	121	-	-	(13.82)	-
1387	1161	V	N0204a	N,N'-dimethyloctane-1,8-diamine	33563-54-1	1.0	522.15	-	-	46.02	121	-	-	522.15	121	-	-	(13.82)	-
1388	1162	V	N0206a	decane-1,10-diamine	646-25-3	1.0	345.0	-	-	73.60	114	332.85	120	485.03	121	-	-	(13.82)	-
1389	1163	V	D7401a	heptanamide	628-62-6	1.0	298.15	-	-	82.40	118	368.6	118	527.15	121	-	-	(43.86)	-

Table S.1 – Reference experimental data (continued)

n_{sim}	n_{iso}	Set	Code	Name	CAS	P [bar]	T [K]	ρ_{liq} [kg·m^{-3}]	Src	ΔH_{vap} [kJ·mol^{-1}]	Src	T_m [K]	Src	T_b [K]	Src	T_c [K]	Src	ϵ	Src
1390	1164	V	D8402a	2-propylpentanamide	2430-27-5	1.0	298.0	-	-	83.60	[114]	-	-	472.28	[121]	-	-	(43.86)	-
1391	1165	V	D8403a	octanamide	629-01-6	1.0	383.15	845.00	[120]	-	-	378.15	[120]	512.15	[121]	-	-	(43.86)	-
1392	1165	V	D8403b	octanamide	629-01-6	1.0	512.15	-	-	45.05	[121]	378.15	[120]	512.15	[121]	-	-	(43.86)	-
1393	1166	V	D7201a	N,N,2,2-tetramethylpropanamide	24331-71-3	1.0	298.0	-	-	55.10	[114]	-	-	-	-	-	-	(35.30)	-
1394	1167	V	D7202a	N,N-diethylpropanamide	1114-51-8	1.0	293.15	897.20	[120]	-	-	-	-	464.15	[121]	-	-	(35.30)	-
1395	1167	V	D7202b	N,N-diethylpropanamide	1114-51-8	1.0	464.15	-	-	40.45	[121]	-	-	464.15	[121]	-	-	(35.30)	-
1396	1168	V	D7203a	N,N-dimethylpentanamide	6225-06-5	1.0	298.15	896.20	[120]	-	-	222.15	[120]	458.76	[121]	-	-	(35.30)	-
1397	1169	V	D8201a	N,N-di(propan-2-yl)acetamide	759-22-8	0.06	389.2	808.80	[121]	46.07	[121]	-	-	469.15	[121]	700.00	[121]	(35.30)	-
1398	1170	V	D8202a	N,N-diethylbutanamide	1114-76-7	1.0	293.15	888.40	[120]	-	-	-	-	479.15	[121]	-	-	(35.30)	-
1399	1170	V	D8202b	N,N-diethylbutanamide	1114-76-7	1.0	313.0	-	-	38.70	[114]	-	-	479.15	[121]	-	-	(35.30)	-
1400	1171	V	D8203a	N,N-dimethylhexanamide	5830-30-8	1.0	408.15	-	-	35.13	[121]	-	-	408.15	[121]	-	-	(35.30)	-
1401	1172	V	D8204a	N,N-dipropylacetamide	1116-24-1	1.0	290.15	899.20	[120]	-	-	-	-	482.65	[121]	700.00	[121]	(35.30)	-
1402	1173	V	D9201a	N,N-diethyl-2,2-dimethylpropanamide	24331-72-4	1.0	479.15	-	-	41.88	[121]	-	-	479.15	[121]	-	-	(35.30)	-
1403	1174	V	D9202a	N,N-diethyl-3-methylbutanamide	533-32-4	1.0	293.15	876.40	[120]	-	-	-	-	484.15	[121]	-	-	(35.30)	-
1404	1174	V	D9202b	N,N-diethyl-3-methylbutanamide	533-32-4	1.0	484.15	-	-	42.36	[121]	-	-	484.15	[121]	-	-	(35.30)	-
1405	1175	V	D0202a	N,N-diethylhexanamide	6282-97-9	1.0	388.0	-	-	47.70	[114]	-	-	-	-	-	-	(35.30)	-

S.3 Covalent Interaction Parameters

The covalent interaction parameters were not subject to optimization, and ported directly from the 2016H66 parameter set.[112] The corresponding values are provided in Tab. S.2. For the torsional-dihedral potentials, the 2016H66 parameter set includes 12 types A-L relevant for the molecules of the O+N family. These are shown in Fig. S.3a, and the corresponding parameters are listed in Tab. S.2. Due to the inclusion of polyfunctional compounds in the present calculations (multiple occurrences of the same functional group), the assignment of these torsional-dihedral types has been generalized as shown in Fig. S.3b.

Bond stretching		
Quartic force constant [10^6 kJ·mol^{-1}·nm^{-4}]	Reference bond length [nm]	Usage
15.70	0.1000	H - OA
18.70	0.1000	H - N
12.30	0.1090	HC - C
16.60	0.1230	C = O
11.80	0.1330	C, CR1 - N, NR
10.20	0.1360	C - OA,OE
8.18	0.1430	CHn - OA,OE
8.71	0.1470	CHn - N, NR
7.15	0.1530	C,CHn - C,CHn
Bond-angle bending		
Cosine-harmonic force constant [kJ·mol^{-1}]	Reference bond angle [deg]	Usage
380	109.50	H - NL, NT - H, CHn - OA - CHn
425	109.50	H - NL - C, CHn H - NT - CHn
450	109.50	X - OA, SI - X
520	109.50	CHn,C - CHn - C, CHn, OA, OM, N, NE
530	111.00	CHn - CHn - C,CHn,OA,OE,NR,NT,NL
545	113.00	CHn - CH2 - S or CHn - C - OA,OE
460	115.00	H - N - CHn
610	115.00	CHn, C - C - OA, N, NT, NL
620	116.00	CH2 - N - CH1 or CHn - C - CHn,HC
635	117.00	CH3 - N - C or CHn - C - OM or C - OE - CHn
390	120.00	H - NT, NZ, NE - C
445	120.00	H - NT, NZ - H
505	120.00	H - N - CH3, H / H - NT - CHn / HC - C - O
685	121.00	O - C - CHn, C CH3 - N - CHn
700	122.00	CH1, CH2 - N - C / O - C - OA, OE, CHn
415	123.00	H - N - C
730	124.00	O - C - OA, N, NT, NL C - NE - CH2
750	125.00	CHn - C - O (carb. acids and esters)
Improper-dihedral distortion		
Harmonic force constant [kJ·mol^{-1} deg^{-2}]	Reference improper dihedral angle [deg]	Usage
0.051	0.0	planar groups
0.102	35.26439	tetrahedral centers

Torsional-dihedral rotation				
Type	Force constant [kJ·mol^{-1}]	Phase shift	Multiplicity	Usage
A	5.920	0.0	3	X,C - C - C - C,X
B	0.931	180.0	1	CHn-CHn-OE-CHn
C	0.569	0.0	2	CHn-CHn-OE-CHn
D	4.682	0.0	3	CHn-CHn-OE-CHn
E	6.942	180.0	1	OE-CHn-CHn-OE
F	3.312	0.0	2	OE-CHn-CHn-OE
G	6.787	0.0	3	OE-CHn-CHn-OE
H	3.770	0.0	3	-C,CHn,SI-
I	1.000	0.0	6	-CHn-C,NR(ring), CR1-
J	1.260	0.0	3	-CHn-OA(no sugar)-
K	3.500	180.0	2	-C-N,NT,NE,NZ,NR-
L	16.700	180.0	2	-C-OA,OE-

Table S.2: Covalent types of the proposed GROMOS-compatible force field for the O+N family, along with the values of the associated parameters. These $N_{\text{prm}}^{\text{cov}} = 94$ covalent interaction parameters are ported from the 2016H66 parameter set[112] and not subject to optimization. The application of the torsional-dihedral types is further detailed in Fig. S.3.

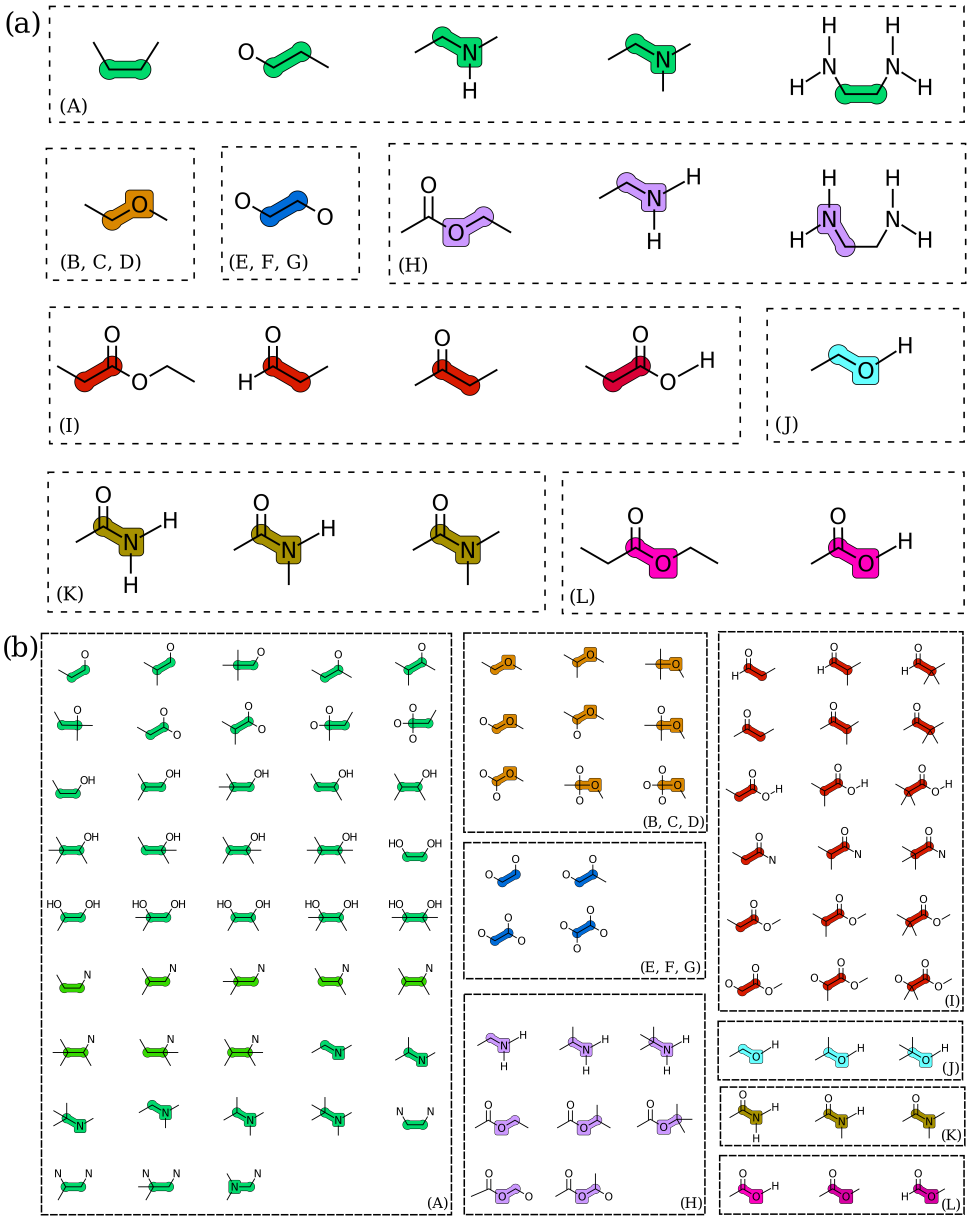


Figure S.3: Application of the different torsional-dihedral types considering (a) the 2016H66 parameter set [112] and (b) the proposed GROMOS-compatible force field for the O+N family. The parameters associated with the 12 types A-L are reported in Tab. S.2.

S.4 Initial Values of the Non-Bonded Interaction Parameters

The initial values of the non-bonded interaction parameters, used to start the optimization, are reported in Tab. S.3 for the 47 EE-types and in Tab. S.4 for the 12 LJ-types.

Idx	Atom type (EE-type)	LJ-type	η [e^{-1}·V]	χ [V]	Usage
Aliphatic carbon (united-)atoms					
1	CH0	CH0	-	-	CH_0 carbon atom (methanetetryl group)
2	CH1	CH1	-	-	CH_1 carbon united-atom (methanetriyl group)
3	CH2	CH2	-	-	CH_2 carbon united-atom (methylene group)
4	CH3	CH3	-	-	CH_3 carbon united-atom (methyl group)
Ether					
5	O_eth	OR	33.917	38.772	ether oxygen alkoxy
6	CH0_O_eth	CH0	2.937	19.820	alkoxylated CH_0 atom
7	CH1_O_eth	CH1	6.440	19.123	alkoxylated CH_1 united-atom
8	CH2_O_eth	CH2	12.894	17.428	alkoxylated CH_2 united-atom
9	CH3_O_eth	CH3	21.565	14.641	alkoxylated CH_3 united-atom
Aldehyde					
10	H_CO_ald	HC	15.789	20.677	aldehyde hydrogen atom
11	C_ald	C=O	15.271	17.113	aldehyde carbonyl carbon atom
12	O_ald	O=C	8.334	23.794	aldehyde carbonyl oxygen atom
Ketone					
13	C_ket	C=O	35.039	15.340	ketone carbonyl carbon atom
14	O_ket	O=C	16.586	39.562	ketone carbonyl oxygen atom
Ester					
15	H_CO_est	HC	15.789	20.677	formate ester hydrogen atom
16	C_est	C=O	23.835	12.918	ester carbonyl carbon atom
17	O_est	O=C	13.065	31.947	ester carbonyl oxygen atom
18	O_R_est	OR	22.659	33.044	ester acylated oxygen atom
19	CH0_O_est	CH0	9.199	22.355	ester oxygen-linked CH_0 atom
20	CH1_O_est	CH1	12.974	21.229	ester oxygen-linked CH_1 united-atom
21	CH2_O_est	CH2	38.375	13.922	ester oxygen-linked CH_2 united-atom
22	CH3_O_est	CH3	21.822	18.698	ester oxygen-linked CH_3 united-atom
Alcohol					
23	H_ol	HB	34.153	16.504	hydroxyl hydrogen atom
24	O_ol	OH	31.328	46.650	hydoxyl oxygen atom
25	CH0_O_ol	CH0	32.971	18.556	hydroxylated CH_0 atom
26	CH1_O_ol	CH1	33.267	18.687	hydroxylated CH_1 united-atom
27	CH2_O_ol	CH2	33.378	18.838	hydroxylated CH_2 united-atom
28	CH3_O_ol	CH3	33.683	18.848	hydroxylated CH_3 united-atom
Carboxylic acid					
29	H_CO_acd	HC	30.481	13.942	formic acid hydrogen atom
30	C_acd	C=O	30.317	13.694	carboxylic acid carbonyl carbon atom
31	O_acd	O=C	34.360	45.492	carboxylic acid carbonyl oxygen atom
32	H_O_acd	HB	30.481	13.942	carboxylic acid hydroxyl hydrogen atom
33	O_H_acd	OH	37.502	37.512	carboxylic acid hydroxyl oxygen atom
Amine					
34	H_N_amn	HB	43.176	7.209	amine hydrogen atom
35	N_amn	N_amn	38.110	50.797	amine nitrogen atom
36	CH0_N_amn	CH0	30.075	12.090	aminated CH_0 atom
37	CH1_N_amn	CH1	28.519	13.156	aminated CH_1 united-atom
38	CH2_N_amn	CH2	33.772	12.233	aminated CH_2 united-atom
39	CH3_N_amn	CH3	30.311	14.639	aminated CH_3 united-atom
Amide					
40	H_N_amd	HB	27.009	11.761	amide nitrogen-linked hydrogen atom
41	C_amd	C=O	30.587	14.430	amide carbonyl carbon atom
42	O_amd	O=C	29.866	43.332	amide carbonyl oxygen atom
43	N_amd	N_amd	32.398	36.131	amide acylated nitrogen atom
44	CH0_N_amd	CH0	35.585	15.614	amide nitrogen-linked CH_0 atom (estimated)
45	CH1_N_amd	CH1	35.488	17.475	amide nitrogen-linked CH_1 united-atom
46	CH2_N_amd	CH2	42.041	15.944	amide nitrogen-linked CH_2 united-atom
47	CH3_N_amd	CH3	38.845	16.767	amide nitrogen-linked CH_3 united-atom

Table S.3: Initial values of the EE parameters, used to start the optimization. This table is similar to Main Article Tab. 3 (see the corresponding caption for details), but reports the initial instead of the final (optimized) values.

LJ type	σ	$\tilde{\sigma}$ [nm]	σ^*	ϵ [kJ·mol^{-1}]	ϵ^*	Usage
Carbon						
CH0	0.664	-	0.336	0.007	0.406	CH_0 carbon atom (methanetetryl group)
CH1	0.502	-	0.330	0.095	0.567	CH_1 carbon united-atom (methanetriyl group)
CH2	0.407	-	0.316	0.411	1.176	CH_2 carbon united-atom (methylene group)
CH3	0.375	-	0.309	0.867	1.946	CH_3 carbon united-atom (methyl group)
C=O	0.358	-	0.336	0.277	0.406	carbonyl carbon
Oxygen						
OR	0.333	0.333	0.287	0.309	1.011	alkoxy oxygen
O=C	0.289	0.289	0.262	0.739	1.725	carbonyl oxygen
OH	0.295	0.295	0.287	0.775	1.011	hydoxyl oxygen
Nitrogen						
N_amn	0.318	0.318	0.298	0.308	0.598	nitrogen in amine
N_amd	0.328	0.328	0.298	0.312	0.459	nitrogen in amide
Hydrogen						
HC	0.237	-	0.237	0.118	0.118	aliphatic hydrogen
HB	0.000	-	0.000	0.000	0.000	hydrogen donor (not optimized)

Table S.4: Initial values of the LJ parameters, used to start the optimization. This table is similar to Main Article Tab. 4 (see the corresponding caption for details), but reports the initial instead of the final (optimized) values.

S.5 Observable-to-parameter Ratio for the LJ- and EE- Types

In this section, the observable-to-parameter ratio is analyzed separately for each of the LJ- and EE-types of the force field, see Tabs. S.5 and S.6. A favorable observable-to-parameter ratio is observed in most cases, except for EE-types occurring in a single molecule. These are the CH3 united-atom of EE-type CH3_O_ol (only found in methanol), the carbonyl-bound hydrogen atom of EE-type H_CO_acd (only found in formic acid) and the CH1 united-atom of EE-type CH1_N_amd (only included *via* compound D5302 of the calibration set, namely N-isopropyl acetamide). In one case, for the EE-type CH0_N_amd, no representative molecule is available at all, and the corresponding EE parameters η and χ are estimated using the average values over the three other CHn_N_amd types.

LJ type	N^{cal}	N_{ρ}^{cal}	$N_{\Delta H}^{\mathrm{cal}}$	N^{val}	N_{ρ}^{val}	$N_{\Delta H}^{\mathrm{val}}$
Carbon						
C=O	110	100	95	336	299	198
Oxygen						
OR	89	82	81	278	239	161
O=C	110	100	95	336	299	198
OH	100	100	58	345	340	76
Nitrogen						
N_amn	100	88	84	88	73	55
N_amd	17	12	13	13	7	11
Hydrogen						
HC	34	32	28	25	25	11

Table S.5: Representation of the different LJ-types in the molecules of the calibration and validation sets, including availability of experimental ρ_{liq} and ΔH_{vap} values. The entries N^{cal}, N_{ρ}^{cal} and $N_{\Delta H}^{\mathrm{cal}}$ provide numbers of molecules, of ρ_{liq} values and of ΔH_{vap} values, respectively, in the calibration set ($N_{\mathrm{iso}}^{\mathrm{cal}} = 339$ compounds depicted in Fig. S.1). The entries N^{val}, N_{ρ}^{val} and $N_{\Delta H}^{\mathrm{val}}$ provide the corresponding information for the validation set ($N_{\mathrm{iso}}^{\mathrm{val}} = 836$ compounds depicted in Fig. S.2). The values reported correspond to the number of molecules including at least one occurrence of the specific atom type. The LJ-types are those listed in Tab. 4, except for the (united-)atom aliphatic types CH0, CH1, CH2, CH3, and HB (not subject to optimization).

Idx	Atom type (EE-type)	N^{cal}	N_{ρ}^{cal}	$N_{\Delta H}^{\mathrm{cal}}$	N^{val}	N_{ρ}^{val}	$N_{\Delta H}^{\mathrm{val}}$
Ether							
5	O_eth	46	43	41	108	93	50
6	CH0_O_eth	6	6	6	23	14	19
7	CH1_O_eth	18	14	15	35	30	12
8	CH2_O_eth	28	26	25	92	81	41
9	CH3_O_eth	33	30	28	25	19	10
Aldehyde							
10	H_CO_ald	19	18	15	21	21	8
11	C_ald	19	18	15	21	21	8
12	O_ald	19	18	15	21	21	8
Ketone							
13	C_ket	14	14	14	91	85	57
14	O_ket	14	14	14	91	85	57
Ester							
15	H_CO_est	14	13	12	4	4	3
16	C_est	43	39	40	170	146	111
17	O_est	43	39	40	170	146	111
18	O_R_est	43	39	40	170	146	111
19	CH0_O_est	3	3	2	12	4	10
20	CH1_O_est	9	7	8	32	29	10
21	CH2_O_est	20	17	20	108	95	82
22	CH3_O_est	14	12	13	22	20	13
Alcohol							
23	H_ol	83	83	45	304	300	65
24	O_ol	83	83	45	304	300	65
25	CH0_O_ol	15	15	6	109	109	16
26	CH1_O_ol	42	42	17	116	115	28
27	CH2_O_ol	53	53	26	109	105	24
28	CH3_O_ol	1	1	1	0	0	0
Carboxylic acid							
29	H_CO_acd	1	1	1	0	0	0
30	C_acd	17	17	13	41	40	11
31	O_acd	17	17	13	41	40	11
32	H_O_acd	17	17	13	41	40	11
33	O_H_acd	17	17	13	41	40	11
Amine							
34	H_N_amn	86	73	70	51	37	32
35	N_amn	100	88	84	88	73	55
36	CH0_N_amn	37	36	32	33	29	18
37	CH1_N_amn	72	57	62	67	53	47
38	CH2_N_amn	28	23	24	26	21	13
39	CH3_N_amn	9	9	7	9	9	4
Amide							
40	H_N_amd	13	8	11	3	1	3
41	C_amd	17	12	13	13	7	11
42	O_amd	17	12	13	13	7	11
43	N_amd	17	12	13	13	7	11
44	CH0_N_amd	0	0	0	0	0	0
45	CH1_N_amd	1	0	1	1	1	1
46	CH2_N_amd	4	3	4	6	4	5
47	CH3_N_amd	6	5	4	3	1	2

Table S.6: Representation of the different EE-types (or, equivalently, atom types) in the molecules of the calibration and validation sets, including availability of experimental ρ_{liq} and ΔH_{vap} values. The entries N^{cal}, N_{ρ}^{cal} and $N_{\Delta H}^{\mathrm{cal}}$ provide numbers of molecules, of ρ_{liq} values and of ΔH_{vap} values, respectively, in the calibration set ($N_{\mathrm{iso}}^{\mathrm{cal}} = 339$ compounds depicted in Fig. S.1). The entries N^{val}, N_{ρ}^{val} and $N_{\Delta H}^{\mathrm{val}}$ provide the corresponding information for the validation set ($N_{\mathrm{iso}}^{\mathrm{val}} = 836$ compounds depicted in Fig. S.2). The values reported correspond to the number of molecules including at least one occurrence of the specific atom type. The atom types (EE-types) are those listed in Tab. 3.

S.6 Comparison of Experimental and Simulated Properties

In this section, we provide a detailed comparison between the experimental properties and their values calculated using the final (refined) force-field parameters listed in Main Article Tabs. 3 and 4, along with Tab. S.2. The experimental and simulated values are reported in Tab. S.7 for the $N_{\mathrm{sim}}^{\mathrm{tot}} = 1405$ compounds/P,T-points ($N_{\mathrm{sim}}^{\mathrm{cal}} = 408$, $N_{\mathrm{sim}}^{\mathrm{val}} = 997$) considered in the simulations (Tab. S.1). Simulation results with errors larger than 80.0 kg·m^{-3} for ρ_{liq} and/or larger than 8.0 kJ·mol^{-1} for ΔH_{vap} (62 simulations concerning 58 molecules) are marked as outliers, and are discussed specifically in Sec. S.7.

Table S.7: Experimental and simulated properties of the 1405 compounds/P, T-points considered in the simulations.

n_{sim}	n_{iso}	Set	Code	Outlier	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq} [kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap} [kJ·mol^{-1}] exp	sim	dev	err [%]
1	1	C	O2101a		131.66	248.31	248.12	1.0	735.0	737.8	2.7	0.4	21.6	23.5	1.9	8.9
2	1	C	O2101b		131.66	248.31	298.28	9.06	661.9	668.4	6.5	1.0	-	-	-	-
3	1	C	O2101c		131.66	248.31	298.15	5.77	-	-	-	-	17.8	21.3	3.6	20.0
4	2	C	O3101a		160.15	280.50	273.15	1.0	726.0	712.6	-13.4	-1.9	-	-	-	-
5	2	C	O3101b		160.15	280.50	298.15	1.82	691.9	681.3	-10.6	-1.5	-	-	-	-
6	2	C	O3101c		160.15	280.50	280.5	1.0	-	-	-	-	31.2	25.3	-5.9	-18.9
7	3	C	O4101a		-	303.92	298.15	1.0	709.0	679.7	-29.3	-4.1	26.4	26.6	0.2	0.9
8	4	C	O4102a		-	311.72	298.15	1.0	719.2	708.2	-11.0	-1.5	27.9	28.8	0.9	3.3
9	5	C	O4103a		156.93	307.58	298.15	1.0	707.8	693.2	-14.6	-2.1	27.2	27.8	0.6	2.2
10	6	C	O5101a		164.55	328.35	298.15	1.0	735.2	708.5	-26.8	-3.6	30.4	29.3	-1.1	-3.7
11	7	C	O5102a		-	331.70	298.15	1.0	727.2	714.4	-12.8	-1.8	-	-	-	-
12	7	C	O5102b		-	331.70	298.15	0.26	-	-	-	-	30.1	31.4	1.2	4.2
13	8	C	O5103a		-	332.15	298.15	1.0	736.7	717.1	-19.6	-2.7	-	-	-	-
14	8	C	O5103b		-	332.15	298.15	0.26	-	-	-	-	30.2	31.5	1.3	4.3
15	9	C	O5104a		-	326.15	298.15	1.0	717.3	694.9	-22.4	-3.1	30.0	30.2	0.2	0.6
16	10	C	O5105a		157.45	343.35	298.15	1.0	739.4	729.3	-10.1	-1.4	32.5	33.6	1.1	3.2
17	11	C	O5106a		145.65	337.01	298.15	1.0	727.0	713.3	-13.7	-1.9	31.4	32.1	0.7	2.1
18	12	C	O6101a		-	356.15	298.15	0.08	753.9	735.6	-18.3	-2.4	-	-	-	-
19	13	C	O6102a		-	359.45	298.15	1.0	765.9	747.7	-18.2	-2.4	35.0	34.4	-0.6	-1.6
20	14	C	O6103a		179.15	345.95	298.15	1.0	735.2	724.4	-10.8	-1.5	33.1	34.0	0.9	2.9
21	15	C	O6104a		-	356.15	298.15	1.0	754.2	738.6	-15.6	-2.1	-	-	-	-
22	16	C	O6105a		187.78	341.45	298.15	1.0	718.7	698.3	-20.4	-2.8	32.7	31.6	-1.1	-3.3
23	17	C	O6106a		-	363.15	298.15	0.07	746.1	742.6	-3.4	-0.5	-	-	-	-
24	18	C	O6107a		-	361.15	298.15	0.07	749.0	742.4	-6.5	-0.9	-	-	-	-
25	19	C	O6108a		-	363.15	298.15	1.0	749.0	738.2	-10.9	-1.4	-	-	-	-
26	19	C	O6108b		-	363.15	298.15	0.07	-	-	-	-	35.5	36.6	1.1	3.1
27	20	C	O6109a		-	354.25	298.15	1.0	734.0	716.8	-17.2	-2.4	-	-	-	-
28	20	C	O6109b		-	354.25	298.15	0.1	-	-	-	-	33.6	34.4	0.8	2.4
29	21	C	O6110a		-	364.15	298.15	0.06	749.9	736.2	-13.7	-1.8	35.6	36.2	0.6	1.8
30	22	C	O6111a		-	354.35	298.15	1.0	738.3	723.2	-15.1	-2.0	-	-	-	-
31	22	C	O6111b		-	354.35	298.15	0.11	-	-	-	-	32.6	34.9	2.2	6.8
32	23	C	O6112a		-	353.15	298.15	1.0	732.4	710.6	-21.8	-3.0	-	-	-	-
33	23	C	O6112b		-	353.15	298.15	0.09	-	-	-	-	34.0	34.2	0.2	0.6
34	24	C	O6113a		-	372.15	298.15	1.0	755.2	744.7	-10.5	-1.4	-	-	-	-
35	24	C	O6113b		-	372.15	298.15	0.04	-	-	-	-	36.4	38.3	1.8	5.0
36	25	C	O6114a		149.15	365.35	298.15	1.0	744.7	730.2	-14.5	-1.9	36.3	36.8	0.5	1.2
37	26	C	O6115a		158.35	362.79	298.15	1.0	741.9	727.0	-14.9	-2.0	35.7	36.2	0.6	1.5
38	27	C	O3201a		168.04	315.00	298.15	0.51	854.1	820.5	-33.6	-3.9	-	-	-	-
39	27	C	O3201b		168.04	315.00	298.0	1.0	-	-	-	-	28.9	27.2	-1.7	-5.9
40	28	C	O4201a		159.95	337.65	293.15	1.0	851.6	791.8	-59.8	-7.0	36.4	29.8	-6.6	-18.2
41	29	C	O4202a		204.15	357.20	298.15	1.01	861.4	843.2	-18.1	-2.1	36.8	36.8	0.0	0.1
42	30	C	O5201a		226.15	356.15	298.15	1.01	845.1	805.9	-39.2	-4.6	37.6	35.0	-2.6	-7.0
43	31	C	O5202a		-	369.05	369.05	1.0	-	-	-	-	31.5	32.0	0.5	1.7
44	32	C	O5203a		-	359.15	293.15	1.0	864.8	802.7	-62.1	-7.2	-	-	-	-
45	32	C	O5203b		-	359.15	359.15	1.0	-	-	-	-	30.5	30.4	-0.1	-0.3
46	33	C	O5204a		-	375.25	298.15	1.0	846.0	824.4	-21.6	-2.5	39.8	39.6	-0.2	-0.4

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
47	34	C	O5205a		207.15	361.15	298.15	1.0	825.2	790.2	-34.9	-4.2	35.7	33.7	-2.0	-5.7
48	35	C	O6201a		-	-	293.15	1.0	844.6	815.4	-29.2	-3.5	-	-	-	-
49	36	C	O6203a		-	-	317.0	1.0	-	-	-	-	41.2	37.5	-3.7	-9.0
50	37	C	O6204a		167.05	376.75	298.15	1.01	822.0	778.0	-44.0	-5.3	39.6	36.4	-3.2	-8.2
51	38	C	O6205a		-	-	298.15	1.0	852.9	837.1	-15.8	-1.9	-	-	-	-
52	39	C	O6206a		-	-	340.0	1.0	-	-	-	-	38.6	36.4	-2.2	-5.6
53	40	C	O6207a		199.15	392.55	298.15	1.0	836.2	811.8	-24.4	-2.9	43.2	43.1	-0.1	-0.2
54	41	C	O4301a		288.15	377.15	293.15	1.0	967.6	899.6	-68.0	-7.0	38.1	38.1	0.0	0.0
55	42	C	O5301a		-	381.15	298.15	1.0	943.8	892.3	-51.5	-5.5	-	-	-	-
56	42	C	O5301b		-	381.15	381.15	1.0	-	-	-	-	32.6	35.4	2.8	8.7
57	43	C	O6302a		-	421.15	421.15	1.0	-	-	-	-	36.4	40.3	4.0	10.8
58	44	C	O6304a		209.15	432.91	298.15	1.0	939.2	913.2	-26.0	-2.8	48.0	53.1	5.1	10.7
59	45	C	O5401a		270.65	387.15	298.15	1.0	1023.0	958.8	-64.2	-6.3	-	-	-	-
60	45	C	O5401b		270.65	387.15	319.0	1.0	-	-	-	-	41.2	41.5	0.3	0.8
61	46	C	O6401a		-	-	366.0	1.0	-	-	-	-	42.9	43.7	0.8	1.9
62	47	C	A1101a		181.15	254.05	250.68	1.36	805.2	884.0	78.9	9.8	-	-	-	-
63	47	C	A1101b		181.15	254.05	293.15	1.0	814.0	811.5	-2.5	-0.3	-	-	-	-
64	47	C	A1101c		181.15	254.05	254.05	1.0	-	-	-	-	23.2	25.6	2.4	10.4
65	48	C	A2101a		149.75	293.55	298.15	1.0	772.0	779.5	7.5	1.0	26.9	26.5	-0.4	-1.6
66	49	C	A3101a		193.15	321.15	298.15	1.0	791.2	772.7	-18.5	-2.3	29.6	29.7	0.1	0.2
67	50	C	A4101a		201.05	337.25	298.15	1.0	796.6	752.1	-44.5	-5.6	32.3	31.0	-1.3	-4.0
68	51	C	A4102a		176.29	347.95	298.15	1.0	796.6	785.7	-10.9	-1.4	33.7	34.2	0.5	1.6
69	52	C	A5101a		274.15	347.15	298.15	0.14	783.1	765.2	-17.9	-2.3	-	-	-	-
70	52	C	A5101b		274.15	347.15	322.0	1.0	-	-	-	-	34.2	30.8	-3.5	-10.1
71	53	C	A5102a		-	365.15	298.15	0.06	804.1	778.2	-25.9	-3.2	34.8	35.9	1.2	3.4
72	54	C	A5103a		222.15	365.75	298.15	1.0	794.2	783.2	-11.0	-1.4	-	-	-	-
73	54	C	A5103b		222.15	365.75	298.15	0.06	-	-	-	-	34.8	36.6	1.8	5.2
74	55	C	A5104a		191.65	376.15	298.15	1.0	806.2	795.4	-10.8	-1.3	38.1	39.0	0.9	2.4
75	56	C	A6101a		-	377.15	298.15	0.03	801.0	797.5	-3.6	-0.4	36.2	37.2	1.0	2.8
76	57	C	A6103a		-	386.15	298.15	1.0	809.7	791.4	-18.3	-2.3	-	-	-	-
77	58	C	A6104a		-	389.95	298.15	0.02	814.1	796.5	-17.6	-2.2	38.6	40.7	2.1	5.4
78	59	C	A6105a		-	390.15	298.15	0.02	808.0	789.5	-18.6	-2.3	38.8	40.7	1.9	5.0
79	60	C	A6106a		-	395.15	299.47	0.01	806.6	801.5	-5.1	-0.6	-	-	-	-
80	61	C	A6108a		214.95	401.45	298.15	1.01	833.1	801.8	-31.3	-3.8	42.3	43.7	1.4	3.4
81	62	C	A4201a		-	443.15	293.15	1.0	1065.0	1009.4	-55.6	-5.2	-	-	-	-
82	63	C	A5201b		259.15	461.15	342.0	1.0	-	-	-	-	56.2	53.7	-2.5	-4.5
83	64	C	A6201a	×	-	439.15	439.15	1.0	-	-	-	-	38.1	48.1	10.1	26.4
84	65	C	A6202a		265.15	435.22	292.15	1.0	1003.0	959.1	-43.9	-4.4	-	-	-	-
85	66	C	K3101a		178.25	329.44	298.15	1.0	784.4	803.1	18.7	2.4	31.3	31.5	0.2	0.5
86	67	C	K4101a		186.48	352.79	298.15	1.0	799.9	793.8	-6.2	-0.8	34.5	34.2	-0.3	-1.0
87	68	C	K5101a		180.02	367.55	298.15	1.0	809.4	781.8	-27.6	-3.4	36.8	35.8	-1.0	-2.6
88	69	C	K5102a		234.17	375.14	298.15	1.0	809.6	789.1	-20.5	-2.5	38.5	37.1	-1.4	-3.7
89	70	C	K5103a		196.32	375.46	298.15	1.0	801.8	799.3	-2.5	-0.3	38.3	38.8	0.5	1.2
90	71	C	K6101a		221.75	379.25	298.15	1.0	804.3	803.6	-0.7	-0.1	38.3	37.3	-1.0	-2.5
91	72	C	K6102a		-	386.55	298.15	1.0	806.6	782.4	-24.2	-3.0	39.8	39.0	-0.8	-2.0
92	73	C	K6103a		-	390.55	298.15	1.0	808.3	799.2	-9.1	-1.1	39.8	40.6	0.8	1.9
93	74	C	K6104a		188.15	389.65	298.15	1.0	796.3	795.1	-1.2	-0.2	41.0	40.9	-0.1	-0.2
94	75	C	K6105a		217.75	396.65	298.15	1.0	811.1	794.3	-16.8	-2.1	40.6	41.7	1.1	2.7

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
95	76	C	K6106a		217.70	400.85	298.15	1.0	807.1	804.4	-2.7	-0.3	42.2	43.4	1.2	2.9
96	77	C	K6201a		-	444.65	332.77	0.01	946.8	921.7	-25.1	-2.6	46.8	50.7	3.9	8.4
97	78	C	K6204a		-	433.15	293.15	1.0	959.0	949.0	-10.0	-1.0	-	-	-	-
98	78	C	K6204b		-	433.15	323.57	0.01	-	-	-	-	44.2	52.0	7.8	17.7
99	79	C	K6205a		267.65	467.15	350.77	0.01	884.6	918.2	33.5	3.8	-	-	-	-
100	79	C	K6205b		267.65	467.15	401.0	1.0	-	-	-	-	50.1	50.6	0.5	1.0
101	80	C	E3201a		174.95	330.09	298.15	1.01	927.5	914.7	-12.8	-1.4	32.3	32.9	0.6	1.9
102	81	C	E4201a		185.65	352.60	298.15	1.0	909.1	880.9	-28.2	-3.1	35.7	35.7	0.0	0.1
103	82	C	E4202a		189.35	350.21	298.15	1.0	894.3	873.4	-20.9	-2.3	35.1	35.3	0.2	0.6
104	83	C	E5201a		188.55	365.65	298.15	1.0	883.3	849.3	-34.0	-3.9	37.3	37.3	-0.0	-0.1
105	84	C	E5202a		199.75	361.65	298.15	1.0	869.0	844.3	-24.7	-2.8	37.0	37.1	0.1	0.3
106	85	C	E5203a		187.35	375.90	298.15	1.01	892.5	871.4	-21.2	-2.4	39.8	40.1	0.3	0.7
107	86	C	E5204a		199.55	372.25	298.15	1.0	884.0	851.8	-32.2	-3.6	39.3	38.1	-1.2	-3.0
108	87	C	E5205a		180.15	374.65	298.15	1.01	882.8	863.3	-19.5	-2.2	39.1	39.3	0.2	0.6
109	88	C	E6201a		-	374.25	293.15	1.0	850.0	860.7	10.7	1.3	38.8	38.8	0.0	0.0
110	89	C	E6202a		-	369.15	298.15	1.0	861.6	845.1	-16.4	-1.9	38.0	38.4	0.4	1.1
111	90	C	E6203a		-	-	293.15	1.0	884.7	861.0	-23.7	-2.7	-	-	-	-
112	91	C	E6204a		175.35	383.00	298.15	1.0	864.0	828.3	-35.8	-4.1	39.8	39.6	-0.1	-0.4
113	92	C	E6205a		-	389.65	298.15	1.0	875.9	856.6	-19.3	-2.2	-	-	-	-
114	92	C	E6205b		-	389.65	298.15	0.02	-	-	-	-	39.4	42.3	2.9	7.3
115	93	C	E6206a		-	383.15	298.15	1.0	860.1	828.8	-31.3	-3.6	-	-	-	-
116	93	C	E6206b		-	383.15	298.15	0.03	-	-	-	-	38.4	39.8	1.4	3.5
117	94	C	E6207a		176.05	389.80	298.15	1.0	866.3	845.2	-21.1	-2.4	-	-	-	-
118	94	C	E6207b		176.05	389.80	298.15	0.02	-	-	-	-	39.5	41.6	2.1	5.3
119	95	C	E6208a		174.25	385.15	298.15	1.0	866.0	848.9	-17.2	-2.0	40.7	41.4	0.7	1.6
120	96	C	E6209a		-	400.55	298.15	1.0	885.2	867.1	-18.1	-2.0	43.7	44.9	1.1	2.6
121	97	C	E6210a		176.15	394.65	298.15	1.0	873.8	847.7	-26.1	-3.0	42.0	42.6	0.6	1.3
122	98	C	E6211a		197.25	395.65	298.15	1.0	876.4	845.0	-31.4	-3.6	43.2	42.1	-1.1	-2.5
123	99	C	E6212a		196.15	399.15	298.15	1.0	876.4	860.1	-16.2	-1.9	42.7	44.0	1.4	3.2
124	100	C	E5402a		211.15	454.55	298.15	1.0	1146.7	1103.6	-43.1	-3.8	57.5	57.2	-0.3	-0.6
125	101	C	E5403a		-	437.65	298.15	1.0	1135.5	1083.3	-52.2	-4.6	56.4	55.0	-1.4	-2.5
126	102	C	E6401a		-	447.15	298.15	1.0	1093.6	1048.9	-44.8	-4.1	-	-	-	-
127	102	C	E6401b		-	447.15	293.0	1.0	-	-	-	-	57.8	59.3	1.5	2.5
128	103	C	E6402a		-	-	352.0	1.0	-	-	-	-	52.9	52.3	-0.6	-1.2
129	104	C	E6403a		292.05	442.15	298.15	1.0	1070.0	1022.6	-47.4	-4.4	59.0	54.7	-4.3	-7.3
130	105	C	E6405a		291.75	469.55	298.15	1.0	1114.0	1068.2	-45.9	-4.1	60.9	61.7	0.8	1.4
131	106	C	E6406a	×	-	-	350.0	1.0	-	-	-	-	68.0	57.1	-10.9	-16.0
132	107	C	E6407a	×	-	452.15	452.15	1.0	-	-	-	-	39.3	47.6	8.3	21.1
133	108	C	E6408a		242.15	463.65	298.15	1.0	1098.7	1060.5	-38.2	-3.5	61.0	63.1	2.1	3.4
134	109	C	F2201a		173.45	304.90	298.15	1.0	966.8	948.2	-18.6	-1.9	28.4	28.4	-0.1	-0.2
135	110	C	F3201a		193.55	327.46	298.15	1.0	915.9	896.8	-19.1	-2.1	31.5	30.7	-0.8	-2.4
136	111	C	F4201a		-	341.25	298.15	0.17	870.2	856.5	-13.8	-1.6	31.6	34.2	2.6	8.4
137	112	C	F4202a		180.25	353.97	298.15	1.0	899.9	882.0	-17.9	-2.0	36.6	34.9	-1.7	-4.5
138	113	C	F5201a		-	355.95	298.15	0.09	871.9	862.2	-9.7	-1.1	33.6	36.4	2.8	8.3
139	114	C	F5202a		177.65	371.22	298.15	1.0	875.7	865.7	-10.0	-1.1	-	-	-	-
140	114	C	F5202b		177.65	371.22	298.15	0.05	-	-	-	-	36.1	37.6	1.4	4.0
141	115	C	F5203a		-	363.55	298.15	0.06	878.6	869.2	-9.4	-1.1	36.8	37.1	0.3	0.8
142	116	C	F5204a		183.15	379.25	298.15	1.0	887.6	878.6	-9.0	-1.0	40.5	39.5	-1.0	-2.4

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m	T_b	T	P	ρ_{liq}[kg·m^{-3}]				ΔH_{vap}[kJ·mol^{-1}]			
					[K]	[K]	[K]	[bar]	exp	sim	dev	err [%]	exp	sim	dev	err [%]
143	117	C	F6202a		-	385.65	298.15	0.02	883.7	878.8	-4.9	-0.6	-	-	-	-
144	118	C	F6205a		-	393.76	298.15	0.02	874.3	868.6	-5.6	-0.6	-	-	-	-
145	119	C	F6206a		179.65	397.15	298.15	1.0	877.0	867.9	-9.2	-1.0	-	-	-	-
146	119	C	F6206b		179.65	397.15	298.85	0.01	-	-	-	-	40.8	42.5	1.7	4.2
147	120	C	F6208a		200.15	406.60	298.15	1.0	880.4	872.0	-8.4	-0.9	45.2	44.4	-0.8	-1.8
148	121	C	F4401a		-	447.15	273.15	1.0	1193.0	1185.5	-7.5	-0.6	-	-	-	-
149	121	C	F4401b		-	447.15	447.15	1.0	-	-	-	-	38.8	45.9	7.0	18.1
150	122	C	F5401a	×	-	348.15	348.15	1.0	-	-	-	-	29.5	53.4	23.9	81.1
151	123	C	L1101a	×	175.65	337.85	298.15	1.01	786.7	885.0	98.3	12.5	37.7	42.0	4.3	11.4
152	124	C	L2101a		159.01	351.44	298.15	1.01	786.6	804.9	18.3	2.3	42.3	43.1	0.9	2.0
153	125	C	L3101a		185.24	355.41	298.15	1.0	781.2	733.2	-48.0	-6.1	44.4	43.6	-0.8	-1.9
154	126	C	L3102a		148.76	370.35	298.15	1.0	799.8	796.0	-3.8	-0.5	46.6	46.6	0.0	0.0
155	127	C	L4101a		298.96	355.57	299.15	1.0	779.5	736.2	-43.3	-5.5	46.2	44.9	-1.3	-2.8
156	128	C	L4102a		171.19	380.81	298.15	1.0	797.8	781.4	-16.4	-2.1	50.8	48.2	-2.6	-5.0
157	129	C	L4103a		184.71	372.70	298.15	1.01	803.0	760.0	-43.0	-5.4	48.5	48.4	-0.1	-0.2
158	130	C	L4104a		184.55	390.81	298.15	1.0	805.8	799.9	-5.9	-0.7	52.1	51.4	-0.7	-1.4
159	131	C	L5101a		328.15	386.25	327.15	0.08	780.0	770.7	-9.3	-1.2	-	-	-	-
160	131	C	L5101b		328.15	386.25	345.0	1.0	-	-	-	-	47.5	43.7	-3.8	-8.1
161	132	C	L5102a		264.45	375.15	298.15	1.0	804.7	777.6	-27.1	-3.4	50.1	50.2	0.1	0.2
162	133	C	L5103a		-	384.65	298.15	1.0	815.0	773.1	-41.9	-5.1	-	-	-	-
163	134	C	L5104a		-	401.85	298.15	1.0	815.2	801.0	-14.2	-1.8	54.1	53.3	-0.8	-1.4
164	135	C	L5105a		203.25	388.45	298.15	1.0	815.4	779.1	-36.3	-4.5	52.9	53.6	0.8	1.4
165	136	C	L5106a		155.95	404.35	298.15	1.0	806.9	796.3	-10.6	-1.3	55.3	54.5	-0.8	-1.5
166	137	C	L5107a		200.15	392.15	298.15	1.01	805.3	773.2	-32.1	-4.0	53.6	53.5	-0.1	-0.1
167	138	C	L5108a		195.57	410.95	298.15	1.0	811.3	803.9	-7.5	-0.9	56.9	56.0	-0.9	-1.5
168	139	C	L6101a		-	393.15	298.15	0.01	813.9	808.3	-5.6	-0.7	-	-	-	-
169	139	C	L6101b		-	393.15	298.0	1.0	-	-	-	-	53.8	54.1	0.3	0.5
170	140	C	L6102a		262.65	391.75	298.15	1.0	818.6	807.9	-10.7	-1.3	54.0	54.2	0.2	0.3
171	141	C	L6103a		-	409.95	298.15	1.0	824.5	822.3	-2.2	-0.3	-	-	-	-
172	141	C	L6103b		-	409.95	313.0	1.0	-	-	-	-	52.1	53.0	0.9	1.7
173	142	C	L6104a		249.55	395.56	298.15	1.0	823.8	809.1	-14.7	-1.8	55.7	55.3	-0.4	-0.7
174	143	C	L6105a		213.15	416.15	298.15	1.0	809.7	816.1	6.4	0.8	58.0	57.1	-0.9	-1.6
175	144	C	L6106a		170.15	394.56	298.15	1.0	809.5	789.1	-20.3	-2.5	54.7	55.2	0.5	0.9
176	145	C	L6107a		-	422.15	298.15	1.0	823.7	812.7	-11.0	-1.3	-	-	-	-
177	145	C	L6107b		-	422.15	339.0	1.0	-	-	-	-	51.4	52.4	1.0	1.9
178	146	C	L6108a		-	407.36	298.15	1.0	824.7	796.2	-28.5	-3.5	58.2	57.2	-1.0	-1.8
179	147	C	L6109a		-	399.66	298.15	1.0	820.1	793.3	-26.9	-3.3	56.0	56.9	0.9	1.6
180	148	C	L6110a		183.15	404.85	298.15	1.0	803.0	782.0	-21.1	-2.6	-	-	-	-
181	148	C	L6110b		183.15	404.85	308.0	1.0	-	-	-	-	49.6	56.1	6.5	13.0
182	149	C	L6111a		-	419.65	298.15	1.0	829.3	815.4	-13.9	-1.7	60.3	58.4	-1.9	-3.2
183	150	C	L6112a		-	425.55	298.15	1.0	820.5	812.5	-8.0	-1.0	61.7	59.6	-2.1	-3.4
184	151	C	L6113a		-	421.15	298.15	1.0	820.6	806.6	-14.1	-1.7	59.4	58.3	-1.1	-1.9
185	152	C	L6114a		-	408.55	298.15	1.0	814.5	789.1	-25.4	-3.1	58.6	58.7	0.1	0.2
186	153	C	L6115a		-	424.95	298.15	1.0	809.7	801.0	-8.7	-1.1	-	-	-	-
187	153	C	L6115b		-	424.95	313.0	1.0	-	-	-	-	63.9	57.7	-6.2	-9.7
188	154	C	L6116a		-	413.04	298.15	1.0	810.3	781.6	-28.8	-3.5	58.3	58.4	0.1	0.2
189	155	C	L6117a		226.75	430.15	298.15	1.0	815.5	808.1	-7.5	-0.9	59.6	61.0	1.4	2.4
190	156	C	L2201a		260.15	470.45	298.15	1.0	1109.9	1083.0	-27.0	-2.4	64.8	68.4	3.6	5.6

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
191	157	C	L3201a	×	213.15	460.75	298.15	1.0	1032.5	985.7	-46.8	-4.5	62.2	71.2	9.0	14.5
192	158	C	L3202a		245.55	487.55	298.15	1.0	1050.3	1062.6	12.3	1.2	69.8	75.6	5.8	8.3
193	159	C	L4201a		-	451.15	298.15	1.0	989.6	972.9	-16.7	-1.7	-	-	-	-
194	160	C	L4202a		-	455.15	298.15	1.0	999.8	952.9	-46.9	-4.7	-	-	-	-
195	160	C	L4202b	×	-	455.15	332.0	1.0	-	-	-	-	58.4	67.6	9.2	15.8
196	161	C	L4203a		182.15	487.15	293.15	1.0	1009.0	1002.1	-6.9	-0.7	71.3	74.6	3.3	4.6
197	162	C	L4204a		-	464.15	298.15	1.0	999.2	976.8	-22.4	-2.2	-	-	-	-
198	163	C	L4205a		196.15	480.15	298.15	1.0	1000.2	974.4	-25.8	-2.6	72.6	72.1	-0.5	-0.7
199	164	C	L4206a		293.58	501.15	298.15	1.0	1015.4	1021.7	6.3	0.6	76.6	81.4	4.8	6.2
200	165	C	L5201a		-	447.15	298.15	1.0	968.8	948.0	-20.8	-2.1	-	-	-	-
201	166	C	L5204a		-	472.15	293.15	1.0	964.5	943.5	-21.1	-2.2	-	-	-	-
202	167	C	L5205a		-	473.15	293.15	1.0	991.7	953.7	-38.0	-3.8	-	-	-	-
203	168	C	L5206a		-	473.15	294.65	1.0	984.2	954.8	-29.4	-3.0	-	-	-	-
204	169	C	L5207a		-	460.65	292.15	1.0	979.8	947.4	-32.5	-3.3	-	-	-	-
205	170	C	L5208a		-	472.15	298.15	1.0	956.0	921.6	-34.4	-3.6	72.5	70.3	-2.2	-3.0
206	171	C	L5211a		-	494.15	293.15	1.0	981.0	959.4	-21.6	-2.2	-	-	-	-
207	172	C	L5212a		-	482.15	297.15	1.0	969.1	956.0	-13.1	-1.4	74.6	80.1	5.5	7.4
208	173	C	L5213a		-	497.00	293.15	1.0	989.5	960.5	-29.0	-2.9	-	-	-	-
209	174	C	L5214a		253.15	512.15	298.15	1.0	989.7	987.8	-2.0	-0.2	86.8	89.4	2.6	3.0
210	175	C	L6201a		316.45	445.95	316.45	0.002	970.4	952.1	-18.3	-1.9	-	-	-	-
211	176	C	L6204a		-	505.76	298.15	1.0	963.8	942.9	-20.9	-2.2	-	-	-	-
212	177	C	L6205a		-	478.65	323.15	1.0	940.0	942.4	2.4	0.2	-	-	-	-
213	178	C	L6206a		-	480.00	298.15	1.0	964.5	933.2	-31.3	-3.2	-	-	-	-
214	179	C	L6207a		-	505.76	293.15	1.0	962.7	940.1	-22.6	-2.3	-	-	-	-
215	180	C	L6208a		223.15	470.65	298.15	1.0	918.5	887.5	-31.0	-3.4	68.6	62.8	-5.8	-8.4
216	181	C	L6209a		-	484.65	287.15	1.0	990.6	919.4	-71.2	-7.2	-	-	-	-
217	182	C	L6210a		-	498.95	323.15	1.0	958.2	961.7	3.5	0.4	-	-	-	-
218	183	C	L6212a		-	480.00	277.15	1.0	996.0	999.4	3.4	0.3	-	-	-	-
219	184	C	L6213a		-	482.98	293.15	1.0	969.0	943.3	-25.7	-2.6	-	-	-	-
220	185	C	L6215a		-	494.35	293.15	1.0	964.5	951.5	-13.0	-1.4	-	-	-	-
221	186	C	L6216a		-	496.94	293.15	1.0	976.8	965.8	-11.0	-1.1	-	-	-	-
222	187	C	L6217a		-	480.00	298.15	1.0	967.7	943.8	-23.9	-2.5	-	-	-	-
223	188	C	L6218a		-	-	293.15	1.0	977.1	979.1	2.0	0.2	-	-	-	-
224	189	C	L6219a		-	493.45	295.15	1.0	973.7	940.6	-33.1	-3.4	-	-	-	-
225	190	C	L6220a	×	-	496.94	273.15	1.0	799.3	940.7	141.4	17.7	-	-	-	-
226	191	C	L6221a		-	478.15	288.15	1.0	989.0	927.7	-61.3	-6.2	-	-	-	-
227	192	C	L6222a		-	484.15	294.15	1.0	951.6	916.1	-35.5	-3.7	-	-	-	-
228	193	C	L6223a		316.15	493.95	323.15	1.0	939.8	897.8	-42.0	-4.5	-	-	-	-
229	194	C	L6224a		-	474.16	298.15	1.0	963.6	955.9	-7.7	-0.8	-	-	-	-
230	195	C	L6225a		-	521.55	293.15	1.0	972.6	973.8	1.1	0.1	-	-	-	-
231	196	C	L6226a		-	496.94	293.15	1.0	971.9	967.5	-4.4	-0.5	-	-	-	-
232	197	C	L6227a		-	508.15	295.15	1.0	958.0	940.7	-17.3	-1.8	-	-	-	-
233	198	C	L6228a		-	529.15	289.45	1.0	982.0	950.7	-31.3	-3.2	-	-	-	-
234	199	C	L6230a		-	510.15	298.15	1.0	964.0	941.3	-22.7	-2.4	-	-	-	-
235	200	C	L6231a		314.65	516.15	318.15	1.0	968.3	950.9	-17.4	-1.8	-	-	-	-
236	200	C	L6231b		314.65	516.15	342.0	1.0	-	-	-	-	87.0	86.9	-0.1	-0.1
237	201	C	L3301a		291.35	563.15	298.15	1.0	1258.3	1189.5	-68.8	-5.5	-	-	-	-
238	201	C	L3301b		291.35	563.15	308.0	1.0	-	-	-	-	85.8	87.7	1.9	2.2

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
239	202	C	L4302a		-	-	298.15	1.0	1184.0	1146.3	-37.7	-3.2	-	-	-	-
240	203	C	L5303a		-	460.64	298.15	1.0	1103.6	1117.8	14.2	1.3	-	-	-	-
241	204	C	L6306a		-	-	293.15	1.0	1104.1	1089.9	-14.2	-1.3	-	-	-	-
242	205	C	L6307a		-	472.47	298.15	1.0	1100.0	1071.3	-28.6	-2.6	-	-	-	-
243	206	C	C1201a		281.45	373.71	298.15	1.0	1213.6	1207.0	-6.6	-0.5	46.3	44.0	-2.3	-4.9
244	207	C	C2201a		290.15	391.05	298.15	1.01	1043.5	1073.5	30.0	2.9	50.3	50.1	-0.2	-0.4
245	208	C	C3201a		252.65	414.32	298.15	1.01	988.1	988.2	0.1	0.0	54.9	54.0	-0.9	-1.6
246	209	C	C4201a		227.15	427.55	298.15	1.0	943.9	931.9	-12.0	-1.3	56.3	56.7	0.4	0.7
247	210	C	C4202a		268.03	436.85	298.15	1.0	952.9	959.2	6.2	0.7	58.2	59.1	0.9	1.6
248	211	C	C5201a		309.15	436.95	309.82	1.0	907.5	920.3	12.8	1.4	-	-	-	-
249	211	C	C5201b		309.15	436.95	320.0	1.0	-	-	-	-	57.6	56.2	-1.4	-2.4
250	212	C	C5202a		-	450.15	298.15	1.0	934.7	930.2	-4.5	-0.5	-	-	-	-
251	213	C	C5203a		243.55	448.25	298.15	1.0	924.1	930.7	6.6	0.7	61.2	62.1	0.9	1.5
252	214	C	C5204a		239.52	458.65	298.15	1.0	934.4	940.7	6.3	0.7	63.0	64.3	1.4	2.1
253	215	C	C6201a		258.15	459.15	293.15	1.0	927.5	944.7	17.2	1.9	-	-	-	-
254	215	C	C6201b		258.15	459.15	370.0	1.0	-	-	-	-	59.4	57.3	-2.1	-3.6
255	216	C	C6202a		279.15	457.15	298.05	1.0	908.0	933.1	25.1	2.8	64.0	64.0	-0.1	-0.1
256	217	C	C6203a		-	464.85	293.15	1.0	927.5	930.2	2.7	0.3	-	-	-	-
257	218	C	C6204a		241.35	466.15	298.15	1.0	923.5	927.0	3.5	0.4	-	-	-	-
258	218	C	C6204b		241.35	466.15	388.0	1.0	-	-	-	-	58.2	59.1	0.9	1.6
259	219	C	C6205a		-	-	298.15	1.0	918.2	920.7	2.5	0.3	-	-	-	-
260	220	C	C6206a		-	-	298.15	1.0	923.0	930.7	7.7	0.8	-	-	-	-
261	221	C	C6207a		240.15	473.65	298.15	1.0	917.0	921.6	4.6	0.5	-	-	-	-
262	221	C	C6207b	×	240.15	473.65	354.0	1.0	-	-	-	-	91.7	63.1	-28.6	-31.2
263	222	C	C6208a		269.05	478.85	298.15	1.0	922.9	928.2	5.3	0.6	69.2	69.5	0.3	0.4
264	223	C	M1101a		179.73	266.82	266.85	1.0	694.2	761.5	67.3	9.7	26.1	27.8	1.7	6.5
265	223	C	M1101b		179.73	266.82	298.15	3.52	655.0	698.8	43.8	6.7	-	-	-	-
266	224	C	M2101a		192.15	289.73	288.15	1.0	688.6	701.3	12.8	1.9	27.4	27.5	0.1	0.6
267	225	C	M3101a		178.03	305.55	298.15	1.01	683.9	659.3	-24.7	-3.6	28.4	26.6	-1.8	-6.3
268	226	C	M3102a		188.37	321.65	298.15	1.01	712.8	713.9	1.2	0.2	31.3	30.4	-0.9	-2.8
269	227	C	M4101a		206.23	317.55	298.15	1.0	690.1	655.1	-35.0	-5.1	29.6	23.5	-6.1	-20.6
270	228	C	M4102a		-	336.15	298.15	1.01	717.8	702.4	-15.4	-2.1	32.6	31.0	-1.6	-4.8
271	229	C	M4103a		187.15	340.88	298.15	1.0	729.1	716.1	-13.0	-1.8	33.8	31.9	-1.9	-5.6
272	230	C	M4104a		224.15	350.55	298.15	1.0	736.8	735.6	-1.3	-0.2	35.6	35.1	-0.5	-1.3
273	231	C	M5101a		168.15	350.15	298.15	0.11	727.6	706.8	-20.8	-2.9	32.5	28.6	-3.8	-11.8
274	232	C	M5102a		-	350.15	298.15	0.1	728.1	738.0	9.9	1.4	33.4	32.7	-0.7	-2.0
275	233	C	M5103a		223.15	357.15	298.15	0.08	753.0	724.6	-28.4	-3.8	33.9	33.8	-0.1	-0.1
276	234	C	M5104a		-	362.15	291.35	1.0	711.3	739.2	27.9	3.9	-	-	-	-
277	234	C	M5104b		-	362.15	298.15	0.06	-	-	-	-	34.6	35.3	0.7	2.1
278	235	C	M5105a		-	368.65	298.15	1.0	750.5	746.1	-4.3	-0.6	-	-	-	-
279	235	C	M5105b		-	368.65	298.15	0.04	-	-	-	-	35.6	37.0	1.4	3.9
280	236	C	M5106a		-	364.85	298.15	0.05	735.7	725.3	-10.4	-1.4	34.8	35.8	1.0	2.8
281	237	C	M5107a		-	370.15	298.15	1.0	744.3	744.3	-0.0	-0.0	-	-	-	-
282	237	C	M5107b		-	370.15	298.15	0.04	-	-	-	-	35.1	38.5	3.4	9.6
283	238	C	M5108a		222.15	377.65	298.15	0.04	751.0	751.2	0.2	0.0	-	-	-	-
284	238	C	M5108b		222.15	377.65	298.0	1.0	-	-	-	-	40.1	39.9	-0.2	-0.4
285	239	C	M6101a		-	377.65	298.15	0.03	760.1	745.3	-14.7	-1.9	-	-	-	-
286	240	C	M6102a		253.15	375.15	298.15	0.04	760.1	759.9	-0.2	-0.0	36.1	35.7	-0.4	-1.1

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
287	241	C	M6103a		-	398.45	300.86	0.01	757.9	741.7	-16.1	-2.1	-	-	-	-
288	242	C	M6104a		-	386.65	298.15	0.02	760.1	773.7	13.6	1.8	-	-	-	-
289	243	C	M6105a		-	377.15	298.15	0.03	743.0	729.4	-13.6	-1.8	36.1	33.5	-2.6	-7.2
290	244	C	M6106a		-	405.98	306.83	0.01	753.1	761.4	8.3	1.1	-	-	-	-
291	245	C	M6107a		-	408.33	308.71	0.01	741.7	736.0	-5.6	-0.8	-	-	-	-
292	246	C	M6108a		-	408.33	308.71	0.01	741.7	741.1	-0.5	-0.1	-	-	-	-
293	247	C	M6109a		-	378.15	298.15	0.03	752.8	768.2	15.4	2.0	-	-	-	-
294	248	C	M6110a		-	381.65	298.15	0.02	745.7	740.4	-5.3	-0.7	37.4	39.2	1.8	4.9
295	249	C	M6111a		398.15	408.77	309.07	0.01	751.3	758.7	7.4	1.0	-	-	-	-
296	250	C	M6112a		-	408.77	309.07	0.01	761.1	734.6	-26.5	-3.5	-	-	-	-
297	251	C	M6113a		-	400.00	302.05	0.01	759.8	757.5	-2.3	-0.3	-	-	-	-
298	252	C	M6114a		-	395.15	298.15	0.01	767.0	767.8	0.8	0.1	-	-	-	-
299	253	C	M6115a		-	403.15	305.93	0.01	756.7	732.0	-24.6	-3.3	38.2	39.6	1.4	3.7
300	254	C	M6116a		-	397.05	301.25	0.01	767.5	753.4	-14.1	-1.8	39.8	42.6	2.8	6.9
301	255	C	M6117a		252.15	404.65	298.15	1.0	763.0	763.5	0.5	0.1	45.0	44.7	-0.3	-0.7
302	256	C	N2101a		180.15	280.03	282.82	1.0	667.9	731.0	63.1	9.4	27.2	27.1	-0.1	-0.4
303	256	C	N2101b		180.15	280.03	298.15	1.96	650.0	705.5	55.5	8.6	-	-	-	-
304	257	C	N3101a		-	309.15	298.15	0.65	684.0	700.5	16.5	2.4	26.7	28.2	1.5	5.8
305	258	C	N4101a		-	323.55	288.15	1.0	740.0	701.3	-38.7	-5.2	30.7	29.3	-1.4	-4.4
306	259	C	N4102a		223.15	328.60	298.15	1.0	701.2	707.2	6.0	0.9	31.2	30.8	-0.4	-1.4
307	260	C	N4103a		-	336.15	298.15	0.2	711.9	719.5	7.6	1.1	31.1	31.8	0.6	1.9
308	261	C	N5101a		-	350.15	298.15	1.0	727.0	743.0	16.0	2.2	32.3	29.5	-2.8	-8.6
309	262	C	N5102a		-	351.65	298.15	0.1	720.0	719.8	-0.2	-0.0	33.3	32.8	-0.5	-1.5
310	263	C	N5103a		-	346.15	298.15	0.12	730.0	719.2	-10.8	-1.5	-	-	-	-
311	264	C	N5104a		-	349.15	298.15	0.13	720.0	703.1	-16.9	-2.4	-	-	-	-
312	264	C	N5104b		-	349.15	298.0	1.0	-	-	-	-	33.1	31.6	-1.5	-4.5
313	265	C	N5105a		-	353.45	298.15	0.11	726.7	720.9	-5.8	-0.8	31.9	34.4	2.5	8.0
314	266	C	N5106a		-	364.25	298.15	0.05	728.1	735.6	7.5	1.0	-	-	-	-
315	266	C	N5106b		-	364.25	298.0	1.0	-	-	-	-	38.1	36.4	-1.7	-4.4
316	267	C	N6101a		-	383.62	298.15	0.02	740.1	737.5	-2.6	-0.3	-	-	-	-
317	268	C	N6102a		-	351.15	298.15	1.0	716.1	761.6	45.5	6.3	-	-	-	-
318	268	C	N6102b		-	351.15	298.15	0.1	-	-	-	-	34.1	33.8	-0.3	-0.8
319	269	C	N6103a		-	386.41	298.15	0.02	740.1	736.5	-3.5	-0.5	-	-	-	-
320	270	C	N6104a		212.15	357.05	298.15	1.0	712.3	715.2	2.9	0.4	34.5	34.1	-0.4	-1.2
321	271	C	N6105a		-	381.15	298.15	0.03	740.1	741.8	1.7	0.2	37.4	37.0	-0.4	-1.0
322	272	C	N6106a		-	371.15	298.15	0.04	729.8	725.1	-4.7	-0.6	-	-	-	-
323	272	C	N6106b		-	371.15	298.0	1.0	-	-	-	-	37.9	35.9	-2.0	-5.2
324	273	C	N6107a		-	371.45	298.15	0.04	723.2	716.3	-6.9	-0.9	-	-	-	-
325	273	C	N6107b		-	371.45	298.0	1.0	-	-	-	-	37.3	35.6	-1.7	-4.5
326	274	C	N6108a		-	386.41	298.15	0.02	740.1	744.0	4.0	0.5	-	-	-	-
327	275	C	N6109a		-	371.15	298.15	0.04	730.0	720.9	-9.2	-1.2	36.1	36.0	-0.1	-0.3
328	276	C	N6110a		-	-	295.15	1.0	739.0	746.9	7.9	1.1	-	-	-	-
329	277	C	N6111a		210.15	382.00	298.15	1.0	734.9	731.1	-3.8	-0.5	40.0	38.3	-1.7	-4.2
330	278	C	N6112a		-	381.15	298.15	0.02	735.4	734.9	-0.6	-0.1	-	-	-	-
331	278	C	N6112b		-	381.15	298.0	1.0	-	-	-	-	40.2	39.2	-1.0	-2.6
332	279	C	N6113a		-	390.55	298.15	0.02	743.0	747.9	4.9	0.7	39.9	41.1	1.2	2.9
333	280	C	R3101a	×	156.05	276.02	273.15	1.0	655.7	743.8	88.0	13.4	22.9	28.5	5.6	24.3
334	280	C	R3101b	×	156.05	276.02	298.15	2.33	628.9	718.0	89.1	14.2	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
335	281	C	R4101a		133.15	310.15	298.15	1.0	669.4	727.1	57.7	8.6	-	-	-	-
336	281	C	R4101b		133.15	310.15	298.15	0.67	-	-	-	-	26.7	30.9	4.2	15.9
337	282	C	R5101a		-	339.18	298.15	1.0	710.6	729.5	18.9	2.7	31.9	32.8	0.9	2.8
338	283	C	R5102a		77.15	339.15	298.15	1.0	701.5	735.9	34.4	4.9	31.8	34.5	2.7	8.4
339	284	C	R5103a		-	339.15	298.15	0.21	695.6	742.5	46.9	6.8	31.1	35.5	4.4	14.0
340	285	C	R6101a		-	363.15	298.15	1.0	737.6	758.7	21.1	2.9	34.8	35.0	0.1	0.4
341	286	C	R6102a		-	367.15	298.15	0.05	733.9	752.6	18.7	2.5	35.4	37.5	2.2	6.2
342	287	C	R6103a		-	364.65	298.15	0.06	721.5	739.5	18.1	2.5	35.0	36.5	1.5	4.2
343	288	C	R6104a		-	354.15	298.15	0.1	720.0	747.0	27.0	3.8	33.1	38.0	5.0	14.9
344	289	C	R6105a		158.45	361.92	298.15	1.01	723.0	746.2	23.2	3.2	-	-	-	-
345	289	C	R6105b		158.45	361.92	298.15	0.06	-	-	-	-	34.9	37.9	2.9	8.4
346	290	C	R6106a		-	364.65	298.15	0.06	718.0	747.9	29.9	4.2	35.0	38.9	3.9	11.1
347	291	C	R6107a		-	367.15	298.15	0.06	716.0	755.3	39.3	5.5	35.3	40.3	5.0	14.2
348	292	C	N2201a		284.29	390.41	298.15	0.02	892.8	971.8	78.9	8.8	-	-	-	-
349	292	C	N2201b		284.29	390.41	298.0	1.0	-	-	-	-	45.0	49.0	4.0	9.0
350	293	C	N3201a		-	388.15	298.15	1.0	841.0	899.0	58.0	6.9	-	-	-	-
351	293	C	N3201b		-	388.15	388.15	1.0	-	-	-	-	33.2	36.9	3.6	11.0
352	294	C	N3202a		-	392.45	298.15	0.02	856.0	882.5	26.5	3.1	-	-	-	-
353	294	C	N3202b		-	392.45	298.0	1.0	-	-	-	-	44.2	46.4	2.2	4.9
354	295	C	N3203a		262.25	412.95	298.15	1.0	884.0	919.9	35.9	4.1	50.2	48.4	-1.8	-3.6
355	296	C	N4201a	×	-	378.65	298.15	1.0	803.0	886.9	83.8	10.4	-	-	-	-
356	296	C	N4201b	×	-	378.65	378.65	1.0	-	-	-	-	31.1	41.0	9.9	31.8
357	297	C	N4202a		-	393.15	288.15	1.0	828.0	886.7	58.7	7.1	-	-	-	-
358	297	C	N4202b		-	393.15	393.15	1.0	-	-	-	-	35.0	38.1	3.1	8.9
359	298	C	N4203a		-	396.15	298.15	1.0	841.0	849.8	8.8	1.1	45.8	40.6	-5.2	-11.4
360	299	C	N4204a		-	402.15	298.15	1.0	837.0	861.5	24.5	2.9	-	-	-	-
361	299	C	N4204b		-	402.15	373.0	1.0	-	-	-	-	43.0	39.9	-3.1	-7.2
362	300	C	N4205a		-	413.15	298.0	1.0	-	-	-	-	53.1	47.2	-5.8	-11.0
363	301	C	N4206a		-	-	298.0	1.0	-	-	-	-	46.9	50.1	3.2	6.8
364	302	C	N4207a	×	-	419.15	419.15	1.0	-	-	-	-	43.7	33.3	-10.5	-23.9
365	303	C	N4208a		295.05	431.65	298.15	1.0	877.0	900.8	23.8	2.7	55.2	54.5	-0.7	-1.2
366	304	C	N5201a	×	-	356.15	291.15	1.0	749.1	854.9	105.8	14.1	-	-	-	-
367	304	C	N5201b	×	-	356.15	298.0	1.0	-	-	-	-	33.1	44.4	11.3	34.2
368	305	C	N5202a	×	-	390.15	390.15	1.0	-	-	-	-	29.7	41.3	11.6	39.1
369	306	C	N5203a		-	406.65	293.15	1.0	827.2	872.9	45.7	5.5	42.2	48.7	6.5	15.5
370	307	C	N5204a		-	418.15	418.15	1.0	-	-	-	-	36.9	37.0	0.1	0.2
371	308	C	N5205a		-	409.15	409.15	1.0	-	-	-	-	34.3	35.6	1.2	3.6
372	309	C	N5206a		-	426.15	426.15	1.0	-	-	-	-	39.4	33.2	-6.2	-15.7
373	310	C	N5207a		-	421.65	421.65	1.0	-	-	-	-	38.0	37.1	-0.8	-2.2
374	311	C	N5208a		-	437.15	298.0	1.0	-	-	-	-	54.9	50.2	-4.7	-8.6
375	312	C	N5209a		284.95	452.15	298.15	1.0	873.0	886.9	13.9	1.6	58.7	58.7	-0.0	-0.0
376	313	C	N6201a	×	215.15	394.15	298.15	1.0	770.0	846.6	76.7	9.9	41.4	50.6	9.2	22.2
377	314	C	N6202a	×	-	407.65	298.15	1.0	738.0	836.8	98.8	13.4	-	-	-	-
378	314	C	N6202b		-	407.65	407.65	1.0	-	-	-	-	35.1	42.4	7.3	20.8
379	315	C	N6203a	×	-	414.15	414.15	1.0	-	-	-	-	30.6	41.5	10.9	35.6
380	316	C	N6205a	×	-	417.15	293.15	1.0	828.0	858.9	30.9	3.7	45.8	54.7	8.9	19.4
381	317	C	N6206a		-	419.15	293.15	1.0	828.0	827.2	-0.8	-0.1	-	-	-	-
382	317	C	N6206b	×	-	419.15	419.15	1.0	-	-	-	-	31.7	39.8	8.1	25.5

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
383	318	C	N6207a		-	435.15	435.15	1.0	-	-	-	-	35.8	35.0	-0.8	-2.2
384	319	C	N6208a		-	442.15	442.15	1.0	-	-	-	-	37.9	37.1	-0.8	-2.0
385	320	C	N6209a		-	431.15	431.15	1.0	-	-	-	-	34.8	40.0	5.2	15.1
386	321	C	N6210a		-	466.15	298.0	1.0	-	-	-	-	60.9	60.1	-0.8	-1.4
387	322	C	N6211a		311.95	475.04	298.0	1.0	-	-	-	-	63.1	62.8	-0.3	-0.5
388	323	C	D2401a		353.31	494.3	354.2	0.004	1002.0	1013.8	11.8	1.2	-	-	-	-
389	323	C	D2401b	×	353.31	494.3	396.0	1.0	-	-	-	-	63.8	52.0	-11.8	-18.6
390	324	C	D3401a		353.05	486.15	355.65	1.01	963.2	937.6	-25.6	-2.6	-	-	-	-
391	324	C	D3401b	×	353.05	486.15	390.0	1.0	-	-	-	-	63.9	54.8	-9.1	-14.2
392	325	C	D4401a		389.15	489.15	393.15	1.0	885.0	873.0	-12.0	-1.4	-	-	-	-
393	326	C	D5402a		410.15	499.15	499.15	1.0	-	-	-	-	43.8	50.3	6.5	14.8
394	327	C	D5403a		377.15	498.15	383.15	1.0	873.5	867.2	-6.3	-0.7	-	-	-	-
395	328	C	D6401a		374.15	528.15	528.15	1.0	-	-	-	-	46.6	53.0	6.4	13.7
396	329	C	D3301a		303.75	478.15	308.15	1.01	949.7	949.0	-0.7	-0.1	-	-	-	-
397	329	C	D3301b		303.75	478.15	348.0	1.0	-	-	-	-	54.4	53.7	-0.7	-1.2
398	330	C	D4301a		242.25	421.15	298.15	1.0	930.5	919.6	-10.9	-1.2	66.6	65.2	-1.4	-2.1
399	331	C	D4302a		-	478.15	277.15	1.0	942.0	958.1	16.1	1.7	-	-	-	-
400	331	C	D4302b		-	478.15	298.0	1.0	-	-	-	-	64.9	64.8	-0.1	-0.1
401	332	C	D5301a		-	-	298.0	1.0	-	-	-	-	67.1	67.3	0.2	0.2
402	333	C	D5302a		-	-	298.0	1.0	-	-	-	-	66.4	66.8	0.3	0.5
403	334	C	D5303a		-	-	298.0	1.0	-	-	-	-	69.8	69.3	-0.5	-0.8
404	335	C	D6303a		-	502.15	298.15	1.0	896.0	904.9	8.9	1.0	76.1	68.2	-7.9	-10.4
405	336	C	D4201a		254.15	439.25	298.15	1.01	936.7	940.6	3.9	0.4	50.7	50.1	-0.5	-1.1
406	337	C	D5201a		228.15	444.65	298.15	1.01	920.3	912.2	-8.2	-0.9	-	-	-	-
407	338	C	D6202a		233.15	459.15	298.15	1.0	906.4	899.4	-7.0	-0.8	-	-	-	-
408	339	C	D6203a		-	458.65	290.15	1.0	913.0	899.9	-13.2	-1.4	53.7	54.1	0.4	0.8
409	340	V	O7101a		184.85	378.66	298.15	1.0	736.4	730.4	-6.0	-0.8	34.5	36.1	1.6	4.6
410	341	V	O7102a		-	375.15	298.15	1.0	761.8	753.8	-8.0	-1.0	38.2	38.9	0.7	1.8
411	342	V	O7103a		-	373.15	298.15	1.0	746.7	734.2	-12.4	-1.7	37.2	37.7	0.5	1.2
412	343	V	O7104a		-	371.20	298.15	1.0	734.9	712.2	-22.7	-3.1	-	-	-	-
413	344	V	O7105a		-	-	298.15	1.0	739.6	723.8	-15.8	-2.1	-	-	-	-
414	345	V	O7106a		-	385.65	298.15	1.0	752.1	737.7	-14.4	-1.9	-	-	-	-
415	346	V	O7107a		-	378.15	298.15	1.0	744.0	727.7	-16.3	-2.2	-	-	-	-
416	346	V	O7107b		-	378.15	298.15	0.03	-	-	-	-	38.1	38.5	0.4	1.1
417	347	V	O7108a		-	-	298.15	1.0	750.1	733.3	-16.8	-2.2	-	-	-	-
418	348	V	O7109a		-	380.15	298.15	1.0	746.0	725.9	-20.1	-2.7	-	-	-	-
419	349	V	O7110a		-	398.15	298.15	1.0	766.3	756.6	-9.7	-1.3	-	-	-	-
420	350	V	O7111a		-	391.15	298.15	1.0	757.2	743.8	-13.4	-1.8	-	-	-	-
421	351	V	O7112a		-	390.15	298.15	1.0	754.2	740.3	-13.9	-1.8	-	-	-	-
422	352	V	O8101a		-	380.40	298.15	1.0	757.8	731.0	-26.8	-3.5	37.6	33.9	-3.7	-9.9
423	353	V	O8102a		-	-	298.0	1.0	-	-	-	-	41.6	40.8	-0.8	-1.9
424	354	V	O8103a		-	439.93	298.15	1.0	748.0	733.3	-14.7	-2.0	40.1	39.4	-0.7	-1.7
425	355	V	O8104a		-	-	298.15	1.0	757.1	748.5	-8.6	-1.1	-	-	-	-
426	356	V	O8105a		-	-	298.15	1.0	758.1	744.5	-13.6	-1.8	42.3	42.0	-0.3	-0.8
427	357	V	O8106a		-	395.85	298.15	1.0	745.2	727.1	-18.1	-2.4	41.2	40.6	-0.6	-1.5
428	358	V	O8107a		-	-	298.15	1.0	750.8	732.0	-18.9	-2.5	-	-	-	-
429	359	V	O8108a		-	-	298.15	1.0	754.5	732.4	-22.1	-2.9	-	-	-	-
430	360	V	O8109a		-	394.20	298.15	1.0	758.8	743.0	-15.8	-2.1	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
431	360	V	O8109b		-	394.20	298.15	0.02	-	-	-	-	40.0	41.1	1.1	2.9
432	361	V	O8110a		-	-	298.15	1.0	760.1	745.9	-14.2	-1.9	-	-	-	-
433	362	V	O8111a		-	424.15	298.15	1.0	755.2	739.8	-15.4	-2.0	-	-	-	-
434	362	V	O8111b		-	424.15	319.77	0.01	-	-	-	-	42.9	41.9	-1.0	-2.3
435	363	V	O8112a		-	-	298.15	1.0	761.1	744.9	-16.2	-2.1	-	-	-	-
436	364	V	O8113a		-	-	298.15	1.0	759.8	738.6	-21.2	-2.8	-	-	-	-
437	365	V	O8114a		-	424.15	298.15	1.0	775.6	765.4	-10.2	-1.3	46.9	47.9	1.0	2.1
438	366	V	O8115a		-	415.15	298.15	1.0	768.2	754.6	-13.6	-1.8	-	-	-	-
439	367	V	O8116a		-	-	298.15	1.0	765.3	751.6	-13.7	-1.8	-	-	-	-
440	368	V	O8117a		177.15	413.44	298.15	1.0	764.1	750.7	-13.4	-1.8	44.7	45.8	1.1	2.4
441	369	V	O9101a		-	-	298.15	1.01	792.4	785.5	-6.8	-0.9	-	-	-	-
442	369	V	O9101b		-	-	396.0	1.0	-	-	-	-	38.5	36.9	-1.6	-4.1
443	370	V	O9102a		-	-	298.15	1.0	761.6	747.6	-14.0	-1.8	-	-	-	-
444	371	V	O9103a		-	-	298.15	1.0	766.4	755.0	-11.4	-1.5	-	-	-	-
445	372	V	O9104a		-	-	298.15	1.0	759.4	745.1	-14.3	-1.9	-	-	-	-
446	373	V	O9105a		-	-	298.15	1.0	764.3	748.3	-16.0	-2.1	-	-	-	-
447	374	V	O9106a		-	-	298.15	1.0	767.6	754.9	-12.7	-1.7	-	-	-	-
448	375	V	O9107a		-	-	298.15	1.0	765.6	750.1	-15.5	-2.0	-	-	-	-
449	376	V	O9108a		-	-	298.15	1.0	802.1	767.0	-35.1	-4.4	-	-	-	-
450	377	V	O9109a		-	-	298.15	1.0	768.7	753.9	-14.8	-1.9	-	-	-	-
451	378	V	O9110a		-	-	298.15	1.0	767.8	748.9	-18.9	-2.5	-	-	-	-
452	379	V	O9111a		-	-	298.15	1.0	783.0	772.9	-10.1	-1.3	-	-	-	-
453	380	V	O9112a		-	-	298.15	1.0	775.3	763.2	-12.1	-1.6	-	-	-	-
454	381	V	O9113a		-	-	298.15	1.0	773.0	760.0	-12.9	-1.7	-	-	-	-
455	382	V	O9114a		-	-	298.15	1.0	772.7	760.0	-12.7	-1.6	-	-	-	-
456	383	V	O0101a		-	-	298.0	1.0	-	-	-	-	45.3	46.2	0.9	1.9
457	384	V	O0102a		-	-	298.0	1.0	-	-	-	-	53.2	51.6	-1.6	-3.0
458	385	V	O0103a		-	-	293.15	1.0	784.8	774.6	-10.2	-1.3	-	-	-	-
459	386	V	O0104a		-	445.65	298.15	1.0	771.5	758.6	-12.9	-1.7	51.4	52.1	0.7	1.3
460	387	V	O0105a		-	-	293.15	1.0	777.8	766.9	-10.9	-1.4	-	-	-	-
461	388	V	O0106a		-	-	298.15	1.0	775.1	763.1	-12.0	-1.5	-	-	-	-
462	389	V	O0107a		-	-	298.15	1.0	771.2	758.0	-13.2	-1.7	-	-	-	-
463	390	V	O0108a		-	-	298.15	1.0	782.1	766.7	-15.4	-2.0	-	-	-	-
464	391	V	O0109a		-	-	293.15	1.0	787.4	766.9	-20.5	-2.6	-	-	-	-
465	392	V	O0110a		-	-	298.15	1.0	775.8	762.1	-13.7	-1.8	-	-	-	-
466	393	V	O0111a		-	-	298.15	1.0	773.6	757.2	-16.4	-2.1	-	-	-	-
467	394	V	O0112a		-	-	298.15	1.0	788.6	778.9	-9.7	-1.2	-	-	-	-
468	395	V	O0113a		-	-	298.15	1.0	782.3	770.0	-12.3	-1.6	-	-	-	-
469	396	V	O0114a		-	-	298.15	1.0	779.8	767.4	-12.4	-1.6	-	-	-	-
470	397	V	O0115a		-	-	298.15	1.0	778.8	767.1	-11.7	-1.5	53.2	55.4	2.2	4.2
471	398	V	O0116a		203.95	460.15	298.15	1.0	779.2	766.9	-12.3	-1.6	-	-	-	-
472	398	V	O0116b		203.95	460.15	388.0	1.0	-	-	-	-	46.2	48.7	2.5	5.5
473	399	V	O7201a		-	404.65	404.65	1.0	-	-	-	-	34.8	38.9	4.1	11.8
474	400	V	O7202a		-	387.15	298.15	1.0	868.8	804.6	-64.2	-7.4	43.9	44.1	0.2	0.6
475	401	V	O7203a		-	-	298.15	1.0	813.7	767.4	-46.3	-5.7	-	-	-	-
476	402	V	O7204a		-	396.15	293.15	1.0	825.0	793.2	-31.8	-3.9	-	-	-	-
477	402	V	O7204b		-	396.15	396.15	1.0	-	-	-	-	34.0	34.6	0.6	1.8
478	403	V	O7205a		-	-	298.15	1.0	851.6	836.9	-14.8	-1.7	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
479	404	V	O7206a		-	420.08	298.15	1.0	840.9	819.0	-21.9	-2.6	47.8	47.3	-0.5	-1.0
480	405	V	O7207a		-	-	298.15	1.0	840.3	815.9	-24.4	-2.9	-	-	-	-
481	406	V	O7208a		-	-	298.15	1.0	831.2	806.4	-24.8	-3.0	45.9	45.6	-0.3	-0.7
482	407	V	O7209a		175.85	413.65	293.15	1.0	834.5	797.8	-36.8	-4.4	-	-	-	-
483	407	V	O7209b		175.85	413.65	413.65	1.0	-	-	-	-	35.6	34.8	-0.8	-2.4
484	408	V	O7210a		-	-	298.15	1.0	832.7	808.4	-24.3	-2.9	46.8	46.5	-0.3	-0.7
485	409	V	O8201a		-	-	298.15	1.0	852.7	829.7	-23.0	-2.7	-	-	-	-
486	410	V	O8202a		-	421.15	421.15	1.0	-	-	-	-	36.4	40.3	4.0	10.9
487	411	V	O8203a		-	416.50	416.5	1.0	-	-	-	-	35.9	37.5	1.6	4.4
488	412	V	O8204a		-	478.13	298.15	1.0	825.6	781.5	-44.0	-5.3	-	-	-	-
489	413	V	O8205a		-	-	298.15	1.0	851.8	836.4	-15.4	-1.8	-	-	-	-
490	414	V	O8206a		-	-	298.15	1.0	843.3	825.1	-18.2	-2.2	-	-	-	-
491	415	V	O8207a		-	-	298.15	1.0	840.7	821.2	-19.5	-2.3	-	-	-	-
492	416	V	O8208a		-	-	298.15	1.0	833.5	812.8	-20.8	-2.5	-	-	-	-
493	417	V	O8209a		-	434.03	298.15	1.0	833.1	809.9	-23.2	-2.8	50.9	50.7	-0.2	-0.3
494	418	V	O8210a		-	478.13	298.15	1.0	831.2	806.5	-24.7	-3.0	50.6	49.9	-0.8	-1.5
495	419	V	O9201a		-	438.65	298.15	1.0	820.3	780.9	-39.4	-4.8	-	-	-	-
496	419	V	O9201b		-	438.65	438.65	1.0	-	-	-	-	38.0	37.2	-0.8	-2.1
497	420	V	O9202a		-	520.68	295.15	1.0	829.0	801.9	-27.1	-3.3	-	-	-	-
498	421	V	O9203a		-	-	298.15	1.0	844.0	826.0	-18.0	-2.1	-	-	-	-
499	422	V	O9204a		-	-	298.15	1.0	838.6	815.8	-22.8	-2.7	-	-	-	-
500	423	V	O9205a		-	-	298.15	1.0	840.6	821.7	-18.9	-2.2	-	-	-	-
501	424	V	O9206a		214.15	452.35	298.15	1.0	831.5	800.5	-31.0	-3.7	48.1	50.7	2.6	5.3
502	425	V	O9207a		-	-	298.0	1.0	-	-	-	-	54.7	54.1	-0.6	-1.1
503	426	V	O0201a		-	444.45	298.15	1.0	816.8	770.2	-46.6	-5.7	-	-	-	-
504	426	V	O0201b		-	444.45	351.0	1.0	-	-	-	-	46.1	44.2	-1.9	-4.2
505	427	V	O0203a		-	415.43	298.15	1.0	829.0	790.5	-38.5	-4.6	57.8	53.0	-4.8	-8.4
506	428	V	O0204a		-	-	298.15	1.0	840.9	823.4	-17.5	-2.1	-	-	-	-
507	429	V	O0205a		-	-	293.15	1.0	840.9	814.7	-26.2	-3.1	-	-	-	-
508	430	V	O0206a		204.05	476.45	298.15	1.0	833.7	809.2	-24.5	-2.9	58.8	58.4	-0.5	-0.8
509	431	V	O7301a	×	-	426.15	426.15	1.0	-	-	-	-	36.8	45.1	8.3	22.4
510	432	V	O7302a		-	419.15	419.15	1.0	-	-	-	-	36.2	38.7	2.5	6.9
511	433	V	O7303a		-	430.15	430.15	1.0	-	-	-	-	37.2	41.4	4.2	11.2
512	434	V	O7304a		-	419.15	419.15	1.0	-	-	-	-	36.2	39.5	3.3	9.1
513	435	V	O7305a		-	416.15	298.15	1.0	893.8	838.2	-55.6	-6.2	47.8	45.7	-2.1	-4.5
514	436	V	O7306a		-	416.90	293.15	1.0	922.9	895.0	-27.9	-3.0	-	-	-	-
515	437	V	O8301a		-	438.15	438.15	1.0	-	-	-	-	38.0	40.9	2.9	7.7
516	438	V	O8302a		-	418.15	298.15	1.0	884.7	852.6	-32.1	-3.6	-	-	-	-
517	438	V	O8302b		-	418.15	418.15	1.0	-	-	-	-	36.1	40.7	4.6	12.8
518	439	V	O8303a		228.85	462.15	298.15	1.0	903.3	872.1	-31.2	-3.5	56.4	58.6	2.2	4.0
519	440	V	O9301a		-	444.15	444.15	1.0	-	-	-	-	38.5	40.9	2.4	6.1
520	441	V	O0301a		-	440.15	293.15	1.0	862.1	809.6	-52.5	-6.1	-	-	-	-
521	441	V	O0301b		-	440.15	440.15	1.0	-	-	-	-	38.2	38.9	0.8	2.0
522	442	V	O0303a		-	467.15	467.15	1.0	-	-	-	-	40.7	42.3	1.5	3.7
523	443	V	O0304a		-	-	288.15	1.0	886.9	865.0	-21.9	-2.5	-	-	-	-
524	444	V	O7401a		-	456.15	298.15	1.0	997.0	941.3	-55.7	-5.6	-	-	-	-
525	445	V	O7402a		-	-	298.0	1.0	-	-	-	-	53.6	55.3	1.7	3.1
526	446	V	O8401a		229.35	489.15	293.15	1.0	986.0	954.9	-31.1	-3.2	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
527	446	V	O8401b		229.35	489.15	489.15	1.0	-	-	-	-	50.9	51.0	0.1	0.2
528	447	V	O9401a		-	432.65	293.15	1.0	918.6	883.2	-35.4	-3.9	52.9	54.8	1.9	3.5
529	448	V	A7102a		-	-	298.15	1.0	829.5	806.3	-23.2	-2.8	-	-	-	-
530	449	V	A7104a		-	-	298.15	1.0	823.1	815.0	-8.1	-1.0	-	-	-	-
531	449	V	A7104b		-	-	334.0	1.0	-	-	-	-	42.4	43.3	0.9	2.2
532	450	V	A7107a		-	416.15	298.15	1.0	814.3	809.4	-5.0	-0.6	-	-	-	-
533	450	V	A7107b		-	416.15	329.0	1.0	-	-	-	-	42.8	44.5	1.7	3.9
534	451	V	A7108a		-	-	298.15	1.0	824.0	812.0	-12.0	-1.5	-	-	-	-
535	452	V	A7109a		-	-	293.15	1.0	820.6	805.9	-14.7	-1.8	-	-	-	-
536	453	V	A7110a		229.21	425.95	298.15	1.0	813.3	806.3	-7.0	-0.9	48.0	48.5	0.5	0.9
537	454	V	A8101a		-	-	293.15	1.0	847.6	811.2	-36.4	-4.3	-	-	-	-
538	455	V	A8102a		-	-	293.15	1.0	847.6	813.6	-34.0	-4.0	-	-	-	-
539	456	V	A8103a		-	433.15	329.07	0.01	802.4	784.4	-18.0	-2.2	-	-	-	-
540	457	V	A8104a		-	433.80	298.15	1.0	815.2	807.3	-7.9	-1.0	-	-	-	-
541	457	V	A8104b		-	433.80	329.59	0.01	-	-	-	-	44.7	47.9	3.3	7.3
542	458	V	A8109a		-	447.15	298.15	1.01	821.1	810.3	-10.8	-1.3	51.0	53.3	2.3	4.4
543	459	V	A9101a		-	-	298.15	1.0	827.0	829.2	2.2	0.3	-	-	-	-
544	460	V	A9102a		-	456.62	347.35	0.01	779.0	790.3	11.3	1.4	-	-	-	-
545	461	V	A9103a		-	-	291.15	1.0	884.3	825.8	-58.5	-6.6	-	-	-	-
546	462	V	A9104a		-	-	293.15	1.0	848.3	821.7	-26.6	-3.1	-	-	-	-
547	463	V	A9105a		-	-	293.15	1.0	842.3	815.4	-26.9	-3.2	-	-	-	-
548	464	V	A9106a		-	456.62	347.53	0.01	785.4	767.0	-18.3	-2.3	-	-	-	-
549	465	V	A9109a		-	468.15	298.15	1.01	831.0	813.5	-17.5	-2.1	55.3	58.0	2.8	5.0
550	466	V	A0101a		-	-	293.15	1.0	843.0	824.3	-18.7	-2.2	-	-	-	-
551	467	V	A0103a		-	403.15	298.15	1.0	813.4	813.3	-0.1	-0.0	-	-	-	-
552	467	V	A0103b	×	-	403.15	403.15	1.0	-	-	-	-	24.3	50.8	26.5	109.3
553	468	V	A0107a		-	488.15	298.15	1.0	824.9	816.1	-8.8	-1.1	59.5	62.9	3.4	5.7
554	469	V	K7101a		-	403.75	294.15	1.0	823.0	830.6	7.6	0.9	-	-	-	-
555	469	V	K7101b		-	403.75	300.55	0.01	-	-	-	-	40.7	42.4	1.7	4.2
556	470	V	K7102a		228.15	398.15	298.15	1.0	808.4	804.3	-4.1	-0.5	42.3	40.8	-1.5	-3.5
557	471	V	K7103a		209.15	398.15	298.15	1.0	801.2	811.2	10.0	1.2	-	-	-	-
558	471	V	K7103b		209.15	398.15	298.15	0.02	-	-	-	-	39.7	42.5	2.7	6.9
559	472	V	K7104a		204.75	397.55	298.15	1.0	799.7	780.6	-19.1	-2.4	41.5	41.1	-0.4	-0.9
560	473	V	K7105a		-	405.15	293.15	1.0	827.3	813.8	-13.5	-1.6	-	-	-	-
561	473	V	K7105b		-	405.15	301.67	0.01	-	-	-	-	41.4	43.7	2.4	5.7
562	474	V	K7106a		-	409.15	298.15	1.0	824.0	797.3	-26.7	-3.2	-	-	-	-
563	475	V	K7107a		-	406.15	302.47	0.01	809.5	784.8	-24.7	-3.0	41.1	43.5	2.3	5.6
564	476	V	K7108a		-	411.15	295.15	1.0	815.3	813.9	-1.4	-0.2	-	-	-	-
565	476	V	K7108b		-	411.15	306.47	0.01	-	-	-	-	41.7	44.4	2.7	6.4
566	477	V	K7109a		-	413.15	298.15	1.0	828.0	806.0	-22.1	-2.7	-	-	-	-
567	477	V	K7109b		-	413.15	308.07	0.01	-	-	-	-	41.8	44.7	2.9	6.9
568	478	V	K7110a		-	409.15	293.15	1.0	812.0	796.2	-15.8	-1.9	-	-	-	-
569	478	V	K7110b		-	409.15	304.87	0.01	-	-	-	-	41.6	43.6	2.0	4.9
570	479	V	K7111a		-	412.15	298.15	1.0	808.5	810.8	2.3	0.3	-	-	-	-
571	479	V	K7111b		-	412.15	307.27	0.01	-	-	-	-	42.0	45.3	3.2	7.7
572	480	V	K7112a		-	417.95	293.15	1.0	811.6	807.2	-4.4	-0.5	-	-	-	-
573	480	V	K7112b		-	417.95	311.91	0.01	-	-	-	-	42.2	45.6	3.4	8.1
574	481	V	K7113a		241.05	417.15	298.15	1.0	811.6	798.4	-13.2	-1.6	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
575	481	V	K7113b		241.05	417.15	311.27	0.01	-	-	-	-	42.9	45.6	2.7	6.3
576	482	V	K7114a		235.95	420.55	298.15	1.0	814.6	799.7	-15.0	-1.8	-	-	-	-
577	482	V	K7114b		235.95	420.55	313.99	0.01	-	-	-	-	43.2	45.4	2.2	5.2
578	483	V	K7115a		238.45	424.05	298.15	1.0	811.6	808.5	-3.1	-0.4	46.1	48.2	2.1	4.5
579	484	V	K8101a		-	-	293.15	1.0	839.5	851.1	11.6	1.4	-	-	-	-
580	485	V	K8102a		-	408.25	298.15	1.0	802.3	805.7	3.4	0.4	43.3	43.3	0.0	0.1
581	486	V	K8103a		-	-	293.15	1.0	826.0	838.6	12.6	1.5	-	-	-	-
582	487	V	K8104a		-	426.60	293.15	1.0	838.9	848.2	9.3	1.1	-	-	-	-
583	487	V	K8104b		-	426.60	318.83	0.01	-	-	-	-	43.6	46.0	2.4	5.6
584	488	V	K8105a		-	421.15	293.15	1.0	829.8	828.5	-1.4	-0.2	-	-	-	-
585	488	V	K8105b		-	421.15	314.47	0.01	-	-	-	-	43.2	44.9	1.7	4.0
586	489	V	K8106a		-	420.15	293.15	1.0	825.7	835.8	10.1	1.2	-	-	-	-
587	490	V	K8107a		-	419.15	298.15	1.0	810.5	807.7	-2.8	-0.3	-	-	-	-
588	490	V	K8107b		-	419.15	312.87	0.01	-	-	-	-	42.3	44.6	2.2	5.3
589	491	V	K8108a		-	-	293.15	1.0	829.0	835.4	6.4	0.8	-	-	-	-
590	492	V	K8109a		-	-	293.15	1.0	812.0	811.5	-0.6	-0.1	-	-	-	-
591	493	V	K8110a		-	-	365.0	1.0	-	-	-	-	42.5	41.9	-0.6	-1.4
592	494	V	K8111a		-	420.65	293.15	1.0	812.1	790.5	-21.6	-2.7	-	-	-	-
593	494	V	K8111b		-	420.65	314.07	0.01	-	-	-	-	42.6	45.0	2.4	5.7
594	495	V	K8112a		-	427.65	319.67	0.01	791.0	804.4	13.4	1.7	43.5	46.8	3.3	7.7
595	496	V	K8113a		-	431.15	295.15	1.0	829.5	825.4	-4.1	-0.5	-	-	-	-
596	496	V	K8113b		-	431.15	322.47	0.01	-	-	-	-	44.1	47.3	3.1	7.1
597	497	V	K8114a		-	426.15	298.15	1.0	817.0	801.0	-16.0	-2.0	-	-	-	-
598	498	V	K8115a		-	-	298.15	1.0	820.0	803.6	-16.4	-2.0	-	-	-	-
599	499	V	K8116a		-	431.15	293.15	1.0	817.5	797.9	-19.6	-2.4	-	-	-	-
600	499	V	K8116b		-	431.15	322.47	0.01	-	-	-	-	44.1	46.8	2.7	6.1
601	500	V	K8117a		-	437.15	327.27	0.01	794.2	786.5	-7.7	-1.0	43.8	48.0	4.2	9.6
602	501	V	K8118a		-	435.14	297.15	1.0	829.0	806.7	-22.3	-2.7	-	-	-	-
603	501	V	K8118b		-	435.14	322.36	0.01	-	-	-	-	44.4	47.3	2.9	6.4
604	502	V	K8119a		-	427.15	295.15	1.0	813.0	798.5	-14.5	-1.8	-	-	-	-
605	502	V	K8119b		-	427.15	319.27	0.01	-	-	-	-	43.5	47.3	3.8	8.8
606	503	V	K8120a		-	437.15	293.15	1.0	830.4	803.1	-27.3	-3.3	-	-	-	-
607	504	V	K8122a		-	437.00	298.15	1.0	811.0	816.5	5.5	0.7	-	-	-	-
608	504	V	K8122b		-	437.00	327.15	0.01	-	-	-	-	44.2	49.5	5.3	11.9
609	505	V	K8123a		-	440.15	298.15	1.0	810.0	807.7	-2.3	-0.3	-	-	-	-
610	505	V	K8123b		-	440.15	329.67	0.01	-	-	-	-	46.3	49.1	2.8	6.0
611	506	V	K8124a		-	436.15	298.15	1.0	814.7	802.8	-11.9	-1.5	-	-	-	-
612	506	V	K8124b		-	436.15	326.47	0.01	-	-	-	-	45.5	49.2	3.7	8.2
613	507	V	K8125a		-	440.65	298.15	1.0	822.0	804.1	-17.9	-2.2	-	-	-	-
614	507	V	K8125b		-	440.65	308.0	1.0	-	-	-	-	43.8	50.5	6.7	15.3
615	508	V	K8126a		252.84	445.75	298.15	1.0	815.2	811.8	-3.5	-0.4	51.8	52.9	1.1	2.2
616	509	V	K9101a		247.95	425.15	298.15	1.0	820.2	831.9	11.7	1.4	45.4	45.6	0.2	0.4
617	510	V	K9102a		-	-	296.15	1.0	812.0	806.5	-5.5	-0.7	-	-	-	-
618	511	V	K9103a		-	-	293.15	1.0	816.8	815.0	-1.8	-0.2	-	-	-	-
619	512	V	K9104a		-	-	298.15	1.0	809.0	809.4	0.4	0.1	-	-	-	-
620	513	V	K9105a		-	435.15	287.15	1.0	826.0	814.5	-11.5	-1.4	-	-	-	-
621	513	V	K9105b		-	435.15	325.67	0.01	-	-	-	-	44.2	48.9	4.7	10.6
622	514	V	K9106a		-	445.00	298.15	1.0	813.5	793.9	-19.6	-2.4	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
623	514	V	K9106b		-	445.00	333.55	0.01	-	-	-	-	45.6	49.0	3.3	7.2
624	515	V	K9107a		227.15	441.41	298.15	1.0	802.4	794.3	-8.1	-1.0	50.9	50.9	0.0	0.1
625	516	V	K9108a		-	-	293.15	1.0	833.5	829.1	-4.4	-0.5	-	-	-	-
626	517	V	K9109a		-	-	298.15	1.0	817.0	817.4	0.4	0.1	-	-	-	-
627	518	V	K9110a		-	447.15	287.15	1.0	829.0	812.9	-16.1	-1.9	-	-	-	-
628	518	V	K9110b		-	447.15	335.27	0.01	-	-	-	-	46.0	50.5	4.6	9.9
629	519	V	K9111a		-	456.62	298.15	1.0	820.0	807.3	-12.7	-1.6	-	-	-	-
630	520	V	K9112a		-	456.00	293.15	1.0	821.2	802.3	-18.9	-2.3	-	-	-	-
631	520	V	K9112b		-	456.00	342.35	0.01	-	-	-	-	47.4	50.1	2.7	5.7
632	521	V	K9113a		-	-	293.15	1.0	824.6	821.2	-3.4	-0.4	-	-	-	-
633	522	V	K9114a		-	456.62	300.15	1.0	832.0	810.3	-21.7	-2.6	-	-	-	-
634	523	V	K9115a		-	-	298.15	1.0	815.0	800.5	-14.5	-1.8	-	-	-	-
635	524	V	K9116a		-	451.15	293.15	1.0	823.9	805.9	-18.0	-2.2	-	-	-	-
636	524	V	K9116b		-	451.15	338.47	0.01	-	-	-	-	46.6	51.3	4.7	10.2
637	525	V	K9120a		-	-	298.15	1.0	822.0	818.6	-3.4	-0.4	-	-	-	-
638	526	V	K9121a		269.31	461.60	298.15	1.0	817.8	806.4	-11.4	-1.4	53.3	55.9	2.6	4.9
639	527	V	K9122a		-	460.65	298.15	1.0	819.7	806.6	-13.1	-1.6	-	-	-	-
640	527	V	K9122b		-	460.65	346.07	0.01	-	-	-	-	48.1	52.4	4.3	8.9
641	528	V	K9123a		265.15	463.15	298.15	1.0	820.4	807.4	-13.0	-1.6	55.6	55.9	0.3	0.6
642	529	V	K9124a		265.75	467.15	298.15	1.0	817.8	814.5	-3.3	-0.4	-	-	-	-
643	529	V	K9124b		265.75	467.15	351.27	0.01	-	-	-	-	49.4	53.7	4.3	8.7
644	530	V	K0101a		-	-	298.15	1.0	816.9	816.6	-0.3	-0.0	48.8	49.1	0.3	0.6
645	531	V	K0102a		-	-	298.15	1.0	825.2	825.0	-0.2	-0.0	-	-	-	-
646	532	V	K0103a		-	-	288.65	1.0	825.2	837.3	12.1	1.5	-	-	-	-
647	533	V	K0104a		-	-	293.15	1.0	832.0	817.5	-14.4	-1.7	-	-	-	-
648	534	V	K0105a		-	-	293.15	1.0	814.3	816.4	2.1	0.3	-	-	-	-
649	535	V	K0106a		-	473.00	293.15	1.0	822.6	806.0	-16.6	-2.0	-	-	-	-
650	535	V	K0106b		-	473.00	355.95	0.01	-	-	-	-	49.4	53.7	4.2	8.5
651	536	V	K0107a		-	-	298.15	1.0	818.0	804.1	-13.9	-1.7	-	-	-	-
652	537	V	K0108a		-	476.65	293.15	1.0	821.3	809.5	-11.8	-1.4	-	-	-	-
653	537	V	K0108b		-	476.65	358.87	0.01	-	-	-	-	50.0	54.3	4.2	8.4
654	538	V	K0109a		-	-	293.15	1.0	838.4	825.5	-12.9	-1.5	-	-	-	-
655	539	V	K0110a		-	477.05	298.15	1.0	820.5	809.3	-11.2	-1.4	-	-	-	-
656	539	V	K0110b		-	477.05	359.19	0.01	-	-	-	-	50.1	55.9	5.8	11.6
657	540	V	K0111a		264.15	479.65	293.65	1.0	822.0	812.7	-9.3	-1.1	-	-	-	-
658	540	V	K0111b		264.15	479.65	361.27	0.01	-	-	-	-	50.5	55.8	5.2	10.3
659	541	V	K0112a		275.15	476.15	298.15	1.0	821.9	810.6	-11.3	-1.4	-	-	-	-
660	541	V	K0112b		275.15	476.15	358.47	0.01	-	-	-	-	50.3	56.0	5.8	11.5
661	542	V	K0113a		287.15	483.35	298.15	1.0	820.1	817.1	-3.0	-0.4	60.9	62.5	1.6	2.6
662	543	V	K7201a		-	446.15	333.97	0.01	923.3	928.2	5.0	0.5	-	-	-	-
663	544	V	K7202a		-	411.15	295.15	1.0	908.0	933.4	25.4	2.8	-	-	-	-
664	545	V	K7203a		-	451.65	292.15	1.0	953.1	947.6	-5.5	-0.6	-	-	-	-
665	546	V	K7204a		-	469.15	352.37	0.01	902.9	891.7	-11.1	-1.2	-	-	-	-
666	547	V	K7205a		-	417.15	291.15	1.0	919.0	944.1	25.1	2.7	-	-	-	-
667	548	V	K7206a		-	449.15	293.15	1.0	945.0	924.7	-20.3	-2.1	-	-	-	-
668	549	V	K7207a	×	-	447.20	447.2	1.0	-	-	-	-	38.8	47.9	9.1	23.4
669	550	V	K7208a		-	495.15	373.17	0.01	885.3	885.7	0.4	0.0	-	-	-	-
670	551	V	K8202a	×	-	417.65	311.17	0.01	909.0	883.9	-25.2	-2.8	41.8	56.1	14.2	34.1

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
671	552	V	K8206a	×	-	441.15	329.97	0.01	907.8	888.9	-18.9	-2.1	45.3	62.5	17.2	37.9
672	553	V	K8207a		-	467.15	350.77	0.01	882.2	875.7	-6.5	-0.7	-	-	-	-
673	554	V	K9201a		-	339.15	298.0	1.0	-	-	-	-	56.1	59.7	3.6	6.4
674	555	V	K9202a		-	467.93	351.39	0.01	893.7	867.9	-25.8	-2.9	-	-	-	-
675	556	V	K0201a		-	442.15	442.15	1.0	-	-	-	-	38.4	45.5	7.1	18.5
676	557	V	K0202a		-	-	298.0	1.0	-	-	-	-	57.7	61.7	4.0	7.0
677	558	V	K7301a	×	-	476.65	384.0	1.0	-	-	-	-	54.9	75.1	20.2	36.8
678	559	V	K7302a		322.15	455.78	313.15	1.0	1059.9	1050.3	-9.6	-0.9	-	-	-	-
679	559	V	K7302b	×	322.15	455.78	455.78	1.0	-	-	-	-	39.6	59.9	20.2	51.0
680	560	V	E7201a		183.65	391.55	298.15	1.0	849.5	833.5	-15.9	-1.9	41.3	40.5	-0.8	-1.9
681	561	V	E7202a		-	-	293.15	1.0	870.0	869.4	-0.6	-0.1	43.9	44.0	0.1	0.3
682	562	V	E7203a		-	-	298.15	1.0	853.9	852.5	-1.4	-0.2	-	-	-	-
683	562	V	E7203b		-	-	300.07	0.01	-	-	-	-	43.5	43.1	-0.3	-0.8
684	563	V	E7204a		-	-	297.85	1.0	872.5	857.4	-15.1	-1.7	40.3	42.9	2.5	6.3
685	564	V	E7205a		-	414.55	293.15	1.0	864.7	835.6	-29.1	-3.4	-	-	-	-
686	564	V	E7205b		-	414.55	414.55	1.0	-	-	-	-	41.1	34.1	-6.9	-16.9
687	565	V	E7206a		-	396.15	294.5	1.0	846.7	814.4	-32.3	-3.8	-	-	-	-
688	565	V	E7206b		-	396.15	272.0	1.0	-	-	-	-	43.3	43.1	-0.2	-0.4
689	566	V	E7207a		-	401.65	298.15	1.0	866.0	850.4	-15.6	-1.8	-	-	-	-
690	567	V	E7208a		-	409.15	293.15	1.0	879.7	865.2	-14.5	-1.6	-	-	-	-
691	568	V	E7209a		-	-	293.15	1.0	876.5	861.1	-15.4	-1.8	-	-	-	-
692	569	V	E7210a		-	-	293.15	1.0	867.8	841.1	-26.7	-3.1	44.7	44.4	-0.3	-0.8
693	570	V	E7211a		-	407.15	298.15	1.0	859.5	824.8	-34.7	-4.0	-	-	-	-
694	570	V	E7211b		-	407.15	282.0	1.0	-	-	-	-	50.5	44.7	-5.8	-11.4
695	571	V	E7212a		173.85	408.15	298.15	1.0	861.2	836.9	-24.3	-2.8	-	-	-	-
696	571	V	E7212b		173.85	408.15	282.0	1.0	-	-	-	-	44.5	45.6	1.1	2.6
697	572	V	E7213a		201.75	409.15	298.15	1.0	867.5	830.8	-36.7	-4.2	-	-	-	-
698	572	V	E7213b		201.75	409.15	286.0	1.0	-	-	-	-	44.9	45.1	0.2	0.5
699	573	V	E7214a		-	406.15	298.15	1.0	861.2	834.6	-26.6	-3.1	-	-	-	-
700	574	V	E7215a		-	402.15	298.15	1.0	853.9	827.9	-26.1	-3.0	-	-	-	-
701	575	V	E7216a		-	413.15	293.15	1.0	867.8	859.4	-8.4	-1.0	-	-	-	-
702	575	V	E7216b		-	413.15	309.67	0.01	-	-	-	-	42.9	45.8	2.9	6.7
703	576	V	E7217a		-	405.15	303.27	0.01	861.5	849.1	-12.4	-1.4	41.8	45.1	3.3	7.8
704	577	V	E7218a		194.65	414.75	298.75	1.0	864.8	851.9	-12.9	-1.5	46.4	47.1	0.7	1.4
705	578	V	E7219a		-	406.15	298.15	1.0	863.1	849.5	-13.5	-1.6	-	-	-	-
706	578	V	E7219b		-	406.15	304.07	0.01	-	-	-	-	42.0	45.6	3.6	8.6
707	579	V	E7220a		203.15	422.65	298.15	1.0	880.4	864.3	-16.1	-1.8	47.7	49.6	1.9	4.0
708	580	V	E7221a		181.95	419.25	298.15	1.01	869.4	846.8	-22.7	-2.6	47.0	47.3	0.3	0.7
709	581	V	E7222a		177.95	416.45	298.15	1.0	868.2	841.9	-26.3	-3.0	-	-	-	-
710	581	V	E7222b		177.95	416.45	286.0	1.0	-	-	-	-	44.3	47.4	3.1	7.1
711	582	V	E7223a		183.65	419.75	298.15	1.0	871.5	844.5	-27.1	-3.1	48.5	46.9	-1.6	-3.4
712	583	V	E7224a		202.25	422.15	298.15	1.0	872.2	857.7	-14.5	-1.7	48.6	48.8	0.2	0.5
713	584	V	E8201a		-	-	293.15	1.0	830.0	822.4	-7.6	-0.9	-	-	-	-
714	585	V	E8202a		-	-	298.15	1.0	874.9	878.9	4.0	0.5	-	-	-	-
715	586	V	E8203a		-	399.85	399.85	1.0	-	-	-	-	30.5	36.6	6.1	20.0
716	587	V	E8204a		-	-	277.15	1.0	883.0	867.2	-15.8	-1.8	-	-	-	-
717	588	V	E8205a		-	421.15	316.07	0.01	860.1	853.6	-6.6	-0.8	-	-	-	-
718	589	V	E8206a		-	-	293.15	1.0	860.4	849.3	-11.1	-1.3	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
719	590	V	E8208a		-	-	293.15	1.0	867.9	869.1	1.2	0.1	-	-	-	-
720	591	V	E8209b		-	437.43	298.0	1.0	-	-	-	-	45.7	45.7	-0.0	-0.1
721	592	V	E8210b		-	426.15	298.0	1.0	-	-	-	-	45.6	47.7	2.1	4.6
722	593	V	E8211a		-	409.15	409.15	1.0	-	-	-	-	36.4	38.4	2.0	5.6
723	594	V	E8212a		-	-	298.15	1.0	866.0	840.6	-25.4	-2.9	-	-	-	-
724	595	V	E8213a		192.55	421.15	293.15	1.0	847.0	817.6	-29.4	-3.5	48.5	46.1	-2.4	-4.9
725	596	V	E8214a		-	-	289.15	1.0	870.0	825.6	-44.4	-5.1	-	-	-	-
726	597	V	E8216a		-	420.15	298.15	1.0	846.1	820.0	-26.1	-3.1	-	-	-	-
727	598	V	E8217a		-	422.15	316.87	0.01	846.6	839.0	-7.7	-0.9	-	-	-	-
728	599	V	E8218a		-	420.65	298.15	1.0	880.5	848.3	-32.2	-3.7	-	-	-	-
729	600	V	E8219a		-	-	293.15	1.0	875.0	864.6	-10.4	-1.2	-	-	-	-
730	601	V	E8220a		-	-	293.15	1.0	863.3	846.9	-16.4	-1.9	-	-	-	-
731	602	V	E8221a		-	428.3	293.15	1.0	876.5	843.0	-33.5	-3.8	48.4	49.1	0.8	1.6
732	602	V	E8221b		-	428.3	298.15	1.0	-	-	-	-	48.4	48.8	0.4	0.8
733	603	V	E8222a		-	-	293.15	1.0	869.7	836.7	-33.0	-3.8	-	-	-	-
734	604	V	E8223a		-	-	298.15	1.0	857.4	826.4	-31.0	-3.6	-	-	-	-
735	605	V	E8224a		-	-	293.15	1.0	878.0	850.3	-27.7	-3.1	-	-	-	-
736	606	V	E8225a		-	429.05	298.15	1.0	857.5	832.9	-24.6	-2.9	44.3	48.6	4.3	9.7
737	607	V	E8227a		-	436.15	293.15	1.0	870.5	846.6	-23.9	-2.7	-	-	-	-
738	607	V	E8227b		-	436.15	299.0	1.0	-	-	-	-	45.4	50.6	5.2	11.4
739	608	V	E8228a		-	430.15	298.15	1.0	860.6	829.8	-30.8	-3.6	-	-	-	-
740	608	V	E8228b		-	430.15	292.0	1.0	-	-	-	-	41.7	49.2	7.5	18.0
741	609	V	E8229a		-	446.15	298.15	1.0	865.0	839.3	-25.7	-3.0	44.1	50.0	5.8	13.3
742	610	V	E8230a		-	-	298.15	1.0	863.2	833.4	-29.8	-3.5	-	-	-	-
743	611	V	E8231a		-	440.22	298.15	1.0	861.3	836.9	-24.4	-2.8	-	-	-	-
744	612	V	E8232a		-	436.35	293.15	1.0	857.9	833.8	-24.1	-2.8	-	-	-	-
745	613	V	E8233a		-	435.65	293.15	1.0	879.0	866.8	-12.2	-1.4	-	-	-	-
746	613	V	E8233b		-	435.65	327.67	0.01	-	-	-	-	44.9	49.2	4.3	9.6
747	614	V	E8235a		-	436.15	298.15	1.0	869.1	855.2	-13.9	-1.6	-	-	-	-
748	614	V	E8235b		-	436.15	328.07	0.01	-	-	-	-	45.7	49.2	3.5	7.7
749	615	V	E8236a		-	-	298.15	1.0	859.9	849.1	-10.8	-1.3	-	-	-	-
750	616	V	E8237a		217.45	447.15	298.15	1.01	875.9	862.0	-13.9	-1.6	51.6	54.4	2.8	5.4
751	617	V	E8238a		205.55	440.15	298.15	1.0	866.7	847.2	-19.5	-2.2	50.6	52.2	1.6	3.1
752	618	V	E8239a		202.45	440.65	298.15	1.0	865.8	842.2	-23.5	-2.7	-	-	-	-
753	618	V	E8239b		202.45	440.65	329.57	0.01	-	-	-	-	46.6	49.1	2.5	5.3
754	619	V	E8240a		181.65	438.15	298.15	1.01	869.1	841.8	-27.3	-3.1	-	-	-	-
755	619	V	E8240b		181.65	438.15	327.57	0.01	-	-	-	-	46.4	49.2	2.8	6.0
756	620	V	E8241a		200.05	441.90	298.15	1.0	868.1	844.8	-23.4	-2.7	52.2	51.7	-0.5	-1.0
757	621	V	E8242a		212.15	444.65	298.15	1.0	868.6	856.3	-12.3	-1.4	51.9	53.6	1.7	3.3
758	622	V	E9201a		-	-	298.0	1.0	-	-	-	-	48.4	50.7	2.3	4.8
759	623	V	E9202a		-	-	298.0	1.0	-	-	-	-	47.8	47.3	-0.5	-1.0
760	624	V	E9203a		-	-	298.0	1.0	-	-	-	-	50.4	49.1	-1.3	-2.5
761	625	V	E9205b		-	460.31	298.0	1.0	-	-	-	-	50.3	50.1	-0.1	-0.3
762	626	V	E9207a		-	-	301.15	1.0	855.0	837.0	-18.0	-2.1	-	-	-	-
763	627	V	E9209a		-	442.15	293.15	1.0	862.7	828.5	-34.1	-4.0	51.7	51.9	0.2	0.4
764	628	V	E9210a		-	-	298.15	1.0	869.0	851.8	-17.2	-2.0	-	-	-	-
765	629	V	E9212a		-	442.15	298.15	1.0	861.7	822.5	-39.2	-4.6	-	-	-	-
766	629	V	E9212b		-	442.15	304.0	1.0	-	-	-	-	47.3	50.3	3.0	6.3

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
767	630	V	E9213a		-	-	293.15	1.0	848.2	830.2	-18.0	-2.1	-	-	-	-
768	631	V	E9214a		-	-	293.15	1.0	871.0	862.9	-8.1	-0.9	-	-	-	-
769	632	V	E9215a		-	-	293.15	1.0	857.2	847.1	-10.1	-1.2	-	-	-	-
770	633	V	E9216a		-	-	293.15	1.0	868.8	841.5	-27.3	-3.1	-	-	-	-
771	634	V	E9217a		-	-	293.15	1.0	866.9	838.5	-28.4	-3.3	-	-	-	-
772	635	V	E9218a		-	452.15	293.15	1.0	862.0	837.2	-24.8	-2.9	50.6	53.1	2.5	4.9
773	636	V	E9219a		-	-	293.15	1.0	872.1	833.0	-39.1	-4.5	-	-	-	-
774	637	V	E9220a		-	450.15	293.15	1.0	867.9	850.7	-17.2	-2.0	-	-	-	-
775	638	V	E9221a		-	456.91	298.15	1.0	856.7	833.6	-23.1	-2.7	-	-	-	-
776	638	V	E9221b		-	456.91	456.91	1.0	-	-	-	-	39.8	42.1	2.3	5.8
777	639	V	E9222a		-	453.15	293.15	1.0	870.8	854.6	-16.2	-1.9	-	-	-	-
778	640	V	E9223a		-	452.15	336.57	0.01	-	-	-	-	49.2	50.8	1.6	3.3
779	641	V	E9225a		-	452.15	298.15	1.0	860.3	837.9	-22.4	-2.6	-	-	-	-
780	641	V	E9225b		-	452.15	309.0	1.0	-	-	-	-	47.4	53.6	6.2	13.1
781	642	V	E9226a		-	456.15	298.15	1.0	853.6	831.4	-22.1	-2.6	-	-	-	-
782	642	V	E9226b		-	456.15	338.77	0.01	-	-	-	-	48.8	50.5	1.7	3.6
783	643	V	E9227a		-	455.15	298.15	1.0	864.7	835.0	-29.7	-3.4	-	-	-	-
784	644	V	E9228a		-	-	298.15	1.0	854.9	834.5	-20.4	-2.4	-	-	-	-
785	645	V	E9229a		-	-	298.15	1.0	852.5	831.0	-21.5	-2.5	-	-	-	-
786	645	V	E9229b		-	-	322.0	1.0	-	-	-	-	51.6	52.0	0.4	0.7
787	646	V	E9232a		-	-	346.57	0.01	818.2	811.4	-6.8	-0.8	-	-	-	-
788	647	V	E9234a		-	-	298.15	1.0	857.0	847.6	-9.5	-1.1	-	-	-	-
789	648	V	E9235a		236.25	466.05	298.15	1.0	873.1	859.8	-13.3	-1.5	56.4	59.1	2.7	4.8
790	649	V	E9236a		206.95	460.15	298.15	1.0	864.7	846.1	-18.6	-2.1	-	-	-	-
791	650	V	E9237a		199.15	460.15	298.15	1.0	863.0	842.2	-20.8	-2.4	-	-	-	-
792	650	V	E9237b		199.15	460.15	330.0	1.0	-	-	-	-	52.1	53.7	1.6	3.0
793	651	V	E9238a		189.38	459.15	298.15	1.0	863.4	842.1	-21.2	-2.5	-	-	-	-
794	651	V	E9238b		189.38	459.15	344.77	0.01	-	-	-	-	49.2	52.6	3.4	6.9
795	652	V	E9239a		200.49	458.15	298.15	1.0	861.9	842.2	-19.7	-2.3	53.6	56.2	2.6	4.8
796	653	V	E9240a		215.65	463.15	298.15	1.0	865.4	844.1	-21.4	-2.5	57.1	56.4	-0.7	-1.3
797	654	V	E9241a		222.85	465.55	298.15	1.0	866.4	854.5	-11.9	-1.4	56.9	58.4	1.5	2.6
798	655	V	E0201a		-	-	293.15	1.0	843.1	829.1	-13.9	-1.6	48.9	48.5	-0.4	-0.9
799	656	V	E0202a		-	-	298.0	1.0	-	-	-	-	48.0	48.6	0.6	1.3
800	657	V	E0203a		-	461.15	273.15	1.0	872.9	853.9	-19.0	-2.2	-	-	-	-
801	658	V	E0204a		-	-	289.15	1.0	883.7	877.8	-5.9	-0.7	-	-	-	-
802	659	V	E0205a		-	-	293.15	1.0	856.8	845.1	-11.7	-1.4	-	-	-	-
803	660	V	E0209a		-	463.15	298.15	1.0	854.1	831.0	-23.1	-2.7	-	-	-	-
804	660	V	E0209b		-	463.15	315.0	1.0	-	-	-	-	47.2	55.2	8.0	16.9
805	661	V	E0210a		-	445.15	333.17	0.01	819.4	800.1	-19.3	-2.4	-	-	-	-
806	662	V	E0212a		-	457.65	345.27	0.01	810.3	808.2	-2.1	-0.3	-	-	-	-
807	663	V	E0213a		-	460.15	293.15	1.0	847.4	846.2	-1.2	-0.1	-	-	-	-
808	664	V	E0214a		-	-	293.15	1.0	865.9	847.9	-18.0	-2.1	-	-	-	-
809	665	V	E0215a		-	-	298.15	1.0	864.4	855.8	-8.6	-1.0	-	-	-	-
810	666	V	E0216a		-	473.73	298.15	1.0	858.6	842.6	-16.0	-1.9	-	-	-	-
811	667	V	E0217a		-	-	277.15	1.0	875.9	868.3	-7.6	-0.9	-	-	-	-
812	668	V	E0218a		-	-	293.15	1.0	870.0	833.3	-36.7	-4.2	-	-	-	-
813	669	V	E0219a		-	-	292.95	1.0	872.6	850.5	-22.1	-2.5	-	-	-	-
814	670	V	E0220a		-	-	354.97	0.01	826.1	799.5	-26.6	-3.2	51.3	55.0	3.6	7.1

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
815	671	V	E0222a		-	466.15	293.15	1.0	858.0	842.1	-15.8	-1.9	-	-	-	-
816	672	V	E0223a		-	427.05	318.69	0.01	-	-	-	-	53.0	56.8	3.7	7.0
817	673	V	E0224a		-	-	298.15	1.0	857.5	835.1	-22.4	-2.6	-	-	-	-
818	674	V	E0225a		193.15	471.75	298.15	1.0	868.8	859.2	-9.6	-1.1	-	-	-	-
819	674	V	E0225b		193.15	471.75	348.0	1.0	-	-	-	-	50.1	56.6	6.5	13.0
820	675	V	E0227a		-	-	353.67	0.01	805.4	807.9	2.5	0.3	-	-	-	-
821	676	V	E0228a		-	-	348.17	0.01	814.2	810.3	-3.9	-0.5	-	-	-	-
822	677	V	E0230a		-	-	298.15	1.0	858.1	847.3	-10.8	-1.2	-	-	-	-
823	678	V	E0231a		-	486.65	298.15	1.0	870.9	858.3	-12.6	-1.4	61.6	64.0	2.4	3.8
824	679	V	E0232a		228.45	481.65	298.15	1.0	862.9	845.8	-17.1	-2.0	59.5	61.7	2.2	3.7
825	680	V	E0233a		-	481.15	298.15	1.0	861.6	842.3	-19.3	-2.2	-	-	-	-
826	680	V	E0233b		-	481.15	361.97	0.01	-	-	-	-	52.1	55.8	3.6	7.0
827	681	V	E0234a		223.15	481.15	298.15	1.0	862.3	841.9	-20.4	-2.4	-	-	-	-
828	681	V	E0234b		223.15	481.15	361.97	0.01	-	-	-	-	52.1	55.7	3.7	7.0
829	682	V	E0235a		194.35	476.85	298.15	1.0	860.2	842.2	-18.0	-2.1	-	-	-	-
830	682	V	E0235b		194.35	476.85	358.53	0.01	-	-	-	-	51.9	56.1	4.2	8.2
831	683	V	E0236a		195.15	479.15	298.15	1.01	851.0	841.9	-9.1	-1.1	-	-	-	-
832	683	V	E0236b		195.15	479.15	361.97	0.01	-	-	-	-	51.4	55.7	4.3	8.3
833	684	V	E0237a		-	483.15	298.15	1.0	864.0	844.0	-19.9	-2.3	-	-	-	-
834	684	V	E0237b		-	483.15	364.47	0.01	-	-	-	-	52.5	55.9	3.4	6.5
835	685	V	E0238a		235.15	484.45	298.15	1.0	864.3	853.7	-10.6	-1.2	60.7	63.2	2.5	4.2
836	686	V	E7401a		-	-	293.0	1.0	-	-	-	-	55.6	57.5	1.9	3.4
837	687	V	E7403a		-	-	298.15	1.0	1061.4	1027.6	-33.8	-3.2	-	-	-	-
838	688	V	E7404a		-	469.15	298.15	1.0	1076.0	1027.5	-48.5	-4.5	-	-	-	-
839	688	V	E7404b		-	469.15	469.15	1.0	-	-	-	-	40.9	47.4	6.5	15.8
840	689	V	E7405a		-	-	328.0	1.0	-	-	-	-	57.9	55.5	-2.4	-4.2
841	690	V	E7406a		-	463.65	293.15	1.0	1059.0	1023.3	-35.7	-3.4	-	-	-	-
842	690	V	E7406b		-	463.65	323.0	1.0	-	-	-	-	54.9	60.5	5.6	10.2
843	691	V	E7407a		223.15	472.05	298.15	1.0	1049.8	1006.1	-43.7	-4.2	58.7	60.8	2.1	3.5
844	692	V	E7408a		-	481.35	293.15	1.0	1076.0	1027.5	-48.5	-4.5	-	-	-	-
845	692	V	E7408b		-	481.35	481.35	1.0	-	-	-	-	42.1	48.0	5.9	14.0
846	693	V	E7409a		230.65	487.15	293.15	1.01	1087.7	1045.8	-41.9	-3.9	65.7	67.5	1.8	2.7
847	694	V	E7411a	×	-	-	358.0	1.0	-	-	-	-	72.1	57.8	-14.3	-19.9
848	695	V	E7412a		-	482.65	293.15	1.0	1054.7	1036.0	-18.6	-1.8	-	-	-	-
849	695	V	E7412b		-	482.65	482.65	1.0	-	-	-	-	42.2	49.6	7.4	17.5
850	696	V	E8402a		-	463.15	298.15	1.0	989.2	967.2	-22.0	-2.2	60.2	61.1	0.9	1.6
851	697	V	E8403a		-	-	298.15	1.0	1036.9	1008.8	-28.1	-2.7	-	-	-	-
852	698	V	E8404a		-	474.15	298.15	1.0	1017.4	970.7	-46.7	-4.6	-	-	-	-
853	698	V	E8404b		-	474.15	327.0	1.0	-	-	-	-	52.5	58.8	6.3	11.9
854	699	V	E8407a		228.85	484.15	298.15	1.0	1014.0	991.7	-22.3	-2.2	-	-	-	-
855	699	V	E8407b		228.85	484.15	341.0	1.0	-	-	-	-	57.8	62.5	4.7	8.1
856	700	V	E8408a		251.55	489.65	298.15	1.0	1035.3	988.2	-47.1	-4.5	64.5	65.4	0.9	1.4
857	701	V	E8409a		283.45	495.09	298.15	1.0	1057.6	1020.8	-36.7	-3.5	69.0	71.4	2.4	3.5
858	702	V	E8410a		-	484.15	293.15	1.0	1042.0	993.9	-48.1	-4.6	67.6	67.5	-0.1	-0.2
859	703	V	E8411a	×	-	-	367.0	1.0	-	-	-	-	74.7	60.3	-14.4	-19.3
860	704	V	E8412a		285.15	502.15	293.15	1.0	1046.0	1014.5	-31.5	-3.0	-	-	-	-
861	704	V	E8412b		285.15	502.15	502.15	1.0	-	-	-	-	44.1	51.8	7.7	17.4
862	705	V	E9402a		-	470.15	470.15	1.0	-	-	-	-	41.0	45.2	4.2	10.3

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m	T_b	T	P	ρ_{liq}[kg·m^{-3}]				ΔH_{vap}[kJ·mol^{-1}]			
					[K]	[K]	[K]	[bar]	exp	sim	dev	err [%]	exp	sim	dev	err [%]
863	706	V	E9406a		-	509.23	298.0	1.0	-	-	-	-	63.9	62.5	-1.4	-2.2
864	707	V	E9407a		-	481.15	298.15	1.0	1000.7	960.8	-39.9	-4.0	-	-	-	-
865	707	V	E9407b		-	481.15	338.0	1.0	-	-	-	-	55.3	60.6	5.3	9.6
866	708	V	E9408a		-	490.65	490.65	1.0	-	-	-	-	43.0	47.6	4.6	10.8
867	709	V	E9409a		-	-	340.0	1.0	-	-	-	-	63.2	61.7	-1.5	-2.4
868	710	V	E9410a		-	502.15	298.0	1.0	-	-	-	-	66.2	68.1	1.9	2.8
869	711	V	E9411a		249.05	509.65	293.15	1.0	1022.0	980.1	-41.9	-4.1	67.0	71.5	4.5	6.7
870	712	V	E9412a		252.15	509.23	293.15	1.0	1039.1	1007.1	-32.0	-3.1	73.5	76.0	2.5	3.4
871	713	V	E9413a	×	-	-	382.0	1.0	-	-	-	-	75.4	62.7	-12.7	-16.8
872	714	V	E9414a		275.15	514.15	293.15	1.0	1029.6	997.6	-32.0	-3.1	-	-	-	-
873	714	V	E9414b	×	275.15	514.15	514.15	1.0	-	-	-	-	45.2	53.9	8.7	19.2
874	715	V	E0401a		-	-	298.0	1.0	-	-	-	-	63.5	62.2	-1.3	-2.1
875	716	V	E0403a		-	-	332.0	1.0	-	-	-	-	53.2	60.0	6.8	12.9
876	717	V	E0404a	×	-	502.15	351.0	1.0	-	-	-	-	55.5	64.9	9.4	16.9
877	718	V	E0405a		-	488.15	293.15	1.0	996.1	955.9	-40.2	-4.0	-	-	-	-
878	718	V	E0405b		-	488.15	488.15	1.0	-	-	-	-	42.8	49.1	6.3	14.8
879	719	V	E0406a		-	-	298.15	1.0	980.3	935.1	-45.2	-4.6	70.8	67.0	-3.8	-5.4
880	720	V	E0407a		-	494.15	298.15	1.0	982.8	950.6	-32.2	-3.3	-	-	-	-
881	720	V	E0407b		-	494.15	494.15	1.0	-	-	-	-	43.3	50.1	6.8	15.7
882	721	V	E0408a		242.65	514.15	298.15	1.0	983.3	964.9	-18.4	-1.9	71.4	75.8	4.4	6.1
883	722	V	E0409a		267.25	523.95	298.15	1.0	997.4	955.5	-41.8	-4.2	71.0	72.7	1.7	2.5
884	723	V	E0410a		253.15	518.15	298.15	1.0	1003.7	963.9	-39.8	-4.0	73.0	75.3	2.4	3.2
885	724	V	E0411a		279.15	541.15	298.15	1.0	1019.2	988.6	-30.6	-3.0	78.1	80.0	1.9	2.4
886	725	V	E0412a		-	513.15	298.15	1.0	995.3	957.9	-37.4	-3.8	73.2	74.8	1.6	2.1
887	726	V	F7202a		210.55	428.65	298.15	1.0	874.6	873.0	-1.6	-0.2	50.0	49.5	-0.5	-1.0
888	727	V	F8201a		-	451.25	302.25	1.0	869.0	865.8	-3.2	-0.4	53.8	53.9	0.1	0.2
889	728	V	F9201a		234.05	471.95	298.15	1.0	871.0	867.6	-3.4	-0.4	58.2	59.4	1.2	2.1
890	729	V	F0203a		240.15	485.72	293.15	1.0	867.0	865.5	-1.4	-0.2	-	-	-	-
891	730	V	L7101a		290.15	404.15	298.15	1.0	833.5	847.5	14.0	1.7	-	-	-	-
892	730	V	L7101b		290.15	404.15	313.0	1.0	-	-	-	-	48.7	54.8	6.1	12.5
893	731	V	L7102a		-	430.15	293.15	1.0	846.6	849.8	3.1	0.4	-	-	-	-
894	732	V	L7103a		-	420.15	293.15	1.0	827.0	837.4	10.4	1.3	-	-	-	-
895	733	V	L7104a		-	413.15	298.15	1.0	837.3	829.2	-8.1	-1.0	-	-	-	-
896	733	V	L7104b		-	413.15	333.0	1.0	-	-	-	-	53.2	53.6	0.4	0.7
897	734	V	L7105a		-	433.15	298.15	1.0	823.8	842.1	18.4	2.2	-	-	-	-
898	735	V	L7106a		282.45	409.15	298.15	1.0	822.4	821.7	-0.7	-0.1	-	-	-	-
899	735	V	L7106b		282.45	409.15	333.0	1.0	-	-	-	-	51.4	53.7	2.3	4.4
900	736	V	L7107a		-	412.15	298.15	1.0	828.5	823.9	-4.6	-0.6	-	-	-	-
901	737	V	L7108a		-	411.15	293.15	1.0	811.9	806.5	-5.4	-0.7	-	-	-	-
902	738	V	L7109a		-	406.15	298.15	1.0	810.0	800.8	-9.2	-1.1	-	-	-	-
903	738	V	L7109b		-	406.15	343.0	1.0	-	-	-	-	49.7	50.3	0.6	1.2
904	739	V	L7110a		-	426.15	294.15	1.0	836.0	818.9	-17.1	-2.0	-	-	-	-
905	740	V	L7111a		-	411.95	298.15	1.0	824.9	810.0	-14.9	-1.8	-	-	-	-
906	740	V	L7111b		-	411.95	322.0	1.0	-	-	-	-	53.6	56.6	3.0	5.6
907	741	V	L7112a		-	430.15	293.15	1.0	828.2	846.9	18.7	2.3	-	-	-	-
908	741	V	L7112b		-	430.15	373.0	1.0	-	-	-	-	55.7	50.0	-5.8	-10.3
909	742	V	L7113a		260.15	415.65	298.15	1.0	839.6	829.0	-10.5	-1.2	57.3	59.0	1.7	3.0
910	743	V	L7114a		-	438.15	293.15	1.0	832.0	841.6	9.6	1.1	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
911	744	V	L7115a		-	426.15	293.15	1.0	837.9	830.7	-7.2	-0.8	-	-	-	-
912	745	V	L7116a		-	415.95	298.15	1.0	820.2	814.1	-6.0	-0.7	-	-	-	-
913	745	V	L7116b		-	415.95	338.0	1.0	-	-	-	-	53.6	54.7	1.1	2.0
914	746	V	L7117a		-	433.15	293.15	1.0	815.1	822.5	7.4	0.9	-	-	-	-
915	747	V	L7118a		-	415.95	298.15	1.0	809.8	796.3	-13.5	-1.7	58.6	60.3	1.7	2.9
916	748	V	L7119a		-	435.15	298.15	1.0	832.7	827.4	-5.3	-0.6	-	-	-	-
917	749	V	L7120a		-	425.15	298.15	1.0	833.3	814.4	-18.9	-2.3	-	-	-	-
918	750	V	L7121a		-	437.15	296.15	1.0	836.0	829.4	-6.6	-0.8	-	-	-	-
919	751	V	L7122a		-	422.15	314.89	0.01	805.7	797.3	-8.4	-1.0	-	-	-	-
920	752	V	L7123a		-	438.15	297.15	1.0	819.0	823.2	4.2	0.5	-	-	-	-
921	753	V	L7124a		-	425.15	298.15	1.0	822.0	802.3	-19.7	-2.4	-	-	-	-
922	754	V	L7125a		-	418.15	293.15	1.0	823.9	804.5	-19.4	-2.4	-	-	-	-
923	754	V	L7125b		-	418.15	338.0	1.0	-	-	-	-	55.7	56.4	0.7	1.3
924	755	V	L7126a		-	432.15	298.15	1.0	816.0	810.8	-5.2	-0.6	-	-	-	-
925	756	V	L7127a		-	424.15	298.15	1.0	817.7	798.4	-19.3	-2.4	-	-	-	-
926	757	V	L7128a		-	421.15	293.15	1.0	833.1	798.0	-35.1	-4.2	59.8	62.9	3.1	5.2
927	758	V	L7129a		-	424.15	293.15	1.0	813.1	785.9	-27.2	-3.3	-	-	-	-
928	759	V	L7130a		-	439.15	328.67	0.01	803.5	802.5	-1.0	-0.1	-	-	-	-
929	760	V	L7131a		-	439.15	298.15	1.0	828.8	819.3	-9.5	-1.1	-	-	-	-
930	761	V	L7132a		-	445.15	298.15	1.0	824.5	817.0	-7.5	-0.9	-	-	-	-
931	762	V	L7133a		-	446.15	297.15	1.0	821.0	816.1	-4.9	-0.6	-	-	-	-
932	762	V	L7133b		-	446.15	363.0	1.0	-	-	-	-	62.6	56.5	-6.1	-9.7
933	763	V	L7134a		-	436.15	293.15	1.0	827.0	813.9	-13.1	-1.6	-	-	-	-
934	764	V	L7135a		231.95	427.85	298.15	1.0	815.6	795.1	-20.5	-2.5	62.4	63.6	1.2	1.9
935	765	V	L7136a		-	429.85	298.15	1.0	816.5	794.9	-21.6	-2.6	-	-	-	-
936	765	V	L7136b		-	429.85	364.0	1.0	-	-	-	-	53.1	54.4	1.3	2.5
937	766	V	L7137a		-	445.15	298.15	1.0	819.2	806.2	-12.9	-1.6	-	-	-	-
938	767	V	L7138a		-	432.35	298.15	1.0	813.4	788.5	-24.9	-3.1	62.1	63.3	1.2	1.9
939	768	V	L7139a		239.95	449.45	298.15	1.0	819.2	811.2	-7.9	-1.0	66.5	65.7	-0.8	-1.1
940	769	V	L8102a		-	433.15	298.15	1.0	815.1	867.5	52.4	6.4	-	-	-	-
941	770	V	L8103a		-	425.15	298.15	1.0	842.9	856.6	13.7	1.6	-	-	-	-
942	770	V	L8103b		-	425.15	333.0	1.0	-	-	-	-	47.3	54.9	7.6	16.0
943	771	V	L8104a		253.15	419.55	293.15	1.0	823.7	820.2	-3.5	-0.4	-	-	-	-
944	772	V	L8105a		-	438.15	293.15	1.0	855.7	860.8	5.0	0.6	-	-	-	-
945	773	V	L8106a		-	430.15	293.15	1.0	849.2	851.0	1.8	0.2	-	-	-	-
946	774	V	L8107a		-	431.15	293.15	1.0	840.8	846.1	5.3	0.6	-	-	-	-
947	775	V	L8108a		260.15	424.15	293.15	1.0	832.4	837.8	5.4	0.7	-	-	-	-
948	775	V	L8108b		260.15	424.15	343.0	1.0	-	-	-	-	57.1	54.4	-2.7	-4.8
949	776	V	L8109a		-	431.15	293.15	1.0	808.0	839.8	31.8	3.9	-	-	-	-
950	777	V	L8110a		-	433.00	293.15	1.0	857.6	859.3	1.7	0.2	-	-	-	-
951	778	V	L8111a		-	433.15	293.15	1.0	829.5	852.6	23.1	2.8	-	-	-	-
952	779	V	L8112a		-	432.15	293.15	1.0	834.1	849.4	15.2	1.8	-	-	-	-
953	780	V	L8113a		-	433.00	293.15	1.0	845.7	842.2	-3.5	-0.4	-	-	-	-
954	781	V	L8114a		-	425.15	298.15	1.0	834.5	839.8	5.3	0.6	-	-	-	-
955	782	V	L8115a		-	431.35	293.15	1.0	837.1	833.8	-3.3	-0.4	-	-	-	-
956	783	V	L8116a		-	446.00	298.15	1.0	842.5	851.0	8.5	1.0	-	-	-	-
957	784	V	L8118a		-	429.25	293.15	1.0	834.2	830.7	-3.5	-0.4	-	-	-	-
958	785	V	L8119a		-	430.95	298.15	1.0	834.6	834.4	-0.2	-0.0	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
959	786	V	L8120a		-	433.25	298.15	1.0	831.0	828.5	-2.5	-0.3	-	-	-	-
960	787	V	L8121a		-	441.45	293.15	1.0	838.4	834.3	-4.1	-0.5	-	-	-	-
961	787	V	L8121b		-	441.45	348.0	1.0	-	-	-	-	54.7	56.4	1.6	3.0
962	788	V	L8122a		-	425.15	298.15	1.0	827.0	815.9	-11.1	-1.3	-	-	-	-
963	789	V	L8123a		-	444.15	293.15	1.0	833.0	830.4	-2.6	-0.3	-	-	-	-
964	790	V	L8124a		-	426.15	293.15	1.0	833.9	819.7	-14.2	-1.7	-	-	-	-
965	791	V	L8126a		-	423.85	301.15	1.0	806.5	811.1	4.6	0.6	-	-	-	-
966	792	V	L8127a		-	425.65	298.15	1.0	811.5	796.3	-15.2	-1.9	-	-	-	-
967	793	V	L8128a		-	446.15	298.15	1.0	842.5	839.6	-2.9	-0.3	-	-	-	-
968	794	V	L8130a		-	456.15	293.15	1.0	849.8	846.0	-3.8	-0.5	-	-	-	-
969	795	V	L8131a		-	444.15	331.02	0.01	805.0	803.8	-1.2	-0.1	-	-	-	-
970	796	V	L8134a		-	432.15	298.15	1.0	813.5	805.9	-7.6	-0.9	-	-	-	-
971	796	V	L8134b		-	432.15	352.0	1.0	-	-	-	-	55.0	56.3	1.3	2.3
972	797	V	L8137a		-	432.15	298.15	1.0	834.2	830.3	-3.9	-0.5	-	-	-	-
973	797	V	L8137b	×	-	432.15	345.0	1.0	-	-	-	-	49.2	57.3	8.1	16.5
974	798	V	L8138a		-	454.00	293.15	1.0	839.0	843.8	4.8	0.6	-	-	-	-
975	799	V	L8140a		-	445.65	293.15	1.0	826.5	832.6	6.1	0.7	-	-	-	-
976	800	V	L8141a		191.15	434.25	298.15	1.0	820.2	817.8	-2.4	-0.3	-	-	-	-
977	800	V	L8141b		191.15	434.25	345.0	1.0	-	-	-	-	54.8	58.1	3.3	6.0
978	801	V	L8142a		190.15	434.15	298.15	1.0	824.9	816.3	-8.6	-1.0	-	-	-	-
979	801	V	L8142b		190.15	434.15	353.0	1.0	-	-	-	-	54.7	57.0	2.3	4.1
980	802	V	L8144a		222.75	429.85	298.15	1.0	805.0	801.6	-3.4	-0.4	-	-	-	-
981	802	V	L8144b		222.75	429.85	358.0	1.0	-	-	-	-	53.1	56.4	3.3	6.2
982	803	V	L8145a		-	437.15	332.39	0.01	812.9	799.1	-13.8	-1.7	-	-	-	-
983	804	V	L8146a		150.15	428.55	298.15	1.0	794.2	814.9	20.7	2.6	-	-	-	-
984	804	V	L8146b	×	150.15	428.55	318.66	0.01	-	-	-	-	43.5	64.4	20.8	47.8
985	805	V	L8147a		-	437.85	298.15	1.0	833.5	813.6	-19.9	-2.4	-	-	-	-
986	805	V	L8147b	×	-	437.85	355.0	1.0	-	-	-	-	48.0	58.1	10.1	21.0
987	806	V	L8148a		-	439.25	298.15	1.0	817.6	806.5	-11.1	-1.4	-	-	-	-
988	806	V	L8148b	×	-	439.25	356.0	1.0	-	-	-	-	48.0	58.7	10.7	22.3
989	807	V	L8149a		-	440.75	298.15	1.0	821.0	803.9	-17.1	-2.1	-	-	-	-
990	807	V	L8149b		-	440.75	364.0	1.0	-	-	-	-	54.8	56.6	1.8	3.2
991	808	V	L8150a		-	449.65	293.15	1.0	827.3	824.5	-2.8	-0.3	-	-	-	-
992	808	V	L8150b		-	449.65	365.0	1.0	-	-	-	-	53.3	57.7	4.4	8.2
993	809	V	L8152a		181.95	426.75	298.15	1.0	814.1	808.8	-5.4	-0.7	-	-	-	-
994	810	V	L8153a		-	456.15	293.15	1.0	828.2	823.1	-5.1	-0.6	-	-	-	-
995	811	V	L8154a		171.15	444.75	298.15	1.0	799.0	804.6	5.6	0.7	-	-	-	-
996	811	V	L8154b		171.15	444.75	366.0	1.0	-	-	-	-	54.2	57.8	3.6	6.6
997	812	V	L8155a		-	452.15	298.15	1.0	824.5	807.5	-17.0	-2.1	-	-	-	-
998	813	V	L8156a		212.15	445.05	298.15	1.0	810.0	796.9	-13.1	-1.6	-	-	-	-
999	813	V	L8156b	×	212.15	445.05	363.0	1.0	-	-	-	-	47.2	57.9	10.7	22.8
1000	814	V	L8157a		192.15	439.25	298.15	1.0	809.8	799.5	-10.2	-1.3	-	-	-	-
1001	814	V	L8157b		192.15	439.25	363.0	1.0	-	-	-	-	54.8	57.3	2.5	4.6
1002	815	V	L8158a		-	433.00	298.15	1.0	776.6	793.4	16.8	2.2	-	-	-	-
1003	816	V	L8159a		168.15	445.05	298.15	1.0	803.4	789.7	-13.7	-1.7	-	-	-	-
1004	816	V	L8159b		168.15	445.05	369.0	1.0	-	-	-	-	55.2	56.7	1.5	2.6
1005	817	V	L8160a		-	453.00	301.15	1.0	829.0	825.6	-3.4	-0.4	-	-	-	-
1006	818	V	L8161a		-	452.15	294.15	1.0	900.0	824.5	-75.5	-8.4	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1007	819	V	L8162a		203.15	457.75	298.15	1.0	828.7	820.5	-8.2	-1.0	68.5	68.0	-0.5	-0.7
1008	820	V	L8163a		-	456.35	298.15	1.0	806.0	819.4	13.3	1.7	-	-	-	-
1009	820	V	L8163b		-	456.35	372.0	1.0	-	-	-	-	55.9	59.7	3.8	6.8
1010	821	V	L8164a		183.15	459.15	298.15	1.0	784.5	818.9	34.4	4.4	-	-	-	-
1011	821	V	L8164b		183.15	459.15	375.0	1.0	-	-	-	-	53.4	59.0	5.6	10.5
1012	822	V	L8165a		-	459.75	298.15	1.0	815.2	818.8	3.6	0.4	-	-	-	-
1013	822	V	L8165b		-	459.75	379.0	1.0	-	-	-	-	57.6	58.6	1.0	1.8
1014	823	V	L8166a		-	448.75	298.15	1.0	798.7	813.0	14.3	1.8	-	-	-	-
1015	824	V	L8167a		-	449.75	298.15	1.0	815.9	799.9	-16.0	-2.0	67.2	68.7	1.4	2.1
1016	825	V	L8168a		228.15	447.85	298.15	1.0	817.0	799.4	-17.6	-2.2	-	-	-	-
1017	826	V	L8169a		167.15	460.85	298.15	1.0	817.6	810.4	-7.1	-0.9	-	-	-	-
1018	826	V	L8169b		167.15	460.85	383.0	1.0	-	-	-	-	61.0	57.7	-3.3	-5.5
1019	827	V	L8170a		-	452.95	298.15	1.0	817.0	793.8	-23.2	-2.8	67.9	68.3	0.4	0.6
1020	828	V	L8171a		258.45	468.35	298.15	1.0	821.8	815.0	-6.8	-0.8	70.1	70.8	0.7	1.0
1021	829	V	L9103a		-	447.35	344.93	0.01	814.0	834.8	20.9	2.6	-	-	-	-
1022	830	V	L9107a		-	447.15	298.15	1.0	852.6	872.1	19.5	2.3	-	-	-	-
1023	831	V	L9108a		-	439.15	294.15	1.0	832.3	876.1	43.8	5.3	-	-	-	-
1024	832	V	L9109a		-	446.25	293.15	1.0	846.2	860.5	14.3	1.7	-	-	-	-
1025	832	V	L9109b		-	446.25	358.0	1.0	-	-	-	-	55.1	54.9	-0.2	-0.4
1026	833	V	L9110a		-	466.00	293.15	1.0	847.5	839.4	-8.1	-1.0	-	-	-	-
1027	834	V	L9111a		-	439.00	293.15	1.0	835.0	836.6	1.6	0.2	-	-	-	-
1028	835	V	L9113a		-	451.05	298.15	1.0	854.9	866.1	11.2	1.3	-	-	-	-
1029	835	V	L9113b		-	451.05	384.0	1.0	-	-	-	-	50.0	47.7	-2.3	-4.5
1030	836	V	L9115a		-	444.15	293.15	1.0	848.8	855.1	6.3	0.7	-	-	-	-
1031	837	V	L9116a		-	439.00	293.15	1.0	825.6	838.8	13.2	1.6	-	-	-	-
1032	838	V	L9119a		-	433.15	333.57	0.01	758.1	797.1	39.0	5.2	-	-	-	-
1033	839	V	L9120a		-	466.00	288.15	1.0	835.3	854.9	19.6	2.3	-	-	-	-
1034	840	V	L9121a		-	442.00	293.15	1.0	825.0	827.4	2.4	0.3	-	-	-	-
1035	841	V	L9122a		-	466.00	359.85	0.01	778.5	769.8	-8.6	-1.1	-	-	-	-
1036	842	V	L9124a		-	452.00	288.15	1.0	861.0	864.6	3.6	0.4	-	-	-	-
1037	843	V	L9125a		-	457.25	298.15	1.0	844.5	844.8	0.3	0.0	-	-	-	-
1038	844	V	L9128a		-	452.00	298.15	1.0	899.4	847.6	-51.8	-5.8	-	-	-	-
1039	845	V	L9129a		-	447.15	294.15	1.0	838.3	837.8	-0.5	-0.1	-	-	-	-
1040	846	V	L9130a		-	475.15	293.15	1.0	846.0	851.3	5.3	0.6	-	-	-	-
1041	847	V	L9131a		-	451.00	298.15	1.0	823.7	826.7	3.0	0.4	-	-	-	-
1042	848	V	L9132a		-	451.15	298.15	1.0	833.4	837.7	4.3	0.5	-	-	-	-
1043	849	V	L9133a		-	461.15	298.15	1.0	837.0	846.5	9.5	1.1	-	-	-	-
1044	850	V	L9134a		-	445.15	295.15	1.0	839.6	840.5	0.9	0.1	-	-	-	-
1045	851	V	L9136a		-	450.00	298.15	1.0	821.8	827.4	5.6	0.7	-	-	-	-
1046	852	V	L9137a		-	444.55	293.15	1.0	824.2	824.1	-0.1	-0.0	-	-	-	-
1047	853	V	L9138a		-	446.15	289.15	1.0	828.5	822.3	-6.2	-0.8	-	-	-	-
1048	854	V	L9139a		-	466.15	298.15	1.0	823.6	833.7	10.1	1.2	67.9	69.5	1.6	2.4
1049	855	V	L9141a		-	455.00	298.15	1.0	828.0	818.3	-9.7	-1.2	-	-	-	-
1050	856	V	L9142a		-	-	295.15	1.0	830.0	810.8	-19.2	-2.3	-	-	-	-
1051	857	V	L9143a		-	444.15	293.15	1.0	818.6	804.1	-14.5	-1.8	-	-	-	-
1052	858	V	L9144a		-	452.00	293.15	1.0	827.5	838.6	11.1	1.3	-	-	-	-
1053	859	V	L9145a		-	460.15	293.15	1.0	859.2	836.9	-22.3	-2.6	-	-	-	-
1054	860	V	L9147a		-	448.15	293.15	1.0	814.8	805.8	-9.0	-1.1	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1055	861	V	L9148a		-	467.15	273.15	1.0	878.7	826.4	-52.3	-6.0	-	-	-	-
1056	862	V	L9149a		-	451.00	298.15	1.0	806.4	804.2	-2.2	-0.3	65.2	70.9	5.7	8.7
1057	863	V	L9150a		-	452.15	298.15	1.0	829.9	833.9	4.0	0.5	-	-	-	-
1058	864	V	L9151a		-	455.35	298.15	1.0	829.9	831.8	1.9	0.2	-	-	-	-
1059	865	V	L9153a		-	454.15	298.15	1.0	824.6	821.7	-2.9	-0.3	-	-	-	-
1060	866	V	L9154a		-	-	298.15	1.0	827.5	820.5	-7.0	-0.8	-	-	-	-
1061	866	V	L9154b		-	-	368.0	1.0	-	-	-	-	53.2	58.7	5.5	10.3
1062	867	V	L9155a		-	455.00	293.15	1.0	843.9	826.6	-17.3	-2.0	-	-	-	-
1063	868	V	L9156a		-	451.15	298.15	1.0	813.4	805.2	-8.2	-1.0	-	-	-	-
1064	868	V	L9156b		-	451.15	353.0	1.0	-	-	-	-	64.6	62.0	-2.6	-4.0
1065	869	V	L9157a		-	466.15	298.15	1.0	835.8	839.3	3.5	0.4	-	-	-	-
1066	870	V	L9159a		-	455.00	298.15	1.0	815.6	818.7	3.1	0.4	-	-	-	-
1067	871	V	L9160a		-	459.00	298.15	1.0	843.7	816.5	-27.2	-3.2	-	-	-	-
1068	872	V	L9161a		-	453.15	291.15	1.0	834.0	821.2	-12.8	-1.5	-	-	-	-
1069	873	V	L9162a		-	454.00	300.15	1.0	831.0	808.5	-22.5	-2.7	-	-	-	-
1070	874	V	L9163a		-	457.15	293.15	1.0	827.0	811.3	-15.7	-1.9	-	-	-	-
1071	874	V	L9163b		-	457.15	403.0	1.0	-	-	-	-	49.5	53.8	4.3	8.8
1072	875	V	L9164a		-	468.15	293.15	1.0	828.8	833.9	5.1	0.6	-	-	-	-
1073	876	V	L9165a		-	465.15	293.15	1.0	825.6	826.4	0.8	0.1	-	-	-	-
1074	877	V	L9166a		-	466.00	298.15	1.0	820.8	816.8	-4.0	-0.5	-	-	-	-
1075	878	V	L9167a		-	455.00	296.15	1.0	822.0	813.2	-8.8	-1.1	-	-	-	-
1076	879	V	L9169a		-	459.00	301.15	1.0	832.0	804.6	-27.4	-3.3	-	-	-	-
1077	880	V	L9170a		-	-	300.15	1.0	823.0	814.5	-8.5	-1.0	-	-	-	-
1078	881	V	L9171a		-	454.00	298.15	1.0	821.0	803.0	-18.0	-2.2	-	-	-	-
1079	882	V	L9172a		-	457.15	298.15	1.0	815.0	803.4	-11.6	-1.4	-	-	-	-
1080	883	V	L9173a		-	455.00	293.15	1.0	813.6	802.8	-10.8	-1.3	-	-	-	-
1081	884	V	L9174a		-	459.00	285.15	1.0	840.2	807.8	-32.4	-3.9	-	-	-	-
1082	885	V	L9177a		-	480.15	296.15	1.0	834.0	829.8	-4.2	-0.5	-	-	-	-
1083	886	V	L9179a		-	472.00	298.15	1.0	848.0	829.0	-19.0	-2.2	-	-	-	-
1084	887	V	L9181a		-	473.00	300.65	1.0	820.0	819.6	-0.4	-0.1	-	-	-	-
1085	888	V	L9182a		-	473.00	297.15	1.0	828.0	823.0	-5.0	-0.6	-	-	-	-
1086	889	V	L9183a		-	473.00	297.15	1.0	827.0	821.2	-5.8	-0.7	-	-	-	-
1087	890	V	L9184a		-	479.15	370.37	0.01	770.4	768.0	-2.3	-0.3	-	-	-	-
1088	891	V	L9185a		-	473.00	277.15	1.0	841.8	829.9	-11.9	-1.4	-	-	-	-
1089	892	V	L9186a		278.75	468.25	298.15	1.0	818.3	804.3	-14.0	-1.7	71.4	73.8	2.4	3.3
1090	893	V	L9187a		-	466.15	293.15	1.0	826.3	807.2	-19.1	-2.3	71.5	74.1	2.6	3.6
1091	894	V	L9188a		-	467.85	298.15	1.0	823.5	803.7	-19.8	-2.4	70.9	73.4	2.5	3.5
1092	895	V	L9189a		-	479.15	298.15	1.0	826.0	813.5	-12.5	-1.5	-	-	-	-
1093	896	V	L9190a		-	471.65	298.15	1.0	819.4	798.6	-20.7	-2.5	72.9	73.2	0.3	0.4
1094	897	V	L9191a		268.15	486.25	298.15	1.0	824.6	817.6	-7.0	-0.8	72.2	75.6	3.4	4.8
1095	898	V	L0103a		-	464.15	293.15	1.0	862.4	878.8	16.4	1.9	-	-	-	-
1096	899	V	L0104a		-	475.15	293.15	1.0	874.2	905.5	31.3	3.6	-	-	-	-
1097	900	V	L0105a		-	474.15	293.15	1.0	874.5	892.0	17.5	2.0	-	-	-	-
1098	901	V	L0106a		-	465.15	293.15	1.0	858.4	886.5	28.1	3.3	-	-	-	-
1099	902	V	L0107a		-	513.48	293.15	1.0	839.3	867.6	28.3	3.4	-	-	-	-
1100	903	V	L0108a		-	463.15	293.15	1.0	854.9	877.9	23.0	2.7	-	-	-	-
1101	904	V	L0111a		-	468.15	293.15	1.0	862.3	883.8	21.5	2.5	-	-	-	-
1102	905	V	L0112a		-	475.00	293.15	1.0	837.8	849.8	12.0	1.4	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1103	906	V	L0115a		-	467.65	298.15	1.0	859.1	864.5	5.4	0.6	-	-	-	-
1104	907	V	L0117a		-	459.15	293.15	1.0	848.7	857.3	8.6	1.0	-	-	-	-
1105	908	V	L0118a		-	460.00	293.15	1.0	842.8	850.5	7.7	0.9	-	-	-	-
1106	909	V	L0119a		-	468.75	293.15	1.0	854.3	850.6	-3.6	-0.4	-	-	-	-
1107	910	V	L011aa		-	490.15	293.15	1.0	825.2	805.8	-19.4	-2.4	-	-	-	-
1108	911	V	L011ba		280.15	503.35	298.15	1.0	826.5	819.9	-6.7	-0.8	80.9	80.6	-0.3	-0.3
1109	912	V	L0120a		-	454.15	293.15	1.0	833.0	837.6	4.6	0.6	-	-	-	-
1110	913	V	L0121a		-	465.15	293.15	1.0	853.7	860.4	6.7	0.8	-	-	-	-
1111	914	V	L0122a		-	460.00	293.15	1.0	860.6	868.7	8.1	0.9	-	-	-	-
1112	915	V	L0124a		-	463.00	293.15	1.0	839.8	832.0	-7.8	-0.9	-	-	-	-
1113	916	V	L0126a		-	460.15	293.15	1.0	833.9	858.0	24.1	2.9	-	-	-	-
1114	917	V	L0127a		-	463.00	293.15	1.0	823.6	825.9	2.3	0.3	-	-	-	-
1115	918	V	L0128a		-	455.15	294.15	1.0	823.0	829.6	6.7	0.8	-	-	-	-
1116	919	V	L0129a	×	-	455.00	289.15	1.0	751.3	840.1	88.8	11.8	-	-	-	-
1117	920	V	L0130a		-	466.00	293.15	1.0	826.5	827.0	0.5	0.1	-	-	-	-
1118	921	V	L0132a		-	466.15	291.15	1.0	833.0	822.8	-10.2	-1.2	-	-	-	-
1119	922	V	L0134a		-	463.15	298.15	1.0	841.3	845.9	4.6	0.5	-	-	-	-
1120	923	V	L0135a		-	466.15	293.15	1.0	845.5	849.3	3.8	0.5	-	-	-	-
1121	924	V	L0137a		-	462.25	298.15	1.0	824.9	833.3	8.4	1.0	-	-	-	-
1122	925	V	L0139a		-	464.00	301.15	1.0	825.8	826.9	1.1	0.1	-	-	-	-
1123	926	V	L0140a		-	466.00	298.15	1.0	837.0	829.2	-7.8	-0.9	-	-	-	-
1124	927	V	L0141a		-	464.00	293.15	1.0	823.2	825.8	2.6	0.3	-	-	-	-
1125	928	V	L0142a		205.65	465.15	295.15	1.0	834.7	827.2	-7.5	-0.9	-	-	-	-
1126	929	V	L0143a		-	465.15	273.15	1.0	842.1	835.9	-6.2	-0.7	-	-	-	-
1127	930	V	L0144a		-	469.15	298.15	1.0	826.0	817.5	-8.5	-1.0	-	-	-	-
1128	931	V	L0145a		-	463.15	293.15	1.0	821.2	826.3	5.1	0.6	-	-	-	-
1129	932	V	L0146a		-	485.00	293.15	1.0	825.7	824.8	-0.9	-0.1	-	-	-	-
1130	933	V	L0147a		-	485.00	293.15	1.0	827.3	816.5	-10.8	-1.3	-	-	-	-
1131	934	V	L0148a		-	485.00	298.15	1.0	821.1	805.0	-16.1	-2.0	-	-	-	-
1132	935	V	L0149a		-	466.00	290.15	1.0	865.0	849.9	-15.1	-1.7	-	-	-	-
1133	936	V	L0151a		-	486.15	293.15	1.0	832.2	828.8	-3.4	-0.4	-	-	-	-
1134	937	V	L0152a		-	464.00	358.25	0.01	786.1	779.3	-6.8	-0.9	-	-	-	-
1135	938	V	L0153a		-	464.00	298.15	1.0	821.5	822.4	0.9	0.1	-	-	-	-
1136	939	V	L0154a		-	485.00	293.15	1.0	829.1	812.0	-17.1	-2.1	-	-	-	-
1137	940	V	L0155a		-	467.15	293.15	1.0	815.2	810.5	-4.7	-0.6	-	-	-	-
1138	941	V	L0156a		-	477.15	277.15	1.0	846.0	838.1	-7.9	-0.9	-	-	-	-
1139	942	V	L0157a		-	468.15	361.57	0.01	759.7	766.6	6.9	0.9	-	-	-	-
1140	943	V	L0158a		-	475.15	293.15	1.0	814.0	805.8	-8.2	-1.0	-	-	-	-
1141	944	V	L0159a		-	467.15	298.15	1.0	828.3	834.5	6.2	0.8	-	-	-	-
1142	945	V	L0160a		-	466.00	298.15	1.0	826.8	833.5	6.8	0.8	-	-	-	-
1143	946	V	L0161a		-	472.15	298.15	1.0	836.1	831.4	-4.7	-0.6	-	-	-	-
1144	947	V	L0162a		-	481.15	293.15	1.0	830.0	833.9	3.9	0.5	-	-	-	-
1145	948	V	L0163a		-	475.15	298.15	1.0	825.4	823.6	-1.8	-0.2	-	-	-	-
1146	949	V	L0164a		-	482.00	298.15	1.0	827.1	822.9	-4.2	-0.5	-	-	-	-
1147	950	V	L0165a		-	482.00	298.15	1.0	826.5	822.4	-4.0	-0.5	-	-	-	-
1148	951	V	L0166a		-	487.00	298.15	1.0	807.8	809.2	1.4	0.2	-	-	-	-
1149	952	V	L0167a		-	488.35	303.15	1.0	834.1	832.9	-1.2	-0.1	-	-	-	-
1150	953	V	L0169a		-	482.00	300.15	1.0	826.0	818.2	-7.8	-0.9	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1151	954	V	L0170a		-	487.00	295.15	1.0	845.0	814.0	-31.0	-3.7	-	-	-	-
1152	955	V	L0171a		-	481.55	298.15	1.0	824.5	810.6	-13.9	-1.7	-	-	-	-
1153	956	V	L0172a		-	481.15	293.15	1.0	828.6	835.0	6.4	0.8	-	-	-	-
1154	957	V	L0173a		-	472.00	297.65	1.0	839.6	818.1	-21.5	-2.6	-	-	-	-
1155	958	V	L0176a		-	483.00	291.15	1.0	830.0	825.1	-4.9	-0.6	-	-	-	-
1156	959	V	L0179a		-	485.15	298.15	1.0	832.0	818.1	-13.8	-1.7	-	-	-	-
1157	959	V	L0179b	×	-	485.15	356.0	1.0	-	-	-	-	79.1	68.9	-10.2	-12.9
1158	960	V	L0180a		-	-	288.15	1.0	830.3	820.4	-9.9	-1.2	-	-	-	-
1159	961	V	L0182a		-	487.00	293.15	1.0	833.2	810.7	-22.5	-2.7	-	-	-	-
1160	962	V	L0184a		-	482.00	298.15	1.0	820.0	807.0	-13.1	-1.6	-	-	-	-
1161	963	V	L0185a		-	482.00	293.15	1.0	821.5	805.8	-15.7	-1.9	-	-	-	-
1162	964	V	L0186a		-	487.00	376.65	0.01	760.1	742.5	-17.6	-2.3	-	-	-	-
1163	965	V	L0187a		-	482.00	372.65	0.01	763.4	775.9	12.5	1.6	-	-	-	-
1164	966	V	L0188a		-	-	289.15	1.0	836.0	830.1	-5.9	-0.7	-	-	-	-
1165	967	V	L0189a		-	491.05	293.15	1.0	832.2	827.2	-5.0	-0.6	-	-	-	-
1166	968	V	L0191a		-	487.00	297.15	1.0	831.0	824.4	-6.6	-0.8	-	-	-	-
1167	969	V	L0192a		-	489.15	300.15	1.0	826.0	821.6	-4.4	-0.5	-	-	-	-
1168	970	V	L0193a		-	487.00	296.15	1.0	837.0	823.9	-13.1	-1.6	-	-	-	-
1169	971	V	L0194a		-	487.00	298.15	1.0	828.2	823.3	-4.9	-0.6	-	-	-	-
1170	972	V	L0195a		-	495.15	288.15	1.0	833.6	824.8	-8.9	-1.1	-	-	-	-
1171	973	V	L0196a		281.85	474.15	298.15	1.0	820.6	807.4	-13.2	-1.6	-	-	-	-
1172	974	V	L0197a		262.15	483.15	293.15	1.0	825.0	810.8	-14.2	-1.7	-	-	-	-
1173	975	V	L0198a		265.65	483.00	298.15	1.0	822.9	807.7	-15.2	-1.9	-	-	-	-
1174	976	V	L0199a		-	493.00	381.45	0.01	771.1	755.3	-15.8	-2.0	-	-	-	-
1175	977	V	L7201a		-	525.85	293.15	1.0	961.3	967.7	6.4	0.7	-	-	-	-
1176	978	V	L7202a		-	470.00	293.15	1.0	920.6	880.5	-40.0	-4.3	-	-	-	-
1177	979	V	L7204a		-	-	298.15	1.0	961.2	948.5	-12.8	-1.3	-	-	-	-
1178	980	V	L7206a		-	517.03	293.15	1.0	952.8	965.1	12.3	1.3	-	-	-	-
1179	981	V	L7207a		-	517.03	293.15	1.0	929.6	898.2	-31.4	-3.4	-	-	-	-
1180	982	V	L7208a		-	517.03	291.15	1.0	932.1	892.0	-40.1	-4.3	-	-	-	-
1181	983	V	L7212a		334.45	507.15	334.45	1.0	949.0	951.7	2.7	0.3	-	-	-	-
1182	984	V	L7217a		-	494.25	295.15	1.0	967.0	935.4	-31.6	-3.3	-	-	-	-
1183	985	V	L7220a		-	508.21	293.15	1.0	967.2	960.2	-7.0	-0.7	-	-	-	-
1184	986	V	L7221a		-	-	295.15	1.0	943.0	921.1	-21.9	-2.3	-	-	-	-
1185	987	V	L7224a		-	508.21	298.15	1.0	926.0	902.8	-23.2	-2.5	-	-	-	-
1186	988	V	L7226a		-	485.43	293.15	1.0	962.5	955.4	-7.1	-0.7	-	-	-	-
1187	989	V	L7227a		-	485.43	293.15	1.0	967.9	960.1	-7.8	-0.8	-	-	-	-
1188	990	V	L7228a		-	-	298.15	1.0	946.1	940.7	-5.4	-0.6	-	-	-	-
1189	991	V	L7230a		-	515.15	298.15	1.0	950.4	932.3	-18.1	-1.9	-	-	-	-
1190	992	V	L7232a		-	489.79	293.15	1.0	970.5	935.4	-35.1	-3.6	-	-	-	-
1191	993	V	L7234a		-	485.43	298.15	1.0	962.0	927.7	-34.3	-3.6	-	-	-	-
1192	994	V	L7235a		295.05	535.15	298.15	1.0	952.2	947.4	-4.8	-0.5	96.5	97.7	1.1	1.2
1193	995	V	L8202a		-	-	293.35	1.0	922.9	890.7	-32.2	-3.5	-	-	-	-
1194	996	V	L8203a		364.15	487.15	362.0	0.01	852.2	857.3	5.1	0.6	-	-	-	-
1195	997	V	L8204a		328.35	508.15	391.21	0.01	865.1	872.4	7.3	0.8	-	-	-	-
1196	997	V	L8204b		328.35	508.15	428.0	1.0	-	-	-	-	58.5	61.7	3.2	5.5
1197	998	V	L8205a		-	-	298.15	1.0	928.5	928.3	-0.2	-0.0	-	-	-	-
1198	999	V	L8206a		-	-	293.15	1.0	917.2	887.0	-30.2	-3.3	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m	T_b	T	P	ρ_{liq}[kg·m^{-3}]				ΔH_{vap}[kJ·mol^{-1}]			
					[K]	[K]	[K]	[bar]	exp	sim	dev	err [%]	exp	sim	dev	err [%]
1199	1000	V	L8207a		-	-	298.15	1.0	929.0	913.5	-15.6	-1.7	-	-	-	-
1200	1001	V	L8208a		-	478.13	369.56	0.01	875.7	844.6	-31.1	-3.5	-	-	-	-
1201	1002	V	L8209a		-	535.15	415.17	0.01	845.0	856.0	11.1	1.3	-	-	-	-
1202	1003	V	L8210a		-	-	292.15	1.0	970.4	950.0	-20.4	-2.1	-	-	-	-
1203	1004	V	L8211a		-	-	298.15	1.0	959.0	925.2	-33.8	-3.5	-	-	-	-
1204	1005	V	L8212a		233.15	517.15	295.15	1.0	932.5	931.2	-1.2	-0.1	79.5	87.1	7.6	9.5
1205	1006	V	L8213a		-	478.13	298.15	1.0	918.0	895.8	-22.2	-2.4	-	-	-	-
1206	1007	V	L8215a		-	-	298.15	1.0	949.0	921.2	-27.8	-2.9	-	-	-	-
1207	1008	V	L8217a		-	-	298.15	1.0	954.0	919.6	-34.4	-3.6	-	-	-	-
1208	1009	V	L8219a		-	-	298.15	1.0	943.0	916.3	-26.7	-2.8	-	-	-	-
1209	1010	V	L8220b	×	332.75	544.15	356.0	1.0	-	-	-	-	101.0	92.2	-8.8	-8.7
1210	1011	V	L9201a		-	-	301.35	1.0	920.7	894.9	-25.8	-2.8	-	-	-	-
1211	1012	V	L9202a		-	-	290.35	1.0	913.8	890.0	-23.8	-2.6	-	-	-	-
1212	1013	V	L9203a		-	-	291.15	1.0	902.0	880.6	-21.4	-2.4	-	-	-	-
1213	1014	V	L9204a		-	-	434.0	1.0	-	-	-	-	68.0	72.7	4.7	6.9
1214	1015	V	L9205a		316.15	535.15	323.15	1.0	929.0	931.2	2.2	0.2	-	-	-	-
1215	1015	V	L9205b		316.15	535.15	460.0	1.0	-	-	-	-	67.2	66.4	-0.8	-1.1
1216	1016	V	L9206a		-	-	291.15	1.0	958.0	943.8	-14.2	-1.5	-	-	-	-
1217	1017	V	L9207a		-	-	293.15	1.0	941.6	936.1	-5.5	-0.6	-	-	-	-
1218	1018	V	L9208a		-	-	293.15	1.0	937.0	913.6	-23.4	-2.5	-	-	-	-
1219	1019	V	L9209a		-	571.15	293.15	1.0	929.5	912.7	-16.8	-1.8	-	-	-	-
1220	1020	V	L9211a		-	-	298.15	1.0	944.0	911.6	-32.4	-3.4	-	-	-	-
1221	1021	V	L9213b		319.55	558.15	323.0	1.0	-	-	-	-	110.0	102.5	-7.5	-6.8
1222	1022	V	L0201a		-	-	288.15	1.0	910.2	890.6	-19.6	-2.2	-	-	-	-
1223	1023	V	L0202a		-	503.15	298.15	1.0	943.5	960.6	17.1	1.8	-	-	-	-
1224	1023	V	L0202b		-	503.15	389.57	0.01	-	-	-	-	55.0	59.6	4.6	8.3
1225	1024	V	L0203a		-	-	285.15	1.0	911.8	892.5	-19.3	-2.1	-	-	-	-
1226	1025	V	L0204a	×	-	-	353.0	1.0	-	-	-	-	63.4	81.6	18.2	28.7
1227	1026	V	L0205a		-	-	293.15	1.0	916.5	899.1	-17.4	-1.9	-	-	-	-
1228	1027	V	L0206a		-	538.15	293.15	1.0	926.0	914.7	-11.3	-1.2	-	-	-	-
1229	1028	V	L0207a		-	-	293.15	1.0	948.1	913.3	-34.8	-3.7	-	-	-	-
1230	1029	V	L0208a		-	-	293.15	1.0	936.2	940.8	4.6	0.5	-	-	-	-
1231	1030	V	L0209a		-	-	301.15	1.0	915.5	902.2	-13.3	-1.5	-	-	-	-
1232	1031	V	L0210a		-	-	298.15	1.0	930.7	927.2	-3.5	-0.4	-	-	-	-
1233	1032	V	L0213a		345.55	572.15	353.15	1.0	883.0	879.8	-3.2	-0.4	-	-	-	-
1234	1032	V	L0213b	×	345.55	572.15	364.0	1.0	-	-	-	-	112.4	98.8	-13.6	-12.1
1235	1033	V	L7302a		-	416.90	291.0	1.0	1075.0	1066.8	-8.2	-0.8	-	-	-	-
1236	1034	V	C7202a		-	-	293.15	1.0	885.6	935.7	50.1	5.7	-	-	-	-
1237	1035	V	C7203a		-	-	298.15	1.0	934.8	942.8	8.0	0.9	-	-	-	-
1238	1036	V	C7205a		-	-	298.15	1.0	910.0	913.1	3.1	0.3	-	-	-	-
1239	1037	V	C7206a		-	-	298.15	1.0	923.9	929.1	5.2	0.6	-	-	-	-
1240	1038	V	C7207a		-	-	298.15	1.0	909.8	919.0	9.2	1.0	-	-	-	-
1241	1039	V	C7208a		-	482.65	298.15	1.0	909.0	911.9	2.9	0.3	-	-	-	-
1242	1040	V	C7210a		-	486.15	293.15	1.0	918.7	926.2	7.5	0.8	-	-	-	-
1243	1041	V	C7211a		-	489.15	293.15	1.0	916.3	918.1	1.8	0.2	-	-	-	-
1244	1042	V	C7212a		265.98	496.15	298.15	1.0	913.5	918.3	4.8	0.5	72.9	74.2	1.3	1.7
1245	1043	V	C8201a		-	-	298.15	1.0	919.9	947.8	27.9	3.0	-	-	-	-
1246	1044	V	C8202a		-	-	293.15	1.0	929.0	934.7	5.7	0.6	-	-	-	-

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1247	1045	V	C8203a		-	-	374.97	0.01	849.1	861.4	12.3	1.4	-	-	-	-
1248	1046	V	C8204a		-	-	298.15	1.0	900.9	936.9	36.0	4.0	-	-	-	-
1249	1047	V	C8206a		-	-	298.15	1.0	902.0	915.7	13.7	1.5	-	-	-	-
1250	1048	V	C8207a		-	494.15	298.15	1.0	904.0	912.0	8.0	0.9	74.8	76.2	1.4	1.9
1251	1049	V	C8208a		-	501.15	298.15	1.0	903.0	911.3	8.3	0.9	75.6	76.7	1.1	1.5
1252	1050	V	C8212a		-	-	293.15	1.0	910.5	918.7	8.2	0.9	-	-	-	-
1253	1051	V	C8214a		289.66	513.05	298.15	1.01	906.0	910.0	3.9	0.4	81.2	79.4	-1.8	-2.2
1254	1052	V	C9201a		-	456.91	385.37	0.01	839.7	856.4	16.7	2.0	-	-	-	-
1255	1053	V	C9202a		-	456.91	385.37	0.01	849.7	877.9	28.3	3.3	-	-	-	-
1256	1054	V	C9203a		-	-	298.15	1.0	910.2	926.4	16.2	1.8	-	-	-	-
1257	1055	V	C9207a		-	456.91	298.15	1.0	893.5	903.9	10.3	1.2	-	-	-	-
1258	1055	V	C9207b		-	456.91	401.0	1.0	-	-	-	-	63.4	70.9	7.5	11.9
1259	1056	V	C9208a		-	456.91	277.15	1.0	909.7	914.7	5.0	0.6	-	-	-	-
1260	1057	V	C9210a		-	456.91	296.15	1.0	899.0	907.1	8.1	0.9	-	-	-	-
1261	1058	V	C9211a		-	-	395.77	0.01	830.9	838.1	7.2	0.9	-	-	-	-
1262	1059	V	C9214a		285.53	528.75	298.15	1.0	901.6	903.9	2.3	0.2	-	-	-	-
1263	1059	V	C9214b		285.53	528.75	304.0	1.0	-	-	-	-	85.3	84.0	-1.3	-1.5
1264	1060	V	C0201a		-	473.73	293.15	1.0	902.2	910.9	8.7	1.0	-	-	-	-
1265	1061	V	C0202a		-	-	298.15	1.0	912.9	918.6	5.7	0.6	-	-	-	-
1266	1062	V	C0203a		-	-	291.15	1.0	897.0	901.7	4.7	0.5	-	-	-	-
1267	1063	V	C0204a		-	-	291.55	1.0	897.8	903.2	5.4	0.6	-	-	-	-
1268	1064	V	C0206a		-	-	293.15	1.0	848.1	902.2	54.1	6.4	-	-	-	-
1269	1065	V	C0207a		-	-	298.15	1.0	893.0	894.1	1.1	0.1	-	-	-	-
1270	1066	V	C0208a		-	473.73	293.15	1.0	898.3	904.3	6.0	0.7	-	-	-	-
1271	1067	V	C0209a		-	-	293.15	1.0	908.6	914.0	5.4	0.6	-	-	-	-
1272	1068	V	C0212a		304.54	543.15	313.15	1.0	881.7	888.2	6.5	0.7	88.6	88.0	-0.6	-0.7
1273	1069	V	C7403a	×	376.65	464.16	479.85	0.01	1198.8	1029.9	-168.8	-14.1	-	-	-	-
1274	1070	V	C7409a	×	377.55	464.16	486.25	0.01	1100.1	996.4	-103.7	-9.4	-	-	-	-
1275	1070	V	C7409b		377.55	464.16	451.0	1.0	-	-	-	-	88.6	91.6	3.0	3.4
1276	1071	V	C8401a		-	495.09	480.65	0.01	1089.8	1047.6	-42.2	-3.9	-	-	-	-
1277	1072	V	C8403b		415.45	495.09	460.0	1.0	-	-	-	-	91.4	94.2	2.8	3.1
1278	1073	V	C9401a		379.65	633.36	501.5	0.01	999.7	935.5	-64.2	-6.4	-	-	-	-
1279	1073	V	C9401b		379.65	633.36	466.0	1.0	-	-	-	-	89.3	97.0	7.7	8.6
1280	1074	V	C0403a	×	404.15	642.09	507.79	0.01	1026.1	913.1	-113.0	-11.0	-	-	-	-
1281	1074	V	C0403b	×	404.15	642.09	471.0	1.0	-	-	-	-	85.9	99.5	13.7	15.9
1282	1075	V	M7101a		-	-	298.15	1.0	761.5	775.6	14.1	1.9	-	-	-	-
1283	1076	V	M7102a		-	395.15	298.15	0.01	768.2	743.1	-25.1	-3.3	-	-	-	-
1284	1077	V	M7103a		-	-	293.15	1.0	788.2	771.9	-16.3	-2.1	-	-	-	-
1285	1078	V	M7104a		-	405.65	306.57	0.01	755.5	753.6	-1.8	-0.2	-	-	-	-
1286	1079	V	M7106a		-	412.65	312.17	0.01	752.7	745.2	-7.5	-1.0	-	-	-	-
1287	1080	V	M7107a		-	414.15	313.37	0.01	-	-	-	-	41.8	43.1	1.4	3.2
1288	1081	V	M7108a		-	422.15	319.77	0.01	756.1	757.5	1.4	0.2	-	-	-	-
1289	1082	V	M7109a		-	426.15	322.97	0.01	757.4	752.3	-5.0	-0.7	-	-	-	-
1290	1083	V	M7110a		-	415.15	293.15	1.0	762.9	757.2	-5.7	-0.8	-	-	-	-
1291	1084	V	M7111a		250.15	430.05	298.15	1.0	771.3	772.2	0.9	0.1	49.9	49.4	-0.5	-0.9
1292	1085	V	M8101a		-	413.15	312.57	0.01	794.4	749.8	-44.6	-5.6	41.0	36.8	-4.2	-10.3
1293	1086	V	M8102a		-	428.15	298.15	0.002	767.0	756.3	-10.7	-1.4	44.5	48.2	3.7	8.4
1294	1087	V	M8103a		-	442.35	335.93	0.01	-	-	-	-	45.3	46.7	1.4	3.2

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1295	1088	V	M8104a		-	438.15	293.15	1.0	772.0	766.2	-5.8	-0.8	-	-	-	-
1296	1088	V	M8104b		-	438.15	332.57	0.01	-	-	-	-	44.7	46.0	1.3	2.9
1297	1089	V	M8105a		273.15	452.75	298.15	1.01	780.0	779.0	-0.9	-0.1	55.1	54.1	-1.0	-1.8
1298	1090	V	M9101a		-	-	293.15	1.0	771.9	774.5	2.6	0.3	-	-	-	-
1299	1091	V	M9102a		-	-	298.15	1.0	789.2	791.9	2.7	0.3	-	-	-	-
1300	1092	V	M9103a		272.15	475.35	293.15	1.0	788.6	789.2	0.6	0.1	-	-	-	-
1301	1092	V	M9103b		272.15	475.35	362.33	0.01	-	-	-	-	49.5	50.7	1.3	2.5
1302	1093	V	M0101a		288.15	493.65	298.15	1.0	789.0	790.0	1.0	0.1	64.9	63.8	-1.1	-1.8
1303	1094	V	N7101a		-	371.15	298.15	0.03	726.9	760.0	33.1	4.5	-	-	-	-
1304	1094	V	N7101b		-	371.15	287.0	1.0	-	-	-	-	35.7	36.9	1.2	3.3
1305	1095	V	N7102a		-	-	298.0	1.0	-	-	-	-	42.1	40.3	-1.8	-4.3
1306	1096	V	N7103a		-	406.65	307.37	0.01	737.2	734.1	-3.1	-0.4	-	-	-	-
1307	1097	V	N7104a		-	407.15	307.77	0.01	739.6	738.0	-1.6	-0.2	-	-	-	-
1308	1098	V	N7105a		-	415.15	293.15	1.0	778.7	763.7	-15.0	-1.9	-	-	-	-
1309	1098	V	N7105b		-	415.15	314.17	0.01	-	-	-	-	43.0	44.5	1.5	3.5
1310	1099	V	N8101a		-	407.15	298.15	1.0	749.0	747.7	-1.3	-0.2	41.3	43.0	1.7	4.1
1311	1100	V	N8102a		199.65	412.25	298.15	1.0	740.7	728.8	-12.0	-1.6	-	-	-	-
1312	1100	V	N8102b		199.65	412.25	311.85	0.01	-	-	-	-	41.8	41.0	-0.8	-1.9
1313	1101	V	N8104a		-	-	328.0	1.0	-	-	-	-	41.2	42.8	1.6	3.9
1314	1102	V	N8105a		211.35	432.00	298.15	1.0	755.7	752.2	-3.5	-0.5	49.4	47.9	-1.5	-3.0
1315	1103	V	N8106a		-	431.15	326.97	0.01	735.3	732.5	-2.8	-0.4	-	-	-	-
1316	1104	V	N8107a		-	438.15	273.15	1.0	771.2	789.1	17.9	2.3	-	-	-	-
1317	1105	V	N9101a	×	-	417.15	315.77	0.01	756.4	894.2	137.8	18.2	-	-	-	-
1318	1106	V	N9102a		-	453.85	298.15	1.0	767.5	764.1	-3.4	-0.4	-	-	-	-
1319	1107	V	N9103a		-	459.85	293.15	1.0	782.4	777.9	-4.5	-0.6	-	-	-	-
1320	1107	V	N9103b		-	459.85	380.0	1.0	-	-	-	-	49.2	48.5	-0.7	-1.4
1321	1108	V	N0101a		229.15	461.15	298.15	1.0	766.9	759.7	-7.2	-0.9	-	-	-	-
1322	1108	V	N0101b		229.15	461.15	350.97	0.01	-	-	-	-	48.0	50.4	2.4	4.9
1323	1109	V	N0102a		-	476.15	298.15	1.0	773.2	766.9	-6.3	-0.8	61.2	57.8	-3.4	-5.6
1324	1110	V	N0103a		-	475.15	298.15	1.0	774.3	770.9	-3.4	-0.4	-	-	-	-
1325	1111	V	N0104a		-	480.15	292.15	1.0	784.0	784.7	0.7	0.1	-	-	-	-
1326	1112	V	R7101a		-	391.15	298.15	0.02	732.1	786.2	54.1	7.4	-	-	-	-
1327	1113	V	R7102a		-	383.15	298.15	0.02	744.5	766.5	22.0	3.0	37.8	38.8	1.0	2.7
1328	1114	V	R7103a		-	390.50	298.15	0.02	732.2	764.0	31.8	4.3	-	-	-	-
1329	1115	V	R7104a		-	385.15	298.15	0.02	749.5	742.6	-6.8	-0.9	-	-	-	-
1330	1116	V	R7105a		-	390.50	298.15	0.02	732.1	771.5	39.4	5.4	-	-	-	-
1331	1117	V	R7106a		-	389.15	298.15	0.02	750.8	769.8	19.0	2.5	39.0	42.3	3.3	8.6
1332	1118	V	R7107a		-	376.15	298.15	0.03	715.4	758.2	42.9	6.0	-	-	-	-
1333	1119	V	R7108a		-	382.15	298.15	0.02	717.1	765.1	48.0	6.7	-	-	-	-
1334	1120	V	R7109a		-	381.65	298.15	0.03	739.0	752.0	13.0	1.8	37.5	40.4	2.9	7.8
1335	1121	V	R7110a		-	386.00	298.15	0.02	750.0	750.4	0.4	0.1	-	-	-	-
1336	1122	V	R7111a		-	388.00	298.15	0.02	752.1	766.5	14.4	1.9	-	-	-	-
1337	1123	V	R7112a		-	380.15	298.15	0.03	729.5	750.6	21.2	2.9	-	-	-	-
1338	1124	V	R7113a		-	386.65	298.15	0.02	752.0	760.3	8.4	1.1	38.4	43.5	5.0	13.1
1339	1125	V	R7114a		-	385.15	298.15	0.02	738.0	755.5	17.5	2.4	38.2	42.4	4.2	11.0
1340	1126	V	R7115a		-	387.25	298.15	0.02	750.1	757.0	6.9	0.9	38.4	43.4	5.0	12.9
1341	1127	V	R7116a		-	390.15	298.15	0.02	731.9	758.5	26.6	3.6	39.1	43.7	4.7	11.9
1342	1128	V	R7117a		-	395.15	298.15	0.01	731.8	764.8	33.0	4.5	40.0	45.2	5.1	12.8

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1343	1129	V	R8101a		-	400.15	302.17	0.01	763.8	769.2	5.4	0.7	-	-	-	-
1344	1130	V	R8102a		-	399.65	313.15	1.0	749.0	747.9	-1.1	-0.1	-	-	-	-
1345	1130	V	R8102b		-	399.65	301.77	0.01	-	-	-	-	40.0	42.5	2.5	6.3
1346	1131	V	R8103a		-	411.15	310.97	0.01	795.5	753.2	-42.3	-5.3	40.4	45.9	5.5	13.7
1347	1132	V	R8104a		-	409.15	293.15	1.0	742.0	768.0	26.0	3.5	-	-	-	-
1348	1132	V	R8104b		-	409.15	309.37	0.01	-	-	-	-	41.4	46.4	5.0	12.0
1349	1133	V	R8105a		-	-	298.15	1.0	742.0	766.0	24.0	3.2	-	-	-	-
1350	1134	V	R8106a		-	418.15	316.57	0.01	729.5	759.6	30.1	4.1	43.4	48.9	5.5	12.7
1351	1135	V	R9101a		172.65	429.65	298.15	1.0	752.9	769.6	16.8	2.2	46.2	51.1	4.9	10.6
1352	1136	V	R9102a		-	429.15	293.15	1.0	766.3	775.5	9.2	1.2	-	-	-	-
1353	1136	V	R9102b		-	429.15	325.37	0.01	-	-	-	-	43.8	50.1	6.2	14.2
1354	1137	V	R9103a		-	432.75	293.15	1.0	759.3	776.8	17.5	2.3	-	-	-	-
1355	1138	V	R9104a		-	445.15	293.15	1.0	758.0	783.6	25.6	3.4	-	-	-	-
1356	1138	V	R9104b		-	445.15	338.17	0.01	-	-	-	-	45.8	52.2	6.4	14.0
1357	1139	V	R0101a		-	445.00	338.05	0.01	737.6	744.2	6.6	0.9	-	-	-	-
1358	1140	V	R0102a		-	-	293.15	1.0	768.6	796.4	27.8	3.6	-	-	-	-
1359	1141	V	R0103a		-	452.15	343.77	0.01	732.3	744.6	12.3	1.7	46.7	53.5	6.8	14.6
1360	1142	V	R0104a		-	464.15	293.15	1.0	768.7	788.6	19.9	2.6	-	-	-	-
1361	1142	V	R0104b		-	464.15	303.0	1.0	-	-	-	-	54.0	59.5	5.5	10.2
1362	1143	V	N7201a		-	417.15	291.15	1.0	783.7	850.9	67.2	8.6	-	-	-	-
1363	1143	V	N7201b	×	-	417.15	298.0	1.0	-	-	-	-	45.3	54.2	8.9	19.7
1364	1144	V	N7202a		-	429.65	429.65	1.0	-	-	-	-	37.2	38.7	1.5	4.1
1365	1145	V	N7203a		-	431.65	431.65	1.0	-	-	-	-	37.4	42.3	4.9	13.1
1366	1146	V	N7205a		-	441.65	293.15	1.0	822.0	847.5	25.5	3.1	52.4	53.4	1.0	1.8
1367	1147	V	N7206a		298.45	497.15	298.0	1.0	-	-	-	-	67.1	67.2	0.1	0.1
1368	1148	V	N8201a	×	-	437.70	298.0	1.0	-	-	-	-	47.9	56.4	8.5	17.7
1369	1149	V	N8202a		-	441.15	288.15	1.0	794.2	853.1	58.9	7.4	-	-	-	-
1370	1149	V	N8202b	×	-	441.15	441.15	1.0	-	-	-	-	38.3	49.8	11.5	30.1
1371	1150	V	N8204a	×	-	394.15	394.15	1.0	-	-	-	-	33.8	44.6	10.8	31.8
1372	1151	V	N8205a		-	443.15	443.15	1.0	-	-	-	-	38.5	39.6	1.2	3.1
1373	1152	V	N8206a		-	457.15	288.15	1.0	848.5	834.9	-13.6	-1.6	-	-	-	-
1374	1152	V	N8206b		-	457.15	457.15	1.0	-	-	-	-	39.8	32.1	-7.7	-19.2
1375	1153	V	N8207a	×	-	327.65	327.65	1.0	-	-	-	-	27.6	54.1	26.5	95.9
1376	1154	V	N8210a		324.85	498.15	498.15	1.0	-	-	-	-	43.7	43.2	-0.5	-1.1
1377	1155	V	N9201a		-	438.95	293.15	1.0	800.0	824.6	24.6	3.1	-	-	-	-
1378	1155	V	N9201b		-	438.95	438.95	1.0	-	-	-	-	38.0	45.0	7.0	18.3
1379	1156	V	N9203a		-	474.15	293.15	1.0	814.0	833.4	19.4	2.4	-	-	-	-
1380	1156	V	N9203b		-	474.15	474.15	1.0	-	-	-	-	41.4	43.2	1.8	4.3
1381	1157	V	N9204a		-	531.65	298.0	1.0	-	-	-	-	75.5	76.1	0.6	0.8
1382	1158	V	N0201a		326.45	470.15	326.5	1.0	775.7	789.7	14.0	1.8	-	-	-	-
1383	1159	V	N0202a		-	465.15	298.15	1.0	808.0	826.1	18.1	2.2	-	-	-	-
1384	1159	V	N0202b	×	-	465.15	465.15	1.0	-	-	-	-	40.5	49.5	8.9	22.0
1385	1160	V	N0203a		-	482.65	298.15	1.0	806.0	844.1	38.1	4.7	-	-	-	-
1386	1160	V	N0203b	×	-	482.65	482.65	1.0	-	-	-	-	42.2	54.8	12.5	29.7
1387	1161	V	N0204a		-	522.15	522.15	1.0	-	-	-	-	46.0	48.8	2.8	6.0
1388	1162	V	N0206a		332.85	485.03	345.0	1.0	-	-	-	-	73.6	71.1	-2.5	-3.3
1389	1163	V	D7401a		368.6	527.15	298.15	1.0	-	-	-	-	82.4	83.2	0.8	1.0
1390	1164	V	D8402a		-	472.28	298.0	1.0	-	-	-	-	83.6	84.1	0.5	0.6

Table S.7 – Comparison of experimental and simulated properties (continued)

n_{sim}	n_{iso}	Set	Outlier	code	T_m [K]	T_b [K]	T [K]	P [bar]	ρ_{liq}[kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap}[kJ·mol^{-1}] exp	sim	dev	err [%]
1391	1165	V	D8403a		378.15	512.15	383.15	1.0	845.0	842.8	-2.2	-0.3	-	-	-	-
1392	1165	V	D8403b	×	378.15	512.15	512.15	1.0	-	-	-	-	45.0	61.5	16.4	36.5
1393	1166	V	D7201a		-	-	298.0	1.0	-	-	-	-	55.1	54.5	-0.6	-1.1
1394	1167	V	D7202a		-	464.15	293.15	1.0	897.2	881.3	-15.9	-1.8	-	-	-	-
1395	1167	V	D7202b		-	464.15	464.15	1.0	-	-	-	-	40.5	45.5	5.0	12.5
1396	1168	V	D7203a		222.15	458.76	298.15	1.0	896.2	890.7	-5.5	-0.6	-	-	-	-
1397	1169	V	D8201a		-	469.15	389.2	0.06	808.8	813.8	5.0	0.6	46.1	50.2	4.1	8.9
1398	1170	V	D8202a		-	479.15	293.15	1.0	888.4	875.0	-13.4	-1.5	-	-	-	-
1399	1170	V	D8202b	×	-	479.15	313.0	1.0	-	-	-	-	38.7	59.2	20.6	53.1
1400	1171	V	D8203a	×	-	408.15	408.15	1.0	-	-	-	-	35.1	57.9	22.7	64.7
1401	1172	V	D8204a		-	482.65	290.15	1.0	899.2	883.8	-15.4	-1.7	-	-	-	-
1402	1173	V	D9201a		-	479.15	479.15	1.0	-	-	-	-	41.9	45.8	3.9	9.4
1403	1174	V	D9202a		-	484.15	293.15	1.0	876.4	867.4	-9.0	-1.0	-	-	-	-
1404	1174	V	D9202b		-	484.15	484.15	1.0	-	-	-	-	42.4	49.3	7.0	16.5
1405	1175	V	D0202a	×	-	-	388.0	1.0	-	-	-	-	47.7	62.0	14.3	29.9

S.7 Outliers

In this section, we provide more information on the simulation results considered as outliers (62 simulations concerning 58 molecules) in the comparison between experimental and simulated properties. They correspond to errors larger than 80.0 kg·m^{-3} for ρ_{liq} and/or larger than 8.0 kJ·mol^{-1} for ΔH_{vap}. These specific entries of Tab. S.7 are listed again in Tab. S.8, and the corresponding structures are shown in Fig. S.4.

Table S.8: Experimental and simulated properties of the 58 compounds (62 distinct P, T-points) considered as outliers.

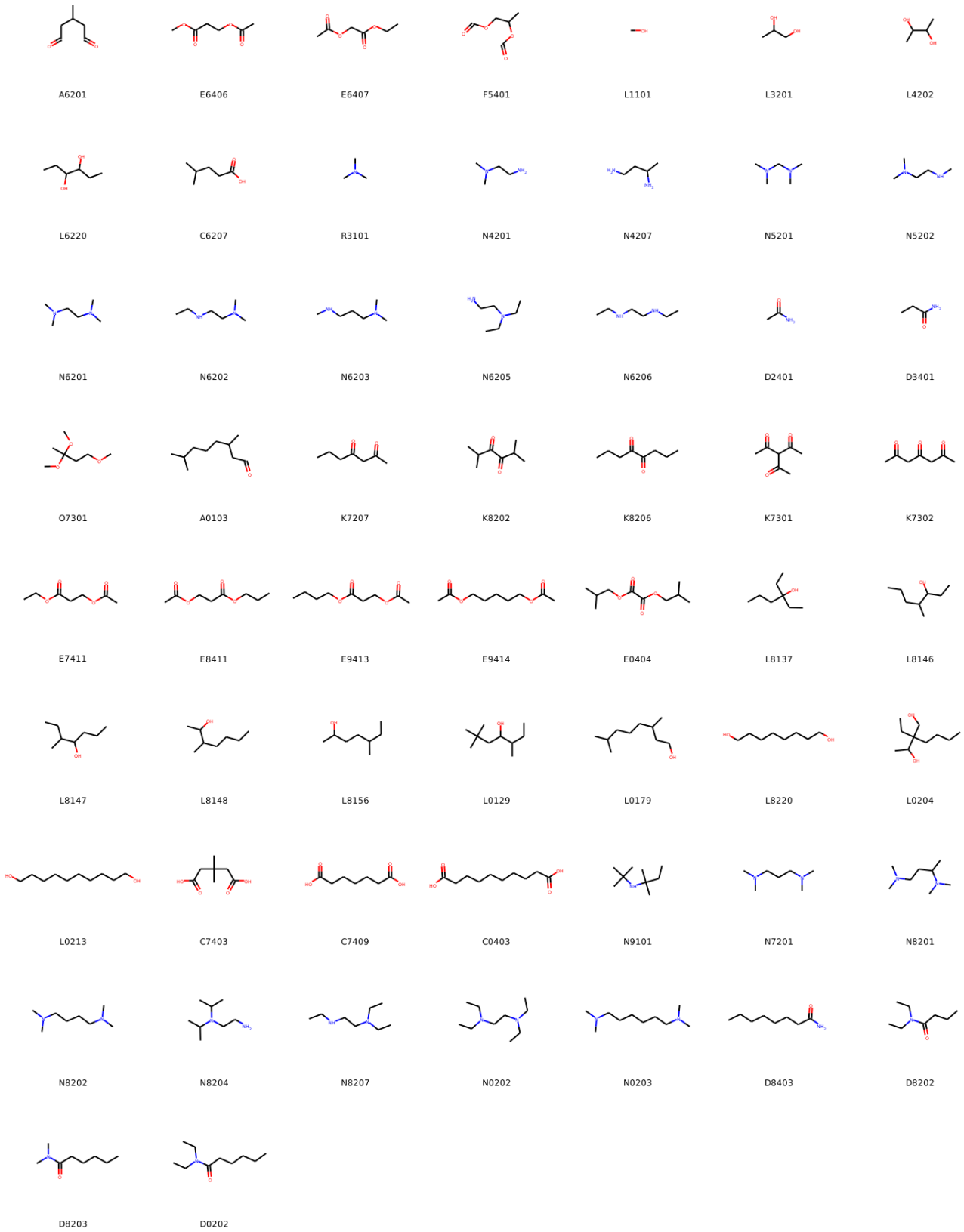
sim	mol	set	code	T_m	T_b	T	P	ρ_{liq}[kg·m^{-3}]				ΔH_{vap}[kJ·mol^{-1}]			
				[K]	[K]	[K]	[bar]	exp	sim	dev	err [%]	exp	sim	dev	err [%]
83	64	C	A6201a	-	439.15	439.15	1.0	-	-	-	-	38.1	48.1	10.1	26.4
131	106	C	E6406a	-	-	350.0	1.0	-	-	-	-	68.0	57.1	-10.9	-16.0
132	107	C	E6407a	-	452.15	452.15	1.0	-	-	-	-	39.3	47.6	8.3	21.1
150	122	C	F5401a	-	348.15	348.15	1.0	-	-	-	-	29.5	53.4	23.9	81.1
151	123	C	L1101a	175.65	337.85	298.15	1.01	786.7	885.0	98.3	12.5	37.7	42.0	4.3	11.4
191	157	C	L3201a	213.15	460.75	298.15	1.0	1032.5	985.7	-46.8	-4.5	62.2	71.2	9.0	14.5
195	160	C	L4202b	-	455.15	332.0	1.0	-	-	-	-	58.4	67.6	9.2	15.8
225	190	C	L6220a	-	496.94	273.15	1.0	799.3	940.7	141.4	17.7	-	-	-	-
262	221	C	C6207b	240.15	473.65	354.0	1.0	-	-	-	-	91.7	63.1	-28.6	-31.2
333	280	C	R3101a	156.05	276.02	273.15	1.0	655.7	743.8	88.0	13.4	22.9	28.5	5.6	24.3
334	280	C	R3101b	156.05	276.02	298.15	2.33	628.9	718.0	89.1	14.2	-	-	-	-
355	296	C	N4201a	-	378.65	298.15	1.0	803.0	886.9	83.8	10.4	-	-	-	-
356	296	C	N4201b	-	378.65	378.65	1.0	-	-	-	-	31.1	41.0	9.9	31.8
364	302	C	N4207a	-	419.15	419.15	1.0	-	-	-	-	43.7	33.3	-10.5	-23.9
366	304	C	N5201a	-	356.15	291.15	1.0	749.1	854.9	105.8	14.1	-	-	-	-
367	304	C	N5201b	-	356.15	298.0	1.0	-	-	-	-	33.1	44.4	11.3	34.2
368	305	C	N5202a	-	390.15	390.15	1.0	-	-	-	-	29.7	41.3	11.6	39.1
376	313	C	N6201a	215.15	394.15	298.15	1.0	770.0	846.6	76.7	9.9	41.4	50.6	9.2	22.2
377	314	C	N6202a	-	407.65	298.15	1.0	738.0	836.8	98.8	13.4	-	-	-	-
379	315	C	N6203a	-	414.15	414.15	1.0	-	-	-	-	30.6	41.5	10.9	35.6
380	316	C	N6205a	-	417.15	293.15	1.0	828.0	858.9	30.9	3.7	45.8	54.7	8.9	19.4
382	317	C	N6206b	-	419.15	419.15	1.0	-	-	-	-	31.7	39.8	8.1	25.5
389	323	C	D2401b	353.31	494.3	396.0	1.0	-	-	-	-	63.8	52.0	-11.8	-18.6
391	324	C	D3401b	353.05	486.15	390.0	1.0	-	-	-	-	63.9	54.8	-9.1	-14.2
509	431	V	O7301a	-	426.15	426.15	1.0	-	-	-	-	36.8	45.1	8.3	22.4
552	467	V	A0103b	-	403.15	403.15	1.0	-	-	-	-	24.3	50.8	26.5	109.3
668	549	V	K7207a	-	447.20	447.2	1.0	-	-	-	-	38.8	47.9	9.1	23.4
670	551	V	K8202a	-	417.65	311.17	0.01	909.0	883.9	-25.2	-2.8	41.8	56.1	14.2	34.1
671	552	V	K8206a	-	441.15	329.97	0.01	907.8	888.9	-18.9	-2.1	45.3	62.5	17.2	37.9
677	558	V	K7301a	-	476.65	384.0	1.0	-	-	-	-	54.9	75.1	20.2	36.8
679	559	V	K7302b	322.15	455.78	455.78	1.0	-	-	-	-	39.6	59.9	20.2	51.0
847	694	V	E7411a	-	-	358.0	1.0	-	-	-	-	72.1	57.8	-14.3	-19.9
859	703	V	E8411a	-	-	367.0	1.0	-	-	-	-	74.7	60.3	-14.4	-19.3
871	713	V	E9413a	-	-	382.0	1.0	-	-	-	-	75.4	62.7	-12.7	-16.8
873	714	V	E9414b	275.15	514.15	514.15	1.0	-	-	-	-	45.2	53.9	8.7	19.2
876	717	V	E0404a	-	502.15	351.0	1.0	-	-	-	-	55.5	64.9	9.4	16.9
973	797	V	L8137b	-	432.15	345.0	1.0	-	-	-	-	49.2	57.3	8.1	16.5
984	804	V	L8146b	150.15	428.55	318.66	0.01	-	-	-	-	43.5	64.4	20.8	47.8
986	805	V	L8147b	-	437.85	355.0	1.0	-	-	-	-	48.0	58.1	10.1	21.0
988	806	V	L8148b	-	439.25	356.0	1.0	-	-	-	-	48.0	58.7	10.7	22.3
999	813	V	L8156b	212.15	445.05	363.0	1.0	-	-	-	-	47.2	57.9	10.7	22.8
1116	919	V	L0129a	-	455.00	289.15	1.0	751.3	840.1	88.8	11.8	-	-	-	-
1157	959	V	L0179b	-	485.15	356.0	1.0	-	-	-	-	79.1	68.9	-10.2	-12.9
1209	1010	V	L8220b	332.75	544.15	356.0	1.0	-	-	-	-	101.0	92.2	-8.8	-8.7
1226	1025	V	L0204a	-	-	353.0	1.0	-	-	-	-	63.4	81.6	18.2	28.7
1234	1032	V	L0213b	345.55	572.15	364.0	1.0	-	-	-	-	112.4	98.8	-13.6	-12.1
1273	1069	V	C7403a	376.65	464.16	479.85	0.01	1198.8	1029.9	-168.8	-14.1	-	-	-	-
1274	1070	V	C7409a	377.55	464.16	486.25	0.01	1100.1	996.4	-103.7	-9.4	-	-	-	-
1280	1074	V	C0403a	404.15	642.09	507.79	0.01	1026.1	913.1	-113.0	-11.0	-	-	-	-
1281	1074	V	C0403b	404.15	642.09	471.0	1.0	-	-	-	-	85.9	99.5	13.7	15.9
1317	1105	V	N9101a	-	417.15	315.77	0.01	756.4	894.2	137.8	18.2	-	-	-	-
1363	1143	V	N7201b	-	417.15	298.0	1.0	-	-	-	-	45.3	54.2	8.9	19.7
1368	1148	V	N8201a	-	437.70	298.0	1.0	-	-	-	-	47.9	56.4	8.5	17.7
1370	1149	V	N8202b	-	441.15	441.15	1.0	-	-	-	-	38.3	49.8	11.5	30.1
1371	1150	V	N8204a	-	394.15	394.15	1.0	-	-	-	-	33.8	44.6	10.8	31.8
1375	1153	V	N8207a	-	327.65	327.65	1.0	-	-	-	-	27.6	54.1	26.5	95.9
1384	1159	V	N0202b	-	465.15	465.15	1.0	-	-	-	-	40.5	49.5	8.9	22.0
1386	1160	V	N0203b	-	482.65	482.65	1.0	-	-	-	-	42.2	54.8	12.5	29.7
1392	1165	V	D8403b	378.15	512.15	512.15	1.0	-	-	-	-	45.0	61.5	16.4	36.5

Table S.8 – *Continued from previous page*

Table S.8 – Experimental and simulated properties of the 62 distinct P, T-points considered as outliers.

sim	mol	set	code	T_m [K]	T_m [K]	T [K]	P [bar]	ρ_{liq} [kg·m^{-3}] exp	sim	dev	err [%]	ΔH_{vap} [kJ·mol^{-1}] exp	sim	dev	err [%]
1399	1170	V	D8202b	-	479.15	313.0	1.0	-	-	-	-	38.7	59.2	20.6	53.1
1400	1171	V	D8203a	-	408.15	408.15	1.0	-	-	-	-	35.1	57.9	22.7	64.7
1405	1175	V	D0202a	-	-	388.0	1.0	-	-	-	-	47.7	62.0	14.3	29.9

Figure S.4: Structure of the 58 compounds considered as outliers.



S.8 Comparison with the 2016H66 Parameter Set

This section provides a comparison between the presently reoptimized force field and the original 2016H66 parameter set.[112] The parametrization of 2016H66 relied on 17 compounds of the O+N family for the calibration and 26 for the validation. The corresponding results are reported in Tab. S.9. The final RMSD values for the calibration set are 19.2 kg·m^{-3} for ρ_{liq} and 3.4 kJ·mol^{-1} for ΔH_{vap}. The corresponding values are slightly higher for the validation set, namely 33.5 kg·m^{-3} for ρ_{liq} and 4.3 kJ·mol^{-1} for ΔH_{vap}.

Code	Name	T K	$\rho_{\mathrm{liq}}^{\mathrm{ref}}$ kg·m^{-3}	$\rho_{\mathrm{liq}}^{\mathrm{sim}}$ kg·m^{-3}	$\Delta H_{\mathrm{vap}}^{\mathrm{ref}}$ kJ·mol^{-1}	$\Delta H_{\mathrm{vap}}^{\mathrm{sim}}$ kJ·mol^{-1}
Calibration						
ETL	ethanol	298	784.9	776.9	42.3	45.9
1PL	propanol	298	799.6	783.1	47.5	50.3
DME	methoxymethane	254	722.0	713.5	21.2	23.8
DEE	ethoxyethane	298	707.8	693.8	27.1	29.1
DXE	1,2-dimethoxyethane	298	863.7	833.2	36.4	40.1
EAL	acetaldehyde	298	778.0	789.5	26.1	31.3
PPN	propanone	298	784.4	811.8	31.3	33.6
BTN	butanone	298	799.7	800.8	34.5	36.0
ACA	acetic acid	298	1043.9	1075.1	51.6	58.2
EAE	ethylacetate	298	894.5	871.1	35.6	36.2
PAE	propylacetate	298	883.0	861.5	39.8	40.1
EAN	ethylamine	298	677.0	692.9	26.6	30.3
DEAN	diethylamine	298	701.6	723.6	31.3	33.6
TEAN	triethylamine	298	723.0	749.9	34.8	39.1
AMD	acetamide	364	989.2	1005.1	56.1	60.6
LNMA	N-methylacetamide	333	926.0	914.0	54.4	57.0
DAMD	dimethylacetamide	298	936.3	930.7	49.1	46.8
Validation						
MTL	methanol	298	784.0	822.5	37.4	43.1
BTL	butanol	298	805.8	791.2	52.3	55.2
PTL	pentanol	298	810.8	797.3	56.9	60.0
HXL	hexanol	298	815.3	803.2	61.9	65.1
HPL	heptanol	298	820.0	806.8	66.8	69.8
OTL	octanol	298	821.6	810.5	71.0	74.8
2PL	propan-2-ol	298	780.0	733.4	45.5	44.5
2BTL	butan-2-ol	298	802.4	763.1	49.7	49.3
2PTL	pentan-2-ol	298	805.4	773.7	53.1	54.0
3PTL	pentan-3-ol	298	816.0	778.1	53.1	53.9
2M2P	2-methylpropan-2-ol	298	781.2	730.8	46.8	41.0
2M2B	2-methylbutan-2-ol	298	805.0	769.2	50.2	46.3
MPH	1-methoxypropane	298	735.6	704.5	27.6	29.8
PAL	propionaldehyde	298	791.2	779.5	29.6	34.5
BAL	butyraldehyde	298	796.4	790.8	33.7	39.0
2PN	pentan-2-one	298	801.5	804.5	38.4	40.5
3PN	pentan-3-one	298	809.5	794.4	38.6	38.7
2HN	hexan-2-one	298	806.7	808.8	42.9	45.1
3HN	hexan-3-one	298	810.0	798.6	42.5	43.2
PPA	propionic acid	298	988.1	978.1	57.3	61.6
BTA	butyric acid	298	953.2	950.5	58.0	66.7
MPE	methylpropionate	298	909.0	872.9	35.9	36.3
BAE	butylacetate	298	876.4	858.1	43.6	44.8
PAN	propylamine	298	712.1	726.4	31.3	34.7
BAN	butylamine	298	736.8	737.8	35.7	38.9
EDAN	ethylenediamine	298	893.1	1009.2	46.0	59.0

Table S.9: Experimental and simulated values of ρ_{liq} and ΔH_{vap} for the 43 O+N compounds from the 2016H66 article.[112] The corresponding RMSD values over the calibration (validation) sets are 19.2 (33.5) kg·m^{-3} for ρ_{liq} and 3.4 (4.3) kJ·mol^{-1} for ΔH_{vap}.

Considering the same 43 molecules, similar values are obtained when using the initial parameters of the present force field (*i.e.* before optimization), as listed in Tab. S.10 (entries "A"). This is expected as these initial parameters are identical (LJ parameters) and very close (charge-fitted EE model) to those of the 2016H66 parameter set (see Sec. S.4).

A statistics extending to the entire set of molecules with up to ten carbon atoms (excluding

Code	m	Calibration						Validation					
		N_ρ^{cal}	ρ_{liq}		$N_{\Delta H}^{\text{cal}}$	ΔH_{vap}		N_ρ^{val}	ρ_{liq}		$N_{\Delta H}^{\text{val}}$	ΔH_{vap}	
			A	B		A	B		A	B		A	B
ROR	1	2	13.3	17.2	2	1.8	1.0	1	14.8	11.0	1	1.5	0.9
	2	1	28.5	10.1	1	2.9	3.3	-	-	-	-	-	-
RCOH	1	1	21.5	10.0	1	4.1	4.8	2	5.1	15.2	2	4.8	0.4
RCOR	1	2	21.6	7.9	2	1.6	2.0	4	9.6	13.4	4	2.0	1.1
RCOOR	1	2	22.8	2.0	2	0.5	0.8	2	29.4	23.1	2	1.1	1.0
ROH	1	2	13.2	21.8	2	3.3	3.3	12	30.6	39.8	12	3.4	1.5
RCOOH	1	1	29.8	1.6	1	5.5	8.1	2	4.9	4.4	2	7.2	0.9
RNH_2	1	1	34.7	8.4	1	4.4	2.8	2	13.6	1.2	2	3.5	0.7
RNHR	1	1	18.6	16.4	1	1.9	2.8	-	-	-	-	-	-
RNR_2	1	1	27.0	3.7	1	3.7	1.2	-	-	-	-	-	-
RN_2*	2	-	-	-	-	-	-	1	118.8	79.0	1	13.8	4.1
$RCONH_2$	1	1	11.1	8.7	1	6.0	5.7	-	-	-	-	-	-
RCONHR	1	1	12.6	35.0	1	2.9	3.7	-	-	-	-	-	-
$RCONR_2$	1	1	4.6	9.9	1	4.2	3.3	-	-	-	-	-	-
All	-	17	20.9	14.6	17	3.3	3.5	26	32.9	32.6	26	4.5	1.4

Table S.10: Statistics concerning the discrepancies between simulated and experimental properties for the 43 O+N compounds from the 2016H66 article,[112] using the initial values A (2016H66-like) and the final values B (reoptimized) of the parameters. The results are reported for the calibration set (left) and the validation set (right). For selected groups of molecules Main Article Tab. 2, the number N_ρ^{cal} of experimental ρ_{liq} values and the number $N_{\Delta H}^{\text{cal}}$ of experimental ΔH_{vap} values are reported, along with the root-mean-square deviation (RMSD) between simulated and experiment for both properties.

the formate esters because they were not included in 2016H66) is shown in Tab. S.11 (entries "A"). When the calibration and validation sets are compared, the increase in the aliphatic content results in smaller deviations for ρ_{liq}, from 37.7 to 23.4 kg·m^{-3}, and slightly higher deviations for ΔH_{vap}, from 5.3 to 6.6 kJ·mol^{-1}. A slight improvement is expected, as the pairwise interactions between aliphatic groups are comparatively easier to describe, and already very well reproduced in the GROMOS force field.[135–137] A very significant difference is observed when comparing mono- and polyfunctional groups. For the monofunctional compounds, the RMSD values are 26.7 (18.4) kg·m^{-3} and 4.2 (5.3) kJ·mol^{-1} for the calibration (validation) set. For the polyfunctional compounds, they are much higher, namely 55.0 (38.0) kg·m^{-3} and 7.2 (8.7) kJ·mol^{-1}, respectively.

After optimization of the non-bonded parameters, the agreement with experiment is improved as shown in Tabs. S.10 and S.11 (entries "B"). The reoptimized parameters lead to a smaller RMSD for the set of 43 compounds (Tab. S.10). The RMSD for the 17 compounds of the calibration set of 2016H66 decreases from 20.9 to 14.6 kg·m^{-3} for ρ_{liq}. For ΔH_{vap} a very slight increase is observed, from 3.3 to 3.5 kJ·mol^{-1}. Improvements in the results for the molecules in the validation set of 2016H66 are only observed for ΔH_{vap}, where the RMSD decreases from 4.5 to 1.4 kJ·mol^{-1}. For ρ_{liq} the results remain essentially the same, with a negligible change from 32.9 to 32.6 kg·m^{-3}. Similar trends are observed when considering the entire set of molecules (Tab. S.11). Note that the inclusion of polyfunctional molecules in the recalibration does not negatively affect the results for the 43 compounds of 2016H66.

Code	m	Calibration						Validation					
		N_ρ^{cal}	ρ_{liq}		$N_{\Delta H}^{\mathrm{cal}}$	ΔH_{vap}		N_ρ^{val}	ρ_{liq}		$N_{\Delta H}^{\mathrm{val}}$	ΔH_{vap}	
			A	B		A	B		A	B		A	B
ROR	1	28	17.8	15.7	23	2.1	1.8	56	15.1	15.4	19	2.0	1.5
	2	11	43.1	37.8	12	3.7	2.7	28	32.5	30.4	17	2.8	2.1
	3	3	67.5	51.5	4	6.5	3.5	6	38.1	39.0	11	3.9	3.7
	4	1	119.0	64.2	2	4.0	0.6	3	58.3	42.1	3	2.6	1.5
	1-4	43	36.4	28.4	41	3.4	2.3	93	25.7	24.0	50	2.8	2.3
RCOH	1	16	20.2	27.3	13	5.1	1.7	21	19.0	21.9	8	12.0	9.6
	2	2	38.8	50.1	2	12.1	7.3	0	-	-	0	-	-
	1-2	18	23.0	30.7	15	6.51	3.1	21	19.0	21.9	8	12.0	9.6
RCOR	1	11	14.4	15.2	11	1.5	0.9	73	11.3	12.8	49	4.1	3.3
	2	3	28.7	24.8	3	7.2	5.1	11	19.0	18.0	6	12.3	10.5
	3	0	-	-	0	-	-	1	11.6	9.6	2	25.0	20.2
	1-3	14	18.4	17.7	14	3.6	2.5	85	12.6	13.5	57	7.2	5.9
RCOOR	1	20	27.0	24.1	19	1.1	1.1	115	21.0	21.1	70	3.5	3.2
	2	6	50.7	45.4	9	5.0	4.9	27	40.3	37.5	38	6.7	5.9
	1-2	26	33.9	30.4	28	3.0	2.9	142	25.8	25.1	108	4.9	4.3
ROH	1	33	24.7	28.4	32	3.3	2.1	247	16.7	16.1	55	5.5	5.1
	2	45	45.6	34.5	12	6.1	5.2	52	26.8	21.6	10	8.6	8.7
	3	5	74.0	38.4	1	1.3	1.9	1	38.1	8.2	0	-	-
	1-3	83	41.2	32.5	45	4.2	3.2	300	18.9	17.2	65	6.1	5.8
RCOOH	1	17	17.5	12.0	13	8.9	8.0	35	16.0	17.1	7	8.9	3.1
	2	0	-	-	0	-	-	5	106.1	107.6	4	20.5	8.1
	1-2	17	17.5	12.0	13	8.9	8.0	40	40.4	41.3	11	13.5	5.5
RNH_2	1	34	27.7	20.2	22	3.8	2.1	17	12.5	14.1	9	3.7	2.2
RNHR	1	25	34.8	22.0	19	2.5	1.4	16	37.9	36.2	10	2.4	1.8
R_3N	1	13	50.3	46.1	12	4.2	3.6	31	27.7	25.6	17	5.5	4.9
RN_2*	2	16	74.1	57.8	31	8.9	6.1	9	40.8	36.2	19	10.6	8.9
	1-2	88	44.9	34.9	84	6.1	4.1	73	29.7	27.8	55	7.2	6.0
$RCONH_2$	1	4	13.2	15.6	4	9.2	8.7	1	0.1	2.2	3	13.9	9.5
RCONHR	1	4	12.2	10.7	7	5.9	3.1	0	-	-	0	-	-
$RCONR_2$	1	4	12.8	8.7	2	3.5	0.5	6	14.5	11.6	8	10.5	12.5
	1	12	12.7	12.0	13	6.8	5.4	7	13.4	10.8	11	11.6	11.8
NHB	-	118	33.8	30.3	112	4.0	2.7	378	23.1	22.4	248	5.9	5.2
HBD	-	183	39.9	30.6	141	4.6	4.6	383	23.6	22.4	117	7.8	6.1
All	1	209	26.7	23.7	177	4.2	3.2	618	18.4	18.3	255	5.3	4.6
	> 1	92	55.0	41.9	76	7.2	5.1	143	38.0	35.1	110	8.7	7.1
	-	301	37.7	30.4	253	5.3	3.9	761	23.4	22.4	365	6.6	5.5

Table S.11: Statistics concerning the discrepancies between simulated and experimental properties using the initial values A (2016H66-like) and the final values B (reoptimized) of the parameters. For selected groups of molecules (Tab. 2) and number m of occurrences of the functional group in the molecule, the number N_ρ^{cal} of experimental ρ_{liq} values and the number $N_{\Delta H}^{\mathrm{cal}}$ of experimental ΔH_{vap} values are reported, along with the root-mean-square deviation (RMSD) and the average deviation (AVED) between simulation and experiment for both properties. The results are reported for the calibration set (left) and the validation set (right) excluding formate esters (because they were not included in 2016H66). The last three lines refer to non-hydrogen-bonding (NHB), hydrogen-bonding (HBD), and the entire set (All) of molecules.