Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information: Rapid Determination of Entropy and Free Energy of Mixtures from Molecular Dynamics Simulations with the Two-Phase Thermodynamic Model

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Table S1. Comparison of excess Gibbs free energy of equimolar LJ mixtures from 2PT with three different methods for estimation of the partial molar volume, one-fluid, molecular size, and Kirkwood-Buff theory, and thermodynamic integration (TI)

	One-fluid		Molecular size		Kirkwood-Buff		TI[35,36]
id	Gex(J/mol)	S.D.[a]	G^{ex}(J/mol)	S.D.[a]	G^{ex}(J/mol)	S.D.[a]	G^{ex}(J/mol)
1	-66	7	-44	5	-46	5	-42
2	-196	6	-118	9	-130	8	-129
3	-442	5	-260	8	-313	8	-288
4	-574	15	-319	15	-381	14	-356
5	-104	5	-26	7	-63	7	-66
6	-374	20	-119	22	-219	21	-228
7	-736	4	-259	17	-437	16	-430
8	-1195	11	-457	43	-791	39	-634
9	-133	29	-1	31	-70	31	-84
10	-492	9	-99	16	-281	15	-284
11	-1066	28	-323	65	-624	59	-523
12	-1727	21	-629	33	-1005	30	-772
13	6	2	1	3	1	3	0
14	23	8	19	12	19	12	26
15	96	13	92	14	91	14	99
16	216	2	208	2	208	3	209
17	336	13	336	13	336	13	350
18	-35	13	-22	10	-29	10	-20
19	-36	9	-19	12	-27	12	-21
20	2	13	20	13	10	13	22
21	61	14	77	16	67	16	82
22	132	25	149	24	139	24	192
23	-470	10	-262	23	-329	22	-235
24	-570	10	-358	8	-423	8	-318
25	-642	6	-446	11	-508	9	-392
26	-691	13	-511	25	-567	24	-417
27	-750	19	-559	16	-613	16	-450
28	374	20	-120	22	-219	21	-228
29	-449	20	-202	31	-300	30	-288
30	-482	7	-239	6	-326	6	-317
31	-531	6	-29	15	-379	13	-322
32	-529	17	-318	33	-395	32	-340

[a] The standard deviation (SD) is determined based on four simulation runs, each having 160ps sampling time.

Table S2. The Fluidicity parameter and partial molar volume (Å^3/particle) of each component in a binary equimolar LJ mixture from different methods

	One-fluid		Size-ratio				Kirkwood-Buff			
id	$f_A = f_B$	$V_A = V_B$	f_A	f_B	V_A	V_B	f_A	f_B	V_A	V_B
1	0.41	74	0.46	0.38	50	97	0.46	0.38	51	96
2	0.40	103	0.49	0.33	47	158	0.48	0.33	52	153
3	0.38	158	0.53	0.28	43	273	0.50	0.28	62	254
4	0.38	188	0.56	0.25	42	334	0.53	0.26	61	315
5	0.60	96	0.65	0.56	65	127	0.64	0.56	74	118
6	0.57	123	0.66	0.50	56	190	0.65	0.50	71	175
7	0.55	158	0.69	0.44	50	266	0.66	0.45	72	244
8	0.53	202	0.71	0.39	45	358	0.67	0.39	83	320
9	0.63	95	0.68	0.58	64	126	0.67	0.59	75	115
10	0.60	120	0.69	0.52	55	185	0.67	0.53	72	167
11	0.56	151	0.70	0.45	48	255	0.67	0.46	70	232
12	0.54	190	0.71	0.40	42	338	0.68	0.40	66	314
13	0.56	59	0.56	0.56	59	59	0.56	0.56	60	59
14	0.54	58	0.54	0.54	58	58	0.54	0.54	59	57
15	0.51	56	0.52	0.51	56	56	0.52	0.51	58	54
16	0.49	54	0.50	0.49	54	54	0.49	0.49	57	52
17	0.48	53	0.49	0.47	53	53	0.49	0.48	56	50
18	0.54	68	0.58	0.52	56	80	0.55	0.52	59	77
19	0.52	66	0.54	0.49	55	78	0.54	0.50	58	75
20	0.49	65	0.52	0.46	53	76	0.52	0.47	58	72
21	0.48	63	0.50	0.45	52	74	0.50	0.45	57	70
22	0.45	62	0.48	0.42	51	73	0.47	0.43	56	68
23	0.49	103	0.58	0.41	47	159	0.57	0.42	58	148
24	0.47	101	0.56	0.38	46	156	0.55	0.39	57	146
25	0.44	100	0.54	0.36	46	154	0.52	0.36	57	143
26	0.42	98	0.51	0.34	45	152	0.50	0.34	56	141
27	0.40	97	0.50	0.32	44	150	0.49	0.32	56	139
28	0.57	123	0.66	0.50	56	190	0.65	0.50	71	175
29	0.54	118	0.64	0.46	54	183	0.62	0.47	70	167
30	0.52	114	0.62	0.43	52	176	0.60	0.44	66	162
31	0.49	111	0.59	0.40	51	171	0.58	0.1	65	156
32	0.46	108	0.56	0.38	49	166	0.55	0.39	63	152