Supporting information: Histogram-free reweighting to estimate vapor-liquid coexistence properties of non-simulated force fields

Richard A. Messerly,[*,†] Mohammad S. Barhaghi,[‡] Jeffrey J. Potoff,[‡] and Michael R. Shirts[¶]

†*Thermodynamics Research Center, National Institute of Standards and Technology, Boulder, Colorado, 80305, United States*

‡*Department of Chemical Engineering and Materials Science, Wayne State University, Detroit, Michigan 48202, United States*

¶*Department of Chemical and Biological Engineering, University of Colorado, Boulder, Colorado, 80309, United States*

E-mail: richard.messerly@nist.gov

Table SI.I: State points simulated for 2-methylpropane with the TraPPE force field.

T (K)	μ (K)	L (nm)
350	-3120	3.0
380	-3120	3.0
405	-3117	3.0
380	-2980	3.0
350	-2880	3.0
320	-2790	3.0
290	-2705	3.0
260	-2645	3.0
230	-2600	3.0
200	-2570	3.0

Table SI.II: State points simulated for 2,2-dimethylpropane with the TraPPE force field.

T (K)	μ (K)	L (nm)
380	-3405	3.0
410	-3405	3.0
440	-3405	3.0
410	-3250	3.0
380	-3140	3.0
350	-3037	3.0
330	-2970	3.0
300	-2900	3.0
270	-2820	3.0

SI.I State Points

SI.II Tabulated MBAR results

SI.III Optimal ψ values

Table SI.III: State points simulated for 2,2-dimethylbutane with the TraPPE force field.

T (K)	μ (K)	L (nm)
420	-3860	3.5
450	-3860	3.5
480	-3860	3.5
450	-3719	3.5
420	-3600	3.5
400	-3524	3.5
380	-3450	3.5
360	-3368	3.5
340	-3288	3.5
310	-3280	3.5

Table SI.IV: State points simulated for 2,3-dimethylbutane with the TraPPE force field.

T (K)	μ (K)	L (nm)
440	-4015	3.0
470	-4015	3.0
500	-4011	3.0
470	-3845	3.0
440	-3735	3.0
410	-3635	3.0
380	-3555	3.0
350	-3480	3.0
320	-3415	3.0

Table SI.V: State points simulated for 3,3-dimethylhexane with the TraPPE force field.

T (K)	μ (K)	L (nm)
500	-4670	3.5
530	-4670	3.5
560	-4670	3.5
520	-4476	3.5
490	-4370	3.5
460	-4268	3.5
430	-4164	3.5
400	-4039	3.5
370	-3925	3.5

Table SI.VI: State points simulated for 3-methyl-3-ethylpentane with the TraPPE force field.

T (K)	μ (K)	L (nm)
500	-4785	4.0
550	-4785	4.0
580	-4785	4.0
550	-4636	4.0
520	-4520	4.0
490	-4400	4.0
460	-4280	4.0
430	-4160	4.0
410	-4080	4.0
390	-3990	4.0

Table SI.VII: State points simulated for 2,3,4-trimethylpentane with the TraPPE force field.

T (K)	μ (K)	L (nm)
480	-4740	3.5
520	-4740	3.5
565	-4735	3.5
530	-4549	3.5
500	-4436	3.5
470	-4337	3.5
440	-4241	3.5
410	-4182	3.5
380	-4090	3.5
350	-4020	3.5

Table SI.VIII: State points simulated for 2,2,4-trimethylpentane with the TraPPE force field.

T (K)	μ (K)	L (nm)
480	-4600	4.0
530	-4600	4.0
560	-4600	4.0
530	-4450	4.0
500	-4330	4.0
470	-4210	4.0
440	-4090	4.0
410	-3960	4.0
380	-3840	4.0

Table SI.IX: State points simulated for cyclohexane with the TraPPE force field.

T (K)	μ (K)	L (nm)
450	-4350	3.0
500	-4350	3.0
550	-4350	3.0
500	-4120	3.0
460	-3977	3.0
410	-3790	3.0
350	-3562	3.0

Table SI.X: State points simulated for cyclohexane with the $\lambda^{(1)}_{\mathrm{CH_2}} = 14$ force field.

T (K)	μ (K)	L (nm)
450	-4389	3.0
500	-4389	3.0
550	-4389	3.0
500	-4164	3.0
460	-4033	3.0
410	-3891	3.0
360	-3780	3.0

Table SI.XI: State points simulated for cyclohexane with the $\lambda^{(1)}_{\mathrm{CH_2}} = 16$ force field.

T (K)	μ (K)	L (nm)
450	-4367	3.0
500	-4367	3.0
550	-4367	3.0
500	-4149	3.0
460	-4024	3.0
410	-3893	3.0
360	-3792	3.0

Table SI.XII: State points simulated for cyclohexane with the $\lambda^{(1)}_{\mathrm{CH_2}} = 18$ force field.

T (K)	μ (K)	L (nm)
450	-4370	3.0
500	-4370	3.0
550	-4370	3.0
500	-4158	3.0
460	-4037	3.0
410	-3912	3.0
360	-3825	3.0

Table SI.XIII: State points simulated for cyclohexane with the $\lambda^{(1)}_{\mathrm{CH_2}} = 20$ force field.

T (K)	μ (K)	L (nm)
450	-4386	3.0
500	-4386	3.0
550	-4386	3.0
500	-4178	3.0
460	-4062	3.0
410	-3946	3.0
360	-3866	3.0

Table SI.XIV: State points simulated for 2-methylpropane with the MiPPE-gen force field.

T (K)	μ (K)	L (nm)
350	-3150	3.0
380	-3150	3.0
410	-3145	3.0
380	-3010	3.0
350	-2910	3.0
320	-2830	3.0
290	-2760	3.0
260	-2700	3.0
230	-2670	3.0
200	-2640	3.0

Table SI.XV: State points simulated for 2,2-dimethylpropane with the MiPPE-gen force field.

T (K)	μ (K)	L (nm)
368	-3344	3.0
398	-3344	3.0
430	-3400	3.0
398	-3216	3.0
372	-3124	3.0
346	-3032	3.0
326	-2961	3.0
299	-2865	3.0
270	-2759	3.0

Table SI.XVI: State points simulated for 2,2-dimethylbutane with the MiPPE-gen force field.

T (K)	μ (K)	L (nm)
415	-3873	3.5
445	-3873	3.5
480	-3895	3.5
450	-3756	3.5
420	-3654	3.5
400	-3588	3.5
380	-3521	3.5
360	-3454	3.5
340	-3384	3.5
310	-3380	3.5

Table SI.XVII: State points simulated for 2,3-dimethylbutane with the MiPPE-gen force field.

T (K)	μ (K)	L (nm)
440	-4010	3.0
470	-4010	3.0
500	-4009	3.0
470	-3860	3.0
440	-3760	3.0
410	-3670	3.0
380	-3600	3.0
350	-3530	3.0
320	-3480	3.0

Table SI.XVIII: State points simulated for 2,3,4-trimethylpentane with the MiPPE-gen force field.

T (K)	μ (K)	L (nm)
480	-4720	3.5
520	-4720	3.5
565	-4713	3.5
530	-4540	3.5
500	-4360	3.5
470	-4355	3.5
440	-4275	3.5
410	-4205	3.5
380	-4165	3.5
350	-4115	3.5

Table SI.XIX: State points simulated for 2,2,4-trimethylpentane with the MiPPE-gen force field.

T (K)	μ (K)	L (nm)
470	-4570	4.0
520	-4570	4.0
550	-4570	4.0
520	-4420	4.0
490	-4300	4.0
460	-4170	4.0
430	-4050	4.0
400	-3920	4.0
370	-3790	4.0

Table SI.XX: GCMC-MBAR results for 2-methylpropane .

T_{sat} (K)	$\rho_{\mathrm{liq}}^{\mathrm{sat}}$ (kg/m^3)	$\rho_{\mathrm{vap}}^{\mathrm{sat}}$ (kg/m^3)	$P_{\mathrm{vap}}^{\mathrm{sat}}$ (MPa)	ΔH_{v} (kJ/mol)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$