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

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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

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

SI.I State Points

SI.II Tabulated GCMC-MBAR results

SI.II.1 Cyclohexane

SI.II.2 Branched alkanes

SI.II.3 Alkynes

SI.III Optimal ψ values

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 2,2,3-trimethylbutane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
520	$427.6_{2.7}$	$90.4_{3.4}$	$23.10_{0.41}$	$14.20_{0.20}$	$0.592_{0.025}$
510	$451.1_{1.5}$	$73.9_{3.6}$	$20.14_{0.30}$	$16.22_{0.27}$	$0.644_{0.033}$
500	$471.00_{0.92}$	$61.5_{2.9}$	$17.48_{0.20}$	$17.84_{0.29}$	$0.684_{0.033}$
490	$488.37_{0.82}$	$51.6_{1.9}$	$15.09_{0.14}$	$19.22_{0.23}$	$0.719_{0.027}$
480	$503.84_{0.76}$	$43.39_{0.99}$	$12.95_{0.11}$	$20.44_{0.15}$	$0.749_{0.018}$
470	$518.11_{0.61}$	$36.42_{0.54}$	$11.046_{0.087}$	$21.544_{0.083}$	$0.778_{0.013}$
460	$531.60_{0.50}$	$30.51_{0.45}$	$9.358_{0.068}$	$22.566_{0.064}$	$0.803_{0.013}$
450	$544.35_{0.55}$	$25.49_{0.41}$	$7.870_{0.049}$	$23.512_{0.070}$	$0.827_{0.014}$
440	$556.68_{0.54}$	$21.21_{0.32}$	$6.564_{0.032}$	$24.402_{0.069}$	$0.848_{0.014}$
430	$568.85_{0.50}$	$17.55_{0.23}$	$5.424_{0.020}$	$25.255_{0.062}$	$0.866_{0.012}$
420	$580.37_{0.55}$	$14.42_{0.15}$	$4.436_{0.014}$	$26.050_{0.058}$	$0.8826_{9.3e-3}$
410	$590.79_{0.86}$	$11.748_{0.088}$	$3.590_{0.014}$	$26.769_{0.064}$	$0.8982_{7.5e-3}$
400	$600.6_{1.0}$	$9.476_{0.069}$	$2.870_{0.014}$	$27.440_{0.077}$	$0.9126_{8.0e-3}$
390	$610.62_{0.83}$	$7.560_{0.096}$	$2.267_{0.013}$	$28.107_{0.086}$	$0.927_{0.013}$
380	$621.8_{1.5}$	$5.96_{0.14}$	$1.765_{0.014}$	$28.82_{0.16}$	$0.940_{0.023}$
370	$633.5_{2.1}$	$4.63_{0.17}$	$1.353_{0.019}$	$29.56_{0.26}$	$0.952_{0.038}$
360	$643.07_{0.71}$	$3.54_{0.20}$	$1.019_{0.029}$	$30.16_{0.26}$	$0.963_{0.060}$

Table SI.XXI: GCMC-MBAR results for 2,2,3-trimethylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap resampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
550	$424.5_{1.7}$	$94.6_{5.8}$	$22.04_{0.85}$	$14.90_{0.26}$	$0.582_{0.042}$
540	$446.63_{0.90}$	$77.5_{4.4}$	$19.31_{0.70}$	$17.04_{0.27}$	$0.634_{0.043}$
530	$466.95_{0.61}$	$64.6_{2.9}$	$16.85_{0.58}$	$18.86_{0.22}$	$0.676_{0.039}$
520	$485.81_{0.76}$	$54.4_{1.9}$	$14.63_{0.50}$	$20.45_{0.13}$	$0.711_{0.035}$
510	$502.62_{0.63}$	$45.9_{1.6}$	$12.63_{0.44}$	$21.840_{0.082}$	$0.742_{0.037}$
500	$517.03_{0.59}$	$38.7_{1.7}$	$10.84_{0.37}$	$23.05_{0.11}$	$0.770_{0.043}$
490	$529.98_{0.76}$	$32.6_{1.9}$	$9.25_{0.29}$	$24.14_{0.18}$	$0.795_{0.053}$
480	$542.7_{1.0}$	$27.4_{1.8}$	$7.84_{0.21}$	$25.18_{0.25}$	$0.818_{0.059}$
470	$555.2_{1.2}$	$23.0_{1.6}$	$6.59_{0.13}$	$26.17_{0.29}$	$0.840_{0.059}$
460	$566.7_{1.3}$	$19.1_{1.2}$	$5.500_{0.068}$	$27.09_{0.30}$	$0.860_{0.054}$
450	$577.6_{1.2}$	$15.82_{0.81}$	$4.550_{0.027}$	$27.94_{0.29}$	$0.878_{0.045}$
440	$588.5_{3.8}$	$13.0_{1.5}$	4_{13}	$28.8_{7.3}$	$0.9_{3.1}$
430	$599.6_{2.4}$	$10.61_{0.31}$	$3.023_{0.035}$	$29.58_{0.30}$	$0.910_{0.029}$
420	$610.1_{2.1}$	$8.58_{0.19}$	$2.423_{0.044}$	$30.34_{0.26}$	$0.923_{0.026}$
410	$619.5_{1.4}$	$6.88_{0.12}$	$1.918_{0.049}$	$31.02_{0.22}$	$0.935_{0.029}$
400	$628.4_{1.5}$	$5.447_{0.098}$	$1.498_{0.051}$	$31.66_{0.24}$	$0.945_{0.036}$
380	$645.33_{0.68}$	$3.285_{0.097}$	$0.874_{0.051}$	$32.86_{0.25}$	$0.961_{0.062}$

Table SI.XXII: GCMC-MBAR results for 2,2,4-trimethylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
530	$400.9_{2.2}$	$97.9_{4.8}$	$21.20_{0.38}$	$13.58_{0.32}$	$0.561_{0.029}$
520	$427.5_{1.3}$	$79.4_{3.2}$	$18.44_{0.28}$	$15.89_{0.27}$	$0.614_{0.027}$
510	$448.78_{0.77}$	$65.1_{1.8}$	$15.97_{0.21}$	$17.79_{0.18}$	$0.661_{0.020}$
500	$466.83_{0.75}$	$53.9_{1.1}$	$13.78_{0.18}$	$19.40_{0.13}$	$0.702_{0.017}$
490	$483.78_{0.81}$	$44.87_{0.89}$	$11.82_{0.15}$	$20.85_{0.12}$	$0.739_{0.017}$
480	$499.84_{0.70}$	$37.41_{0.89}$	$10.09_{0.12}$	$22.18_{0.12}$	$0.772_{0.020}$
470	$514.41_{0.57}$	$31.21_{0.86}$	$8.545_{0.083}$	$23.38_{0.13}$	$0.800_{0.023}$
460	$527.62_{0.53}$	$26.00_{0.75}$	$7.187_{0.053}$	$24.45_{0.13}$	$0.826_{0.025}$
450	$539.75_{0.68}$	$21.58_{0.59}$	$5.995_{0.030}$	$25.42_{0.12}$	$0.848_{0.024}$
440	$551.12_{0.66}$	$17.82_{0.43}$	$4.958_{0.022}$	$26.32_{0.12}$	$0.869_{0.021}$
430	$562.67_{0.50}$	$14.62_{0.31}$	$4.062_{0.027}$	$27.21_{0.13}$	$0.888_{0.020}$
420	$574.59_{0.49}$	$11.89_{0.25}$	$3.292_{0.035}$	$28.09_{0.13}$	$0.906_{0.021}$
410	$585.04_{0.41}$	$9.58_{0.25}$	$2.637_{0.042}$	$28.86_{0.15}$	$0.922_{0.028}$
400	$594.23_{0.30}$	$7.66_{0.27}$	$2.087_{0.051}$	$29.54_{0.20}$	$0.936_{0.040}$
390	$604.33_{0.26}$	$6.05_{0.29}$	$1.630_{0.063}$	$30.26_{0.28}$	$0.949_{0.058}$
380	$615.43_{0.23}$	$4.72_{0.30}$	$1.252_{0.077}$	$31.01_{0.41}$	$0.958_{0.084}$
370	$625.27_{0.23}$	$3.63_{0.29}$	$0.946_{0.092}$	$31.68_{0.58}$	$0.97_{0.12}$

Table SI.XXIII: GCMC-MBAR results for ethyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
290	$421.3_{3.5}$	$69.7_{3.3}$	$40.83_{0.20}$	$8.80_{0.21}$	$0.632_{0.030}$
280	$450.7_{1.9}$	$50.69_{0.91}$	$31.96_{0.26}$	$10.27_{0.12}$	$0.705_{0.014}$
270	$474.9_{3.0}$	$37.66_{0.39}$	$24.65_{0.24}$	$11.390_{0.086}$	$0.759_{0.011}$
260	$497.3_{1.1}$	$27.95_{0.53}$	$18.65_{0.17}$	$12.361_{0.034}$	$0.804_{0.017}$
250	$517.91_{0.59}$	$20.53_{0.34}$	$13.78_{0.12}$	$13.214_{0.042}$	$0.841_{0.016}$
240	$536.87_{0.67}$	$14.82_{0.12}$	$9.92_{0.10}$	$13.975_{0.028}$	$0.874_{0.011}$
230	$554.12_{0.54}$	$10.447_{0.095}$	$6.925_{0.089}$	$14.649_{0.037}$	$0.903_{0.014}$
220	$570.90_{0.53}$	$7.155_{0.097}$	$4.667_{0.082}$	$15.283_{0.049}$	$0.929_{0.021}$

Table SI.XXIV: GCMC-MBAR results for propyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
380	$441.0_{7.9}$	$82.2_{3.1}$	$38.39_{0.90}$	$10.96_{0.34}$	$0.592_{0.026}$
370	$472.7_{5.0}$	$62.7_{2.7}$	$31.64_{0.73}$	$12.83_{0.31}$	$0.657_{0.033}$
360	$498.3_{2.8}$	$48.6_{1.9}$	$25.84_{0.57}$	$14.34_{0.24}$	$0.711_{0.032}$
350	$520.1_{2.4}$	$38.1_{1.3}$	$20.88_{0.45}$	$15.58_{0.19}$	$0.754_{0.030}$
340	$539.4_{2.1}$	$29.88_{0.90}$	$16.67_{0.35}$	$16.65_{0.15}$	$0.791_{0.029}$
330	$556.6_{1.4}$	$23.31_{0.72}$	$13.13_{0.27}$	$17.58_{0.11}$	$0.822_{0.031}$
320	$572.1_{1.3}$	$18.02_{0.60}$	$10.18_{0.19}$	$18.41_{0.11}$	$0.850_{0.032}$
310	$587.6_{1.3}$	$13.76_{0.47}$	$7.76_{0.12}$	$19.20_{0.12}$	$0.876_{0.033}$
300	$603.3_{1.5}$	$10.35_{0.32}$	$5.799_{0.068}$	$19.97_{0.13}$	$0.900_{0.030}$
290	$617.9_{2.2}$	$7.65_{0.20}$	$4.240_{0.040}$	$20.67_{0.15}$	$0.921_{0.025}$

Table SI.XXV: GCMC-MBAR results for 1-butyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
410	$445.1_{5.3}$	76_{12}	$29.5_{1.0}$	$12.82_{0.72}$	$0.620_{0.097}$
400	$472.3_{3.4}$	$59.2_{6.8}$	$24.64_{0.50}$	$14.61_{0.60}$	$0.677_{0.079}$
390	$495.0_{2.6}$	$47.1_{2.3}$	$20.38_{0.30}$	$16.08_{0.32}$	$0.722_{0.037}$
380	$515.5_{2.0}$	$37.54_{0.86}$	$16.69_{0.23}$	$17.37_{0.16}$	$0.761_{0.020}$
370	$534.5_{1.3}$	$29.90_{0.70}$	$13.51_{0.18}$	$18.53_{0.13}$	$0.795_{0.021}$
360	$552.0_{1.6}$	$23.69_{0.62}$	$10.81_{0.13}$	$19.57_{0.16}$	$0.824_{0.024}$
350	$567.8_{1.9}$	$18.62_{0.51}$	$8.524_{0.086}$	$20.50_{0.18}$	$0.851_{0.025}$
340	$582.2_{1.1}$	$14.49_{0.38}$	$6.623_{0.060}$	$21.34_{0.13}$	$0.874_{0.024}$
330	$595.8_{1.1}$	$11.15_{0.24}$	$5.061_{0.049}$	$22.112_{0.082}$	$0.895_{0.021}$
320	$610.6_{2.8}$	$8.45_{0.14}$	$3.795_{0.049}$	$22.905_{0.095}$	$0.913_{0.019}$
310	$624.6_{1.8}$	$6.284_{0.087}$	$2.782_{0.051}$	$23.650_{0.059}$	$0.929_{0.021}$

Table SI.XXVI: GCMC-MBAR results for 2-butyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
450	$431.8_{7.4}$	$93.5_{4.3}$	$36.24_{0.50}$	$11.93_{0.26}$	$0.561_{0.027}$
440	$466.0_{5.5}$	$74.1_{3.5}$	$30.73_{0.28}$	$14.00_{0.24}$	$0.613_{0.029}$
430	$491.6_{2.0}$	$59.1_{1.9}$	$25.87_{0.16}$	$15.71_{0.17}$	$0.662_{0.022}$
420	$512.10_{0.77}$	$47.58_{0.69}$	$21.63_{0.14}$	$17.114_{0.094}$	$0.704_{0.011}$
410	$530.5_{1.1}$	$38.42_{0.30}$	$17.95_{0.13}$	$18.346_{0.054}$	$0.7411_{7.7e-3}$
400	$548.28_{0.94}$	$30.99_{0.31}$	$14.76_{0.11}$	$19.487_{0.051}$	$0.7745_{9.6e-3}$
390	$565.05_{0.94}$	$24.89_{0.27}$	$12.013_{0.089}$	$20.533_{0.061}$	$0.805_{0.011}$
380	$580.6_{1.1}$	$19.89_{0.25}$	$9.674_{0.068}$	$21.483_{0.073}$	$0.833_{0.012}$
370	$594.97_{0.83}$	$15.78_{0.25}$	$7.697_{0.050}$	$22.349_{0.074}$	$0.858_{0.014}$
360	$608.65_{0.59}$	$12.41_{0.22}$	$6.041_{0.038}$	$23.157_{0.070}$	$0.880_{0.017}$
350	$621.69_{0.66}$	$9.66_{0.19}$	$4.672_{0.041}$	$23.912_{0.091}$	$0.899_{0.019}$
340	$633.85_{0.59}$	$7.42_{0.16}$	$3.552_{0.052}$	$24.60_{0.12}$	$0.916_{0.024}$
330	$646.13_{0.73}$	$5.62_{0.13}$	$2.651_{0.064}$	$25.26_{0.16}$	$0.930_{0.031}$

Table SI.XXVII: GCMC-MBAR results for 1-pentyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
450	$433.7_{2.3}$	$85.6_{2.5}$	$27.32_{0.22}$	$13.15_{0.18}$	$0.581_{0.018}$
440	$461.7_{1.7}$	$66.9_{2.0}$	$23.04_{0.15}$	$15.29_{0.18}$	$0.641_{0.020}$
430	$485.2_{1.5}$	$53.1_{1.2}$	$19.32_{0.12}$	$17.06_{0.16}$	$0.693_{0.016}$
420	$505.4_{1.6}$	$42.65_{0.51}$	$16.08_{0.12}$	$18.54_{0.11}$	$0.735_{0.010}$
410	$523.3_{1.4}$	$34.37_{0.30}$	$13.27_{0.10}$	$19.810_{0.078}$	$0.7714_{8.8e-3}$
400	$539.7_{1.2}$	$27.67_{0.31}$	$10.844_{0.077}$	$20.949_{0.055}$	$0.803_{0.011}$
390	$555.3_{1.1}$	$22.17_{0.30}$	$8.770_{0.052}$	$21.998_{0.041}$	$0.831_{0.012}$
380	$570.2_{1.0}$	$17.64_{0.27}$	$7.009_{0.033}$	$22.977_{0.033}$	$0.857_{0.014}$
370	$584.03_{0.90}$	$13.91_{0.25}$	$5.528_{0.028}$	$23.874_{0.050}$	$0.880_{0.016}$
360	$596.86_{0.83}$	$10.86_{0.22}$	$4.300_{0.040}$	$24.697_{0.083}$	$0.901_{0.020}$
350	$609.71_{0.69}$	$8.37_{0.19}$	$3.291_{0.055}$	$25.49_{0.11}$	$0.920_{0.026}$
340	$622.58_{0.99}$	$6.37_{0.15}$	$2.474_{0.070}$	$26.27_{0.13}$	$0.936_{0.035}$

Table SI.XXVIII: GCMC-MBAR results for 2-pentyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
470	$445.8_{3.1}$	$83.4_{6.2}$	$27.7_{1.2}$	$14.09_{0.22}$	$0.578_{0.049}$
460	$473.8_{1.9}$	$65.6_{5.4}$	$23.43_{0.88}$	$16.27_{0.30}$	$0.636_{0.057}$
450	$496.8_{1.0}$	$52.5_{3.7}$	$19.73_{0.64}$	$18.06_{0.28}$	$0.685_{0.053}$
440	$516.64_{0.73}$	$42.4_{2.3}$	$16.50_{0.48}$	$19.56_{0.22}$	$0.725_{0.045}$
430	$534.83_{0.74}$	$34.3_{1.7}$	$13.69_{0.36}$	$20.89_{0.19}$	$0.761_{0.042}$
420	$551.57_{0.81}$	$27.7_{1.4}$	$11.26_{0.25}$	$22.08_{0.19}$	$0.792_{0.044}$
410	$566.89_{0.86}$	$22.3_{1.2}$	$9.17_{0.16}$	$23.16_{0.22}$	$0.821_{0.048}$
400	$581.3_{1.1}$	$17.9_{1.0}$	$7.394_{0.080}$	$24.15_{0.26}$	$0.847_{0.049}$
390	$595.3_{1.6}$	$14.24_{0.71}$	$5.890_{0.039}$	$25.09_{0.28}$	$0.869_{0.043}$
380	$608.6_{1.7}$	$11.23_{0.40}$	$4.631_{0.052}$	$25.95_{0.25}$	$0.889_{0.034}$
370	$621.0_{1.3}$	$8.76_{0.19}$	$3.587_{0.066}$	$26.75_{0.19}$	$0.907_{0.026}$
360	$632.99_{0.96}$	$6.75_{0.16}$	$2.735_{0.069}$	$27.52_{0.12}$	$0.922_{0.031}$
350	$644.7_{1.0}$	$5.12_{0.20}$	$2.049_{0.065}$	$28.249_{0.10}$	$0.937_{0.047}$

Table SI.XXIX: GCMC-MBAR results for 1-hexyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
490	$423.3_{3.5}$	$87.3_{2.1}$	$25.38_{0.68}$	$14.25_{0.14}$	$0.586_{0.021}$
480	$453.3_{2.0}$	$69.9_{1.5}$	$21.70_{0.60}$	$16.54_{0.12}$	$0.639_{0.022}$
470	$477.4_{1.3}$	$56.51_{0.96}$	$18.44_{0.56}$	$18.448_{0.089}$	$0.686_{0.024}$
460	$497.3_{1.4}$	$46.06_{0.95}$	$15.56_{0.51}$	$20.041_{0.074}$	$0.726_{0.028}$
450	$514.8_{1.3}$	$37.6_{1.3}$	$13.04_{0.44}$	$21.428_{0.10}$	$0.761_{0.037}$
440	$531.5_{1.2}$	$30.7_{1.7}$	$10.84_{0.35}$	$22.71_{0.16}$	$0.792_{0.050}$
430	$547.4_{1.2}$	$25.0_{1.7}$	$8.93_{0.24}$	$23.91_{0.22}$	$0.820_{0.061}$
420	$561.77_{0.87}$	$20.3_{1.5}$	$7.28_{0.13}$	$24.98_{0.23}$	$0.845_{0.063}$
410	$575.17_{0.62}$	$16.34_{0.99}$	$5.875_{0.050}$	$25.97_{0.20}$	$0.867_{0.053}$
400	$588.08_{0.75}$	$13.04_{0.55}$	$4.682_{0.027}$	$26.90_{0.15}$	$0.887_{0.038}$
390	$599.80_{0.63}$	$10.31_{0.28}$	$3.684_{0.047}$	$27.75_{0.11}$	$0.905_{0.027}$
380	$610.32_{0.79}$	$8.06_{0.17}$	$2.858_{0.061}$	$28.507_{0.080}$	$0.922_{0.027}$
370	$621.3_{2.9}$	$6.23_{0.13}$	$2.185_{0.072}$	$29.267_{0.086}$	$0.937_{0.037}$
360	$634.3_{3.1}$	$4.74_{0.11}$	$1.640_{0.083}$	$30.118_{0.078}$	$0.950_{0.053}$

Table SI.XXX: GCMC-MBAR results for 2-hexyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
500	$438.2_{2.9}$	$85.9_{4.0}$	$24.95_{0.26}$	$14.93_{0.36}$	$0.574_{0.027}$
490	$464.9_{1.8}$	$67.7_{2.5}$	$21.31_{0.16}$	$17.31_{0.29}$	$0.635_{0.024}$
480	$486.7_{1.5}$	$54.7_{1.3}$	$18.11_{0.11}$	$19.18_{0.19}$	$0.682_{0.017}$
470	$505.2_{1.7}$	$44.67_{0.74}$	$15.302_{0.087}$	$20.71_{0.14}$	$0.720_{0.013}$
460	$522.5_{2.3}$	$36.61_{0.52}$	$12.839_{0.074}$	$22.09_{0.14}$	$0.753_{0.012}$
450	$539.3_{2.5}$	$29.96_{0.40}$	$10.686_{0.062}$	$23.39_{0.15}$	$0.783_{0.011}$
440	$555.2_{1.8}$	$24.43_{0.31}$	$8.815_{0.050}$	$24.60_{0.11}$	$0.810_{0.011}$
430	$569.62_{0.68}$	$19.82_{0.28}$	$7.201_{0.040}$	$25.678_{0.066}$	$0.835_{0.013}$
420	$583.3_{1.4}$	$15.98_{0.26}$	$5.821_{0.034}$	$26.69_{0.11}$	$0.857_{0.015}$
410	$597.0_{1.4}$	$12.77_{0.22}$	$4.651_{0.035}$	$27.67_{0.12}$	$0.877_{0.017}$
400	$609.9_{1.1}$	$10.11_{0.16}$	$3.669_{0.039}$	$28.59_{0.11}$	$0.896_{0.017}$
390	$621.7_{1.4}$	$7.92_{0.14}$	$2.857_{0.045}$	$29.42_{0.14}$	$0.914_{0.021}$
380	$633.2_{1.2}$	$6.12_{0.16}$	$2.190_{0.050}$	$30.23_{0.16}$	$0.930_{0.032}$
370	$644.01_{0.40}$	$4.67_{0.18}$	$1.653_{0.059}$	$30.98_{0.19}$	$0.944_{0.049}$

Table SI.XXXI: GCMC-MBAR results for 1-heptyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
520	$427.5_{6.0}$	$82.9_{6.4}$	$22.18_{0.71}$	$16.05_{0.64}$	$0.595_{0.050}$
510	$454.3_{2.5}$	$66.9_{4.8}$	$19.06_{0.55}$	$18.37_{0.49}$	$0.646_{0.050}$
500	$476.5_{1.4}$	$54.5_{3.3}$	$16.29_{0.41}$	$20.34_{0.35}$	$0.691_{0.045}$
490	$495.7_{1.4}$	$44.8_{2.4}$	$13.84_{0.30}$	$22.02_{0.25}$	$0.730_{0.042}$
480	$512.9_{1.6}$	$36.9_{1.8}$	$11.68_{0.20}$	$23.51_{0.18}$	$0.764_{0.040}$
470	$528.7_{2.0}$	$30.3_{1.4}$	$9.79_{0.12}$	$24.85_{0.13}$	$0.794_{0.037}$
460	$543.2_{1.9}$	$24.91_{0.95}$	$8.138_{0.072}$	$26.066_{0.092}$	$0.821_{0.032}$
450	$556.9_{1.5}$	$20.37_{0.57}$	$6.705_{0.058}$	$27.199_{0.070}$	$0.846_{0.025}$
440	$570.2_{1.0}$	$16.57_{0.25}$	$5.472_{0.063}$	$28.279_{0.062}$	$0.868_{0.016}$
430	$583.08_{0.58}$	$13.38_{0.11}$	$4.419_{0.062}$	$29.301_{0.062}$	$0.888_{0.015}$
420	$595.19_{0.32}$	$10.71_{0.23}$	$3.526_{0.055}$	$30.253_{0.097}$	$0.907_{0.024}$
410	$606.63_{0.36}$	$8.50_{0.30}$	$2.779_{0.046}$	$31.14_{0.16}$	$0.923_{0.037}$
400	$617.58_{0.39}$	$6.66_{0.33}$	$2.160_{0.048}$	$31.98_{0.23}$	$0.938_{0.050}$
390	$628.63_{0.36}$	$5.16_{0.31}$	$1.654_{0.061}$	$32.81_{0.31}$	$0.950_{0.067}$

Table SI.XXXII: GCMC-MBAR results for 1-octyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
550	$419.4_{3.6}$	$89.5_{1.2}$	$20.75_{0.15}$	$16.27_{0.24}$	$0.5584_{8.6e-3}$
540	$445.2_{3.0}$	$70.95_{0.88}$	$17.88_{0.15}$	$18.98_{0.20}$	$0.6184_{9.2e-3}$
530	$467.6_{2.6}$	$57.19_{0.55}$	$15.35_{0.15}$	$21.30_{0.17}$	$0.6711_{9.1e-3}$
520	$487.1_{2.4}$	$46.85_{0.42}$	$13.11_{0.14}$	$23.22_{0.15}$	$0.7133_{9.8e-3}$
510	$504.3_{2.0}$	$38.69_{0.48}$	$11.14_{0.12}$	$24.87_{0.13}$	$0.748_{0.012}$
500	$519.8_{1.5}$	$32.01_{0.56}$	$9.395_{0.099}$	$26.33_{0.12}$	$0.778_{0.016}$
490	$534.3_{1.2}$	$26.45_{0.57}$	$7.869_{0.075}$	$27.66_{0.13}$	$0.805_{0.019}$
480	$548.2_{1.2}$	$21.77_{0.52}$	$6.539_{0.053}$	$28.92_{0.15}$	$0.829_{0.021}$
470	$561.6_{1.2}$	$17.83_{0.40}$	$5.385_{0.038}$	$30.10_{0.15}$	$0.852_{0.020}$
460	$574.15_{0.95}$	$14.52_{0.26}$	$4.392_{0.033}$	$31.21_{0.13}$	$0.872_{0.017}$
450	$586.02_{0.57}$	$11.73_{0.12}$	$3.546_{0.033}$	$32.245_{0.084}$	$0.890_{0.012}$
440	$597.51_{0.35}$	$9.404_{0.077}$	$2.830_{0.032}$	$33.229_{0.046}$	$0.907_{0.013}$
430	$608.64_{0.40}$	$7.46_{0.15}$	$2.231_{0.029}$	$34.171_{0.089}$	$0.921_{0.022}$
420	$619.31_{0.42}$	$5.86_{0.20}$	$1.736_{0.027}$	$35.06_{0.16}$	$0.935_{0.036}$
410	$630.00_{0.38}$	$4.55_{0.22}$	$1.330_{0.032}$	$35.94_{0.24}$	$0.946_{0.052}$

Table SI.XXXIII: GCMC-MBAR results for 1-nonyne with the MiPPE force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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)	$Z_{\mathrm{vap}}^{\mathrm{sat}}$
570	$427.1_{1.2}$	$80.5_{1.0}$	$17.76_{0.15}$	$18.58_{0.17}$	$0.5782_{8.9e-3}$
560	$450.9_{1.3}$	$64.43_{0.86}$	$15.31_{0.13}$	$21.28_{0.20}$	$0.6340_{9.9e-3}$
550	$471.7_{1.6}$	$52.31_{0.73}$	$13.15_{0.10}$	$23.58_{0.20}$	$0.683_{0.011}$
540	$489.9_{1.5}$	$43.02_{0.62}$	$11.239_{0.080}$	$25.52_{0.17}$	$0.723_{0.012}$
530	$506.3_{1.1}$	$35.61_{0.52}$	$9.552_{0.059}$	$27.21_{0.13}$	$0.756_{0.012}$
520	$521.47_{0.66}$	$29.51_{0.42}$	$8.067_{0.041}$	$28.739_{0.093}$	$0.785_{0.012}$
510	$535.75_{0.67}$	$24.42_{0.33}$	$6.762_{0.026}$	$30.149_{0.083}$	$0.811_{0.012}$
500	$549.10_{0.85}$	$20.14_{0.26}$	$5.626_{0.015}$	$31.452_{0.094}$	$0.835_{0.011}$
490	$561.65_{0.81}$	$16.54_{0.20}$	$4.6410_{9.7e-3}$	$32.666_{0.094}$	$0.856_{0.010}$
480	$573.68_{0.62}$	$13.50_{0.15}$	$3.792_{0.010}$	$33.811_{0.080}$	$0.8746_{9.9e-3}$
470	$585.26_{0.49}$	$10.94_{0.11}$	$3.068_{0.014}$	$34.896_{0.067}$	$0.892_{0.010}$
460	$596.35_{0.58}$	$8.794_{0.096}$	$2.455_{0.017}$	$35.924_{0.069}$	$0.907_{0.012}$
450	$607.27_{0.71}$	$7.003_{0.091}$	$1.942_{0.020}$	$36.924_{0.081}$	$0.921_{0.015}$
440	$618.21_{0.61}$	$5.516_{0.091}$	$1.516_{0.023}$	$37.91_{0.10}$	$0.933_{0.021}$
430	$628.74_{0.51}$	$4.292_{0.090}$	$1.166_{0.026}$	$38.85_{0.14}$	$0.944_{0.029}$
420	$638.50_{0.50}$	$3.296_{0.086}$	$0.885_{0.030}$	$39.72_{0.18}$	$0.955_{0.040}$