

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

SI.3

SI.IV Minimum number of effective snapshots

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 $\lambda_{\text{CH}_2}^{(1)} = 14$ 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 $\lambda_{\text{CH}_2}^{(1)} = 16$ 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 $\lambda_{\text{CH}_2}^{(1)} = 18$ 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 $\lambda_{\text{CH}_2}^{(1)} = 20$ 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-methylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
470	422.20 _{0.56}	76.7 _{1.5}	20.68 _{0.17}	14.14 _{0.11}	0.595 _{0.012}
460	444.71 _{0.79}	61.2 _{1.2}	17.61 _{0.13}	16.06 _{0.12}	0.649 _{0.013}
450	464.38 _{0.87}	49.31 _{0.88}	14.918 _{0.096}	17.71 _{0.11}	0.697 _{0.013}
440	481.69 _{0.77}	40.17 _{0.64}	12.557 _{0.068}	19.106 _{0.090}	0.736 _{0.012}
430	497.34 _{0.70}	32.86 _{0.47}	10.491 _{0.045}	20.318 _{0.074}	0.770 _{0.012}
420	511.89 _{0.78}	26.86 _{0.36}	8.690 _{0.027}	21.408 _{0.068}	0.798 _{0.011}
410	525.69 _{0.84}	21.87 _{0.29}	7.130 _{0.017}	22.412 _{0.069}	0.824 _{0.011}
400	538.82 _{0.88}	17.70 _{0.25}	5.788 _{0.020}	23.344 _{0.069}	0.848 _{0.012}
390	551.23 _{0.87}	14.21 _{0.22}	4.645 _{0.031}	24.207 _{0.075}	0.869 _{0.014}
380	562.89 _{0.80}	11.30 _{0.19}	3.681 _{0.042}	25.004 _{0.096}	0.888 _{0.018}
370	573.96 _{0.88}	8.90 _{0.16}	2.878 _{0.051}	25.75 _{0.14}	0.906 _{0.023}
360	584.8 _{1.1}	6.92 _{0.14}	2.215 _{0.059}	26.46 _{0.18}	0.922 _{0.031}
350	595.6 _{1.2}	5.31 _{0.12}	1.677 _{0.065}	27.15 _{0.22}	0.935 _{0.042}
340	606.3 _{1.2}	4.01 _{0.10}	1.245 _{0.070}	27.83 _{0.27}	0.947 _{0.059}
330	616.4 _{1.0}	2.969 _{0.085}	0.906 _{0.074}	28.45 _{0.32}	0.958 _{0.083}
320	625.82 _{0.57}	2.156 _{0.068}	0.644 _{0.078}	29.04 _{0.40}	0.97 _{0.12}

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

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
510	406.8 _{3.4}	88.4 _{2.0}	20.92 _{0.11}	14.14 _{0.12}	0.559 _{0.013}
500	431.2 _{2.2}	70.0 _{1.6}	17.989 _{0.052}	16.506 _{0.085}	0.620 _{0.014}
490	452.1 _{1.2}	56.5 _{1.0}	15.403 _{0.041}	18.472 _{0.088}	0.671 _{0.013}
480	470.38 _{0.73}	46.30 _{0.50}	13.120 _{0.056}	20.092 _{0.065}	0.7116 _{8.3e-3}
470	486.88 _{0.50}	38.21 _{0.17}	11.104 _{0.062}	21.497 _{0.034}	0.7453 _{5.3e-3}
460	502.20 _{0.37}	31.56 _{0.16}	9.327 _{0.058}	22.762 _{0.022}	0.7744 _{6.2e-3}
450	516.52 _{0.39}	26.01 _{0.17}	7.772 _{0.050}	23.921 _{0.024}	0.8003 _{7.3e-3}
440	530.01 _{0.34}	21.34 _{0.15}	6.417 _{0.043}	24.994 _{0.024}	0.8236 _{7.9e-3}
430	542.86 _{0.37}	17.41 _{0.14}	5.245 _{0.039}	25.998 _{0.031}	0.8444 _{9.1e-3}
420	554.93 _{0.46}	14.10 _{0.13}	4.241 _{0.037}	26.928 _{0.041}	0.863 _{0.011}
410	566.22 _{0.43}	11.32 _{0.14}	3.390 _{0.036}	27.789 _{0.046}	0.881 _{0.014}
400	577.21 _{0.43}	8.99 _{0.14}	2.674 _{0.037}	28.610 _{0.060}	0.896 _{0.019}
390	588.02 _{0.38}	7.06 _{0.15}	2.080 _{0.039}	29.403 _{0.089}	0.910 _{0.026}
380	598.35 _{0.22}	5.47 _{0.16}	1.593 _{0.044}	30.15 _{0.14}	0.923 _{0.037}
370	608.04 _{0.19}	4.18 _{0.16}	1.200 _{0.050}	30.85 _{0.20}	0.935 _{0.053}
360	617.49 _{0.27}	3.14 _{0.16}	0.888 _{0.057}	31.52 _{0.28}	0.945 _{0.077}
350	627.22 _{0.26}	2.32 _{0.15}	0.644 _{0.065}	32.20 _{0.39}	0.96 _{0.11}

Table SI.XXII: GCMC-MBAR results for 3-methylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
480	415.8 _{1.5}	84 ₂₄	23.1 _{2.4}	13.7 _{1.3}	0.60 _{0.18}
470	440.0 _{2.3}	67 ₂₄	19.9 _{1.4}	15.6 _{1.7}	0.65 _{0.23}
460	459.8 _{2.5}	55 ₁₈	16.98 _{0.59}	17.2 _{1.6}	0.69 _{0.22}
450	477.1 _{1.9}	45.4 _{7.6}	14.43 _{0.12}	18.52 _{0.94}	0.73 _{0.12}
440	493.2 _{1.2}	37.5 _{1.5}	12.17 _{0.14}	19.74 _{0.27}	0.764 _{0.032}
430	508.9 _{1.4}	30.95 _{0.38}	10.19 _{0.15}	20.87 _{0.11}	0.794 _{0.015}
420	523.6 _{1.1}	25.42 _{0.36}	8.45 _{0.14}	21.917 _{0.094}	0.821 _{0.018}
410	536.8 _{1.4}	20.78 _{0.32}	6.95 _{0.14}	22.85 _{0.12}	0.845 _{0.021}
400	548.9 _{1.7}	16.89 _{0.24}	5.65 _{0.13}	23.69 _{0.15}	0.867 _{0.023}
390	560.5 _{1.5}	13.63 _{0.21}	4.55 _{0.12}	24.49 _{0.13}	0.887 _{0.027}
380	571.8 _{1.2}	10.88 _{0.20}	3.61 _{0.10}	25.250 _{0.099}	0.905 _{0.031}
370	582.3 _{1.1}	8.59 _{0.18}	2.829 _{0.089}	25.950 _{0.093}	0.922 _{0.035}
360	593.0 _{1.1}	6.70 _{0.16}	2.185 _{0.077}	26.64 _{0.12}	0.939 _{0.040}
350	603.8 _{1.0}	5.15 _{0.14}	1.661 _{0.067}	27.33 _{0.14}	0.955 _{0.047}

Table SI.XXIII: GCMC-MBAR results for 3-methylhexane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
520	398.4 _{4.6}	98.1 _{1.2}	23.07 _{0.18}	13.25 _{0.29}	0.5453 _{7.9e-3}
510	426.2 _{3.4}	77.3 _{1.3}	19.96 _{0.15}	15.86 _{0.21}	0.610 _{0.011}
500	449.0 _{1.8}	62.6 _{1.1}	17.20 _{0.12}	17.92 _{0.14}	0.662 _{0.013}
490	467.85 _{0.87}	51.64 _{0.76}	14.74 _{0.11}	19.56 _{0.10}	0.702 _{0.011}
480	484.12 _{0.71}	42.82 _{0.51}	12.562 _{0.093}	20.963 _{0.074}	0.737 _{0.010}
470	498.93 _{0.76}	35.54 _{0.44}	10.638 _{0.075}	22.215 _{0.069}	0.768 _{0.011}
460	512.9 _{1.0}	29.46 _{0.42}	8.944 _{0.056}	23.366 _{0.088}	0.796 _{0.012}
450	526.2 _{1.3}	24.34 _{0.36}	7.463 _{0.040}	24.442 _{0.093}	0.821 _{0.013}
440	539.09 _{0.79}	20.03 _{0.26}	6.171 _{0.029}	25.454 _{0.048}	0.844 _{0.011}
430	551.25 _{0.90}	16.38 _{0.15}	5.055 _{0.025}	26.397 _{0.089}	0.8648 _{8.9e-3}
420	563.0 _{1.6}	13.302 _{0.087}	4.097 _{0.025}	27.29 _{0.16}	0.8838 _{7.9e-3}
410	574.5 _{1.4}	10.70 _{0.12}	3.283 _{0.024}	28.15 _{0.18}	0.902 _{0.012}
400	585.3 _{1.3}	8.53 _{0.18}	2.598 _{0.021}	28.96 _{0.19}	0.918 _{0.021}
390	595.7 _{2.4}	6.72 _{0.26}	2.028 _{0.021}	29.72 _{0.30}	0.933 _{0.037}
380	605.9 _{2.8}	5.23 _{0.33}	1.560 _{0.032}	30.45 _{0.41}	0.947 _{0.063}
370	615.4 _{1.3}	4.01 _{0.38}	1.181 _{0.053}	31.13 _{0.47}	0.96 _{0.10}
360	624.92 _{0.55}	3.04 _{0.40}	0.878 _{0.081}	31.78 _{0.63}	0.97 _{0.16}

Table SI.XXIV: GCMC-MBAR results for 2,3-dimethylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_{v} (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
510	427.9 _{1.6}	81 ₁₀	20.82 _{0.91}	15.20 _{0.53}	0.606 _{0.081}
500	451.7 _{1.0}	66.3 _{9.6}	18.00 _{0.57}	17.17 _{0.70}	0.654 _{0.097}
490	471.41 _{0.86}	54.7 _{7.1}	15.49 _{0.28}	18.83 _{0.70}	0.696 _{0.091}
480	488.48 _{0.89}	45.5 _{4.0}	13.245 _{0.092}	20.25 _{0.54}	0.731 _{0.064}
470	503.90 _{0.73}	37.9 _{1.7}	11.257 _{0.050}	21.50 _{0.32}	0.762 _{0.035}
460	518.28 _{0.52}	31.50 _{0.62}	9.501 _{0.072}	22.64 _{0.14}	0.790 _{0.017}
450	532.03 _{0.63}	26.12 _{0.25}	7.956 _{0.080}	23.709 _{0.054}	0.816 _{0.011}
440	545.26 _{0.62}	21.57 _{0.18}	6.606 _{0.080}	24.711 _{0.037}	0.839 _{0.012}
430	557.77 _{0.54}	17.70 _{0.16}	5.435 _{0.075}	25.646 _{0.038}	0.860 _{0.014}
420	569.33 _{0.53}	14.43 _{0.15}	4.426 _{0.070}	26.504 _{0.037}	0.880 _{0.016}
410	580.03 _{0.59}	11.68 _{0.14}	3.565 _{0.063}	27.290 _{0.040}	0.897 _{0.019}
400	590.33 _{0.66}	9.36 _{0.13}	2.837 _{0.057}	28.032 _{0.047}	0.913 _{0.022}
390	600.50 _{0.61}	7.43 _{0.11}	2.229 _{0.052}	28.747 _{0.057}	0.927 _{0.026}
380	610.33 _{0.59}	5.831 _{0.094}	1.726 _{0.048}	29.424 _{0.079}	0.939 _{0.030}
370	620.01 _{0.64}	4.512 _{0.077}	1.315 _{0.046}	30.08 _{0.11}	0.950 _{0.037}
360	630.25 _{0.55}	3.438 _{0.066}	0.984 _{0.045}	30.75 _{0.14}	0.959 _{0.048}
350	640.58 _{0.49}	2.572 _{0.058}	0.722 _{0.046}	31.42 _{0.20}	0.966 _{0.065}

Table SI.XXV: GCMC-MBAR results for 2,3-dimethylhexane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_{v} (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
540	422.2 _{1.1}	84.5 _{3.7}	19.48 _{0.48}	15.98 _{0.12}	0.586 _{0.029}
530	445.87 _{0.82}	68.6 _{3.6}	16.89 _{0.36}	18.23 _{0.22}	0.638 _{0.036}
520	466.30 _{0.66}	56.3 _{3.0}	14.58 _{0.24}	20.17 _{0.26}	0.684 _{0.038}
510	484.13 _{0.59}	46.7 _{2.1}	12.53 _{0.15}	21.81 _{0.23}	0.722 _{0.034}
500	499.99 _{0.52}	39.0 _{1.4}	10.703 _{0.092}	23.24 _{0.18}	0.755 _{0.027}
490	514.34 _{0.48}	32.51 _{0.80}	9.084 _{0.054}	24.51 _{0.13}	0.783 _{0.020}
480	527.67 _{0.54}	27.08 _{0.47}	7.657 _{0.032}	25.677 _{0.096}	0.809 _{0.014}
470	540.41 _{0.64}	22.49 _{0.30}	6.406 _{0.019}	26.765 _{0.082}	0.833 _{0.012}
460	552.77 _{0.76}	18.58 _{0.23}	5.313 _{0.015}	27.797 _{0.085}	0.854 _{0.011}
450	564.84 _{0.87}	15.26 _{0.22}	4.366 _{0.018}	28.78 _{0.11}	0.874 _{0.013}
440	576.56 _{0.95}	12.43 _{0.23}	3.553 _{0.025}	29.73 _{0.14}	0.892 _{0.017}
430	587.55 _{0.97}	10.05 _{0.23}	2.860 _{0.034}	30.60 _{0.18}	0.909 _{0.023}
420	597.72 _{0.83}	8.05 _{0.21}	2.274 _{0.044}	31.40 _{0.21}	0.924 _{0.030}
410	607.46 _{0.53}	6.39 _{0.18}	1.787 _{0.053}	32.16 _{0.22}	0.937 _{0.038}
400	617.12 _{0.48}	5.01 _{0.14}	1.384 _{0.061}	32.90 _{0.24}	0.949 _{0.050}
390	626.72 _{0.62}	3.88 _{0.10}	1.056 _{0.067}	33.64 _{0.28}	0.959 _{0.066}
380	636.43 _{0.54}	2.959 _{0.070}	0.792 _{0.071}	34.36 _{0.35}	0.967 _{0.090}
370	646.47 _{0.59}	2.219 _{0.049}	0.583 _{0.072}	35.10 _{0.46}	0.98 _{0.12}

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

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
540	406.0 _{3.8}	97.8 _{2.1}	20.90 _{0.36}	14.21 _{0.22}	0.543 _{0.015}
530	430.3 _{3.2}	78.1 _{2.3}	18.10 _{0.28}	16.71 _{0.16}	0.601 _{0.020}
520	452.1 _{1.9}	63.1 _{2.2}	15.62 _{0.19}	18.90 _{0.15}	0.654 _{0.024}
510	470.9 _{1.1}	51.8 _{1.9}	13.42 _{0.13}	20.72 _{0.19}	0.698 _{0.026}
500	487.5 _{1.1}	42.9 _{1.4}	11.472 _{0.080}	22.26 _{0.19}	0.734 _{0.024}
490	502.5 _{1.2}	35.72 _{0.85}	9.745 _{0.054}	23.60 _{0.16}	0.765 _{0.019}
480	516.3 _{1.4}	29.69 _{0.47}	8.222 _{0.043}	24.83 _{0.13}	0.793 _{0.013}
470	529.5 _{1.6}	24.62 _{0.27}	6.886 _{0.037}	25.96 _{0.11}	0.8174 _{9.9e-3}
460	542.1 _{1.7}	20.34 _{0.18}	5.720 _{0.031}	27.026 _{0.098}	0.8399 _{8.6e-3}
450	554.3 _{1.8}	16.71 _{0.13}	4.708 _{0.026}	28.031 _{0.098}	0.8603 _{8.3e-3}
440	566.1 _{1.8}	13.63 _{0.10}	3.836 _{0.024}	28.98 _{0.10}	0.8786 _{8.6e-3}
430	577.4 _{1.6}	11.03 _{0.11}	3.092 _{0.023}	29.89 _{0.11}	0.895 _{0.011}
420	588.1 _{1.4}	8.85 _{0.15}	2.463 _{0.022}	30.73 _{0.13}	0.910 _{0.018}
410	598.1 _{1.1}	7.02 _{0.19}	1.937 _{0.024}	31.51 _{0.17}	0.924 _{0.028}
400	607.97 _{0.72}	5.51 _{0.22}	1.503 _{0.031}	32.27 _{0.22}	0.937 _{0.042}
390	617.69 _{0.31}	4.27 _{0.23}	1.148 _{0.042}	33.01 _{0.29}	0.947 _{0.062}
380	627.04 _{0.22}	3.26 _{0.22}	0.862 _{0.055}	33.71 _{0.42}	0.957 _{0.090}
370	635.81 _{0.19}	2.45 _{0.20}	0.636 _{0.068}	34.36 _{0.62}	0.97 _{0.13}
360	644.04 _{0.32}	1.80 _{0.18}	0.460 _{0.080}	34.97 _{0.91}	0.97 _{0.19}

Table SI.XXVII: GCMC-MBAR results for 3,4-dimethylhexane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
550	416.97 _{0.84}	91.7 _{2.1}	21.00 _{0.24}	15.29 _{0.11}	0.572 _{0.015}
540	441.75 _{0.84}	75.2 _{2.0}	18.28 _{0.18}	17.53 _{0.13}	0.619 _{0.017}
530	462.97 _{0.65}	61.9 _{1.6}	15.84 _{0.12}	19.50 _{0.14}	0.664 _{0.018}
520	481.27 _{0.52}	51.4 _{1.2}	13.67 _{0.076}	21.20 _{0.13}	0.703 _{0.017}
510	497.59 _{0.51}	42.88 _{0.80}	11.73 _{0.044}	22.68 _{0.12}	0.737 _{0.014}
500	512.45 _{0.50}	35.87 _{0.49}	10.01 _{0.025}	23.99 _{0.090}	0.767 _{0.011}
490	526.21 _{0.55}	30.00 _{0.31}	8.48 _{0.015}	25.19 _{0.073}	0.793 _{1.8e-3}
480	539.20 _{0.79}	25.02 _{0.22}	7.14 _{0.014}	26.30 _{0.072}	0.816 _{7.4e-3}
470	551.6 _{1.1}	20.79 _{0.18}	5.96 _{0.017}	27.34 _{0.083}	0.838 _{7.6e-3}
460	563.5 _{1.3}	17.18 _{0.15}	4.93 _{0.023}	28.31 _{0.097}	0.858 _{8.7e-3}
450	574.7 _{1.3}	14.10 _{0.14}	4.05 _{0.028}	29.24 _{0.11}	0.877 _{0.011}
440	585.4 _{1.2}	11.49 _{0.12}	3.28 _{0.033}	30.09 _{0.11}	0.893 _{0.013}
430	595.6 _{1.1}	9.29 _{0.11}	2.64 _{0.037}	30.90 _{0.11}	0.909 _{0.017}
420	605.36 _{0.91}	7.43 _{0.097}	2.09 _{0.040}	31.66 _{0.11}	0.922 _{0.021}
410	614.74 _{0.65}	5.89 _{0.085}	1.64 _{0.042}	32.38 _{0.12}	0.935 _{0.027}
400	624.02 _{0.41}	4.61 _{0.075}	1.27 _{0.044}	33.08 _{0.14}	0.946 _{0.036}
390	633.41 _{0.31}	3.56 _{0.067}	0.96 _{0.045}	33.78 _{0.17}	0.955 _{0.048}
380	642.95 _{0.22}	2.71 _{0.059}	0.72 _{0.045}	34.48 _{0.22}	0.964 _{0.064}
370	652.67 _{0.19}	2.03 _{0.051}	0.53 _{0.046}	35.18 _{0.29}	0.970 _{0.087}

Table SI.XXVIII: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXIX: GCMC-MBAR results for 2,2,3-trimethylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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}	21.84 _{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.XXX: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXI: GCMC-MBAR results for 2,3,3-trimethylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

T^{sat} (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
560	426.5 _{9.5}	98.7 _{1.6}	23.04 _{0.24}	14.76 _{0.51}	0.573 _{0.011}
550	452.4 _{5.9}	80.7 _{1.4}	20.23 _{0.20}	17.10 _{0.29}	0.626 _{0.013}
540	473.3 _{2.0}	67.2 _{1.1}	17.69 _{0.18}	18.98 _{0.12}	0.670 _{0.013}
530	490.60 _{0.59}	56.53 _{0.74}	15.40 _{0.16}	20.523 _{0.065}	0.706 _{0.012}
520	505.89 _{0.92}	47.80 _{0.63}	13.35 _{0.14}	21.863 _{0.043}	0.738 _{0.012}
510	520.2 _{1.1}	40.46 _{0.65}	11.51 _{0.12}	23.086 _{0.038}	0.766 _{0.014}
500	534.1 _{1.0}	34.21 _{0.66}	9.866 _{0.088}	24.232 _{0.057}	0.792 _{0.017}
490	546.97 _{0.93}	28.87 _{0.60}	8.402 _{0.063}	25.283 _{0.071}	0.816 _{0.018}
480	558.82 _{0.80}	24.29 _{0.47}	7.108 _{0.044}	26.241 _{0.071}	0.837 _{0.017}
470	570.25 _{0.87}	20.36 _{0.30}	5.967 _{0.036}	27.143 _{0.070}	0.857 _{0.014}
460	581.5 _{1.1}	16.96 _{0.17}	4.969 _{0.037}	28.007 _{0.066}	0.875 _{0.011}
450	592.0 _{1.0}	14.04 _{0.13}	4.101 _{0.041}	28.816 _{0.071}	0.892 _{0.012}
440	602.0 _{1.1}	11.53 _{0.15}	3.353 _{0.046}	29.578 _{0.085}	0.908 _{0.017}
430	612.3 _{1.6}	9.39 _{0.16}	2.714 _{0.052}	30.34 _{0.10}	0.924 _{0.024}
420	622.8 _{1.6}	7.58 _{0.16}	2.171 _{0.058}	31.10 _{0.13}	0.937 _{0.032}
410	632.87 _{0.75}	6.05 _{0.16}	1.716 _{0.064}	31.82 _{0.20}	0.950 _{0.044}
400	642.39 _{0.29}	4.78 _{0.17}	1.338 _{0.070}	32.50 _{0.28}	0.961 _{0.061}
390	651.59 _{0.31}	3.73 _{0.18}	1.028 _{0.075}	33.14 _{0.37}	0.971 _{0.085}

Table SI.XXXII: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXIII: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXIV: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXV: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXVI: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXVII: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXVIII: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XXXIX: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XL: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XLI: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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.XLII: 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)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m ³)	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m ³)	$P_{\text{vap}}^{\text{sat}}$ (MPa)	ΔH_v (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
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}

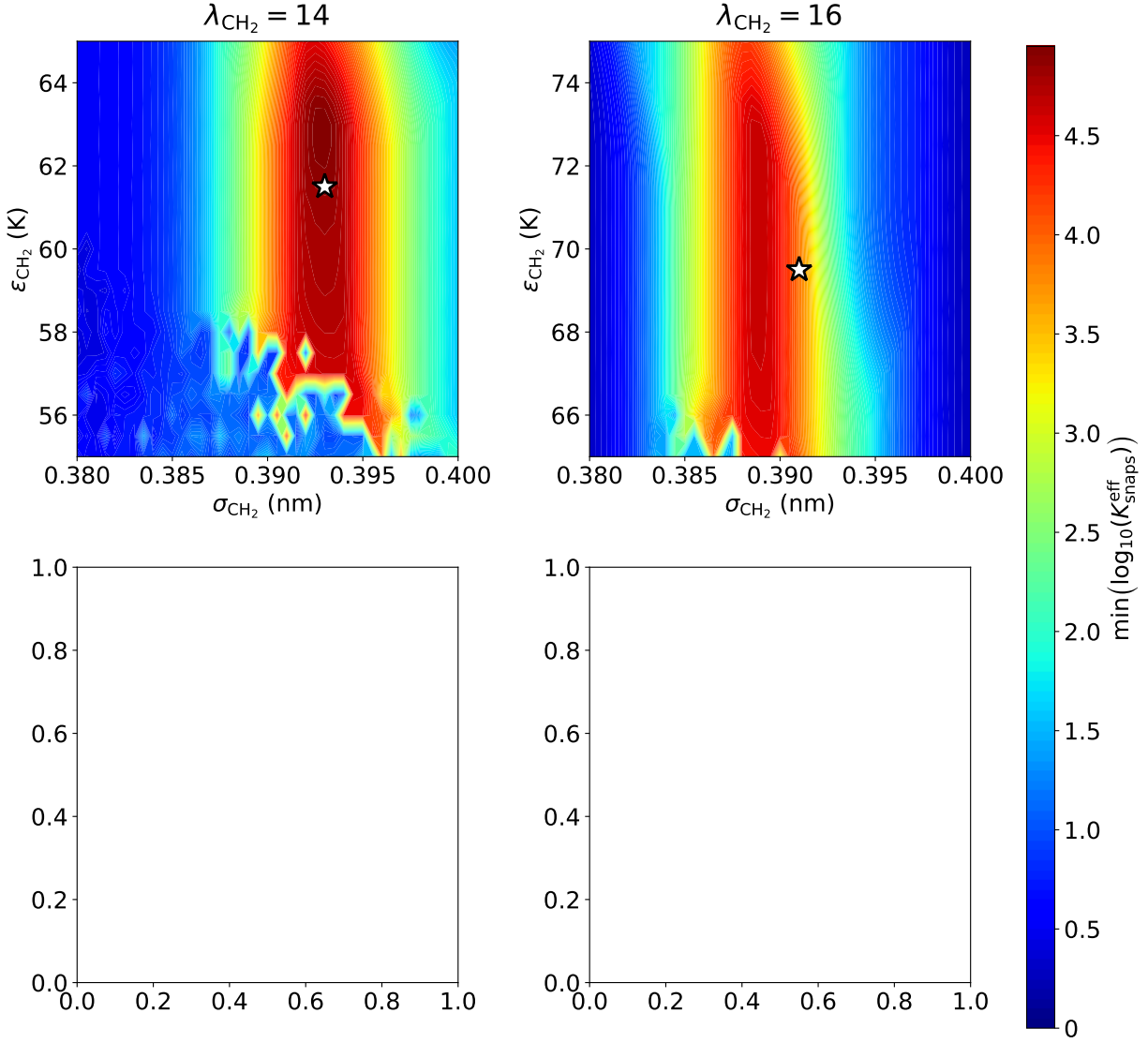


Figure SI.1: Minimum number of effective snapshots ($\min(K_{\text{snaps}}^{\text{eff}})$) with respect to ϵ_{CH_2} and σ_{CH_2} for cyclohexane. Optimization has converged as $\min(K_{\text{snaps}}^{\text{eff}}) \gg 50$ for the optimal ϵ_{CH_2} , σ_{CH_2} , λ_{CH_2} parameter set. Top-left, top-right, bottom-left, and bottom-right panels correspond $\lambda_{\text{CH}_2} = 14$, $\lambda_{\text{CH}_2} = 16$, $\lambda_{\text{CH}_2} = 18$, and $\lambda_{\text{CH}_2} = 12$, respectively. White star represents the optimal parameter set, i.e., the lowest value of S , for a given λ_{CH_2}