

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

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Table SI.I: Equilibrium (fixed) bond lengths ( $r_{\text{eq}}$ ).  $\text{CH}_x$  and  $\text{CH}_y$  represent  $\text{CH}_3$ ,  $\text{CH}_2(\text{sp}^3)$ ,  $\text{CH}(\text{sp}^3)$ , or  $\text{C}(\text{sp}^3)$  sites.

Bending sites	$r_{\text{eq}}$ (nm)		
	TraPPE	MiPPE	NERD
$\text{CH}_x\text{-CH}_y$	0.154	0.154	0.154
$\text{C}(\text{sp})\text{-CH}_x$	–	0.146	–
$\text{CH}\equiv\text{CH}$	–	0.121	–
$\text{C}\equiv\text{CH}$	–	0.121	–

Table SI.II: Equilibrium bond angles ( $\theta_{\text{eq}}$ ) and force constants ( $k_\theta/k_B$ ), where  $k_B$  is the Boltzmann constant.  $\text{CH}_x$  and  $\text{CH}_y$  represent  $\text{CH}_3$ ,  $\text{CH}_2(\text{sp}^3)$ ,  $\text{CH}(\text{sp}^3)$ , or  $\text{C}(\text{sp}^3)$  sites.

Bending sites	$\theta_{\text{eq}}$ (degrees)			$k_\theta/k_B$ (K/rad <sup>2</sup> )
	TraPPE	MiPPE	NERD	
$\text{CH}_x\text{-CH}_2\text{-CH}_y$	114.0	114.0	114.0	62500
$\text{CH}_x\text{-CH-CH}_y$	112.0	112.0	109.5	62500
$\text{CH}_x\text{-C-CH}_y$	109.5	109.5	109.5	62500
$\text{CH}_x\text{-CH}_2\text{-C}(\text{sp})$	–	112	–	62500
$\text{CH}_x\text{-C}(\text{sp})\equiv\text{CH}$	–	180	–	30800
$\text{CH}_x\text{-C}(\text{sp})\equiv\text{C}$	–	180	–	30800

Table SI.III: Fourier constants ( $c_n/k_B$ ) in units of K.  $\text{CH}_x$  and  $\text{CH}_y$  represent  $\text{CH}_3$ ,  $\text{CH}_2(\text{sp}^3)$ ,  $\text{CH}(\text{sp}^3)$ , or  $\text{C}(\text{sp}^3)$  sites.

Torsion sites	$c_0/k_B$	$c_1/k_B$	$c_2/k_B$	$c_3/k_B$
$\text{CH}_x\text{-CH}_2\text{-CH}_2\text{-CH}_y$	0.0	355.03	-68.19	791.32
$\text{CH}_x\text{-CH}_2\text{-CH-CH}_y$	-251.06	428.73	-111.85	441.27
$\text{CH}_x\text{-CH}_2\text{-C-CH}_y$	0.0	0.0	0.0	461.29
$\text{CH}_x\text{-CH-CH-CH}_y$	-251.06	428.73	-111.85	441.27
$\text{CH}_x\text{-CH}_2\text{-CH}_2\text{-C}(\text{sp})$	94.88	162.00	-205.40	980.40
$\text{CH}_x\text{-CH}_2\text{-C}(\text{sp})\equiv\text{C}(\text{sp})$	0	0	0	0
$\text{CH}_x\text{-CH}_2\text{-C}(\text{sp})\equiv\text{CH}(\text{sp})$	0	0	0	0
$\text{CH}_x\text{-C}(\text{sp})\equiv\text{C}(\text{sp})\text{-CH}_y$	0	0	0	0

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

$T$ (K)	$\mu$ (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.V: State points simulated for 2,2-dimethylpropane with the TraPPE force field.

$T$ (K)	$\mu$ (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 Bonded parameters

## SI.II State Points

## SI.III Tabulated GCMC-MBAR results

### SI.III.1 Cyclohexane

### SI.III.2 Branched alkanes

### SI.III.3 Alkynes

SI.3

## SI.IV Optimal $\psi$ values

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

$T$ (K)	$\mu$ (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.VII: State points simulated for 2,3-dimethylbutane with the TraPPE force field.

$T$ (K)	$\mu$ (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.VIII: State points simulated for 3,3-dimethylhexane with the TraPPE force field.

$T$ (K)	$\mu$ (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.IX: State points simulated for 3-methyl-3-ethylpentane with the TraPPE force field.

$T$ (K)	$\mu$ (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.X: State points simulated for 2,3,4-trimethylpentane with the TraPPE force field.

$T$ (K)	$\mu$ (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.XI: State points simulated for 2,2,4-trimethylpentane with the TraPPE force field.

$T$ (K)	$\mu$ (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.XII: State points simulated for cyclohexane with the TraPPE force field.

$T$ (K)	$\mu$ (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.XIII: State points simulated for cyclohexane with the  $\lambda_{\text{CH}_2}^{(1)} = 14$  force field.

$T$ (K)	$\mu$ (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.XIV: State points simulated for cyclohexane with the  $\lambda_{\text{CH}_2}^{(1)} = 16$  force field.

$T$ (K)	$\mu$ (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.XV: State points simulated for cyclohexane with the  $\lambda_{\text{CH}_2}^{(1)} = 18$  force field.

$T$ (K)	$\mu$ (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.XVI: State points simulated for cyclohexane with the  $\lambda_{\text{CH}_2}^{(1)} = 20$  force field.

$T$ (K)	$\mu$ (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.XVII: State points simulated for 2-methylpropane with the MiPPE-gen force field.

$T$ (K)	$\mu$ (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.XVIII: State points simulated for 2,2-dimethylpropane with the MiPPE-gen force field.

$T$ (K)	$\mu$ (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.XIX: State points simulated for 2,2-dimethylbutane with the MiPPE-gen force field.

$T$ (K)	$\mu$ (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.XX: State points simulated for 2,3-dimethylbutane with the MiPPE-gen force field.

$T$ (K)	$\mu$ (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.XXI: State points simulated for 2,3,4-trimethylpentane with the MiPPE-gen force field.

$T$ (K)	$\mu$ (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.XXII: State points simulated for 2,2,4-trimethylpentane with the MiPPE-gen force field.

$T$ (K)	$\mu$ (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.XXIII: GCMC-MBAR results for 2-methylpentane with the MiPPE-SL force field. Subscripts correspond to the 95% confidence interval computed with bootstrap re-sampling.

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

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

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

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

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

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

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

Table SI.XXVII: 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.

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

Table SI.XXVIII: 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.

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



Table SI.XXIX: 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.

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

Table SI.XXX: 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.

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

Table SI.XXXI: 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.

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

Table SI.XXXII: 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.

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
550	424.5 <sub>1.7</sub>	94.6 <sub>5.8</sub>	22.04 <sub>0.85</sub>	14.90 <sub>0.26</sub>	0.582 <sub>0.042</sub>
540	446.63 <sub>0.90</sub>	77.5 <sub>4.4</sub>	19.31 <sub>0.70</sub>	17.04 <sub>0.27</sub>	0.634 <sub>0.043</sub>
530	466.95 <sub>0.61</sub>	64.6 <sub>2.9</sub>	16.85 <sub>0.58</sub>	18.86 <sub>0.22</sub>	0.676 <sub>0.039</sub>
520	485.81 <sub>0.76</sub>	54.4 <sub>1.9</sub>	14.63 <sub>0.50</sub>	20.45 <sub>0.13</sub>	0.711 <sub>0.035</sub>
510	502.62 <sub>0.63</sub>	45.9 <sub>1.6</sub>	12.63 <sub>0.44</sub>	21.84 <sub>0.082</sub>	0.742 <sub>0.037</sub>
500	517.03 <sub>0.59</sub>	38.7 <sub>1.7</sub>	10.84 <sub>0.37</sub>	23.05 <sub>0.11</sub>	0.770 <sub>0.043</sub>
490	529.98 <sub>0.76</sub>	32.6 <sub>1.9</sub>	9.25 <sub>0.29</sub>	24.14 <sub>0.18</sub>	0.795 <sub>0.053</sub>
480	542.7 <sub>1.0</sub>	27.4 <sub>1.8</sub>	7.84 <sub>0.21</sub>	25.18 <sub>0.25</sub>	0.818 <sub>0.059</sub>
470	555.2 <sub>1.2</sub>	23.0 <sub>1.6</sub>	6.59 <sub>0.13</sub>	26.17 <sub>0.29</sub>	0.840 <sub>0.059</sub>
460	566.7 <sub>1.3</sub>	19.1 <sub>1.2</sub>	5.500 <sub>0.068</sub>	27.09 <sub>0.30</sub>	0.860 <sub>0.054</sub>
450	577.6 <sub>1.2</sub>	15.82 <sub>0.81</sub>	4.550 <sub>0.027</sub>	27.94 <sub>0.29</sub>	0.878 <sub>0.045</sub>
440	588.5 <sub>3.8</sub>	13.0 <sub>1.5</sub>	4 <sub>13</sub>	28.8 <sub>7.3</sub>	0.9 <sub>3.1</sub>
430	599.6 <sub>2.4</sub>	10.61 <sub>0.31</sub>	3.023 <sub>0.035</sub>	29.58 <sub>0.30</sub>	0.910 <sub>0.029</sub>
420	610.1 <sub>2.1</sub>	8.58 <sub>0.19</sub>	2.423 <sub>0.044</sub>	30.34 <sub>0.26</sub>	0.923 <sub>0.026</sub>
410	619.5 <sub>1.4</sub>	6.88 <sub>0.12</sub>	1.918 <sub>0.049</sub>	31.02 <sub>0.22</sub>	0.935 <sub>0.029</sub>
400	628.4 <sub>1.5</sub>	5.447 <sub>0.098</sub>	1.498 <sub>0.051</sub>	31.66 <sub>0.24</sub>	0.945 <sub>0.036</sub>
380	645.33 <sub>0.68</sub>	3.285 <sub>0.097</sub>	0.874 <sub>0.051</sub>	32.86 <sub>0.25</sub>	0.961 <sub>0.062</sub>

Table SI.XXXIII: 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.

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
530	400.9 <sub>2.2</sub>	97.9 <sub>4.8</sub>	21.20 <sub>0.38</sub>	13.58 <sub>0.32</sub>	0.561 <sub>0.029</sub>
520	427.5 <sub>1.3</sub>	79.4 <sub>3.2</sub>	18.44 <sub>0.28</sub>	15.89 <sub>0.27</sub>	0.614 <sub>0.027</sub>
510	448.78 <sub>0.77</sub>	65.1 <sub>1.8</sub>	15.97 <sub>0.21</sub>	17.79 <sub>0.18</sub>	0.661 <sub>0.020</sub>
500	466.83 <sub>0.75</sub>	53.9 <sub>1.1</sub>	13.78 <sub>0.18</sub>	19.40 <sub>0.13</sub>	0.702 <sub>0.017</sub>
490	483.78 <sub>0.81</sub>	44.87 <sub>0.89</sub>	11.82 <sub>0.15</sub>	20.85 <sub>0.12</sub>	0.739 <sub>0.017</sub>
480	499.84 <sub>0.70</sub>	37.41 <sub>0.89</sub>	10.09 <sub>0.12</sub>	22.18 <sub>0.12</sub>	0.772 <sub>0.020</sub>
470	514.41 <sub>0.57</sub>	31.21 <sub>0.86</sub>	8.545 <sub>0.083</sub>	23.38 <sub>0.13</sub>	0.800 <sub>0.023</sub>
460	527.62 <sub>0.53</sub>	26.00 <sub>0.75</sub>	7.187 <sub>0.053</sub>	24.45 <sub>0.13</sub>	0.826 <sub>0.025</sub>
450	539.75 <sub>0.68</sub>	21.58 <sub>0.59</sub>	5.995 <sub>0.030</sub>	25.42 <sub>0.12</sub>	0.848 <sub>0.024</sub>
440	551.12 <sub>0.66</sub>	17.82 <sub>0.43</sub>	4.958 <sub>0.022</sub>	26.32 <sub>0.12</sub>	0.869 <sub>0.021</sub>
430	562.67 <sub>0.50</sub>	14.62 <sub>0.31</sub>	4.062 <sub>0.027</sub>	27.21 <sub>0.13</sub>	0.888 <sub>0.020</sub>
420	574.59 <sub>0.49</sub>	11.89 <sub>0.25</sub>	3.292 <sub>0.035</sub>	28.09 <sub>0.13</sub>	0.906 <sub>0.021</sub>
410	585.04 <sub>0.41</sub>	9.58 <sub>0.25</sub>	2.637 <sub>0.042</sub>	28.86 <sub>0.15</sub>	0.922 <sub>0.028</sub>
400	594.23 <sub>0.30</sub>	7.66 <sub>0.27</sub>	2.087 <sub>0.051</sub>	29.54 <sub>0.20</sub>	0.936 <sub>0.040</sub>
390	604.33 <sub>0.26</sub>	6.05 <sub>0.29</sub>	1.630 <sub>0.063</sub>	30.26 <sub>0.28</sub>	0.949 <sub>0.058</sub>
380	615.43 <sub>0.23</sub>	4.72 <sub>0.30</sub>	1.252 <sub>0.077</sub>	31.01 <sub>0.41</sub>	0.958 <sub>0.084</sub>
370	625.27 <sub>0.23</sub>	3.63 <sub>0.29</sub>	0.946 <sub>0.092</sub>	31.68 <sub>0.58</sub>	0.97 <sub>0.12</sub>

Table SI.XXXIV: 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.

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

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

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
290	421.3 <sub>3.5</sub>	69.7 <sub>3.3</sub>	40.83 <sub>0.20</sub>	8.80 <sub>0.21</sub>	0.632 <sub>0.030</sub>
280	450.7 <sub>1.9</sub>	50.69 <sub>0.91</sub>	31.96 <sub>0.26</sub>	10.27 <sub>0.12</sub>	0.705 <sub>0.014</sub>
270	474.9 <sub>3.0</sub>	37.66 <sub>0.39</sub>	24.65 <sub>0.24</sub>	11.390 <sub>0.086</sub>	0.759 <sub>0.011</sub>
260	497.3 <sub>1.1</sub>	27.95 <sub>0.53</sub>	18.65 <sub>0.17</sub>	12.361 <sub>0.034</sub>	0.804 <sub>0.017</sub>
250	517.91 <sub>0.59</sub>	20.53 <sub>0.34</sub>	13.78 <sub>0.12</sub>	13.214 <sub>0.042</sub>	0.841 <sub>0.016</sub>
240	536.87 <sub>0.67</sub>	14.82 <sub>0.12</sub>	9.92 <sub>0.10</sub>	13.975 <sub>0.028</sub>	0.874 <sub>0.011</sub>
230	554.12 <sub>0.54</sub>	10.447 <sub>0.095</sub>	6.925 <sub>0.089</sub>	14.649 <sub>0.037</sub>	0.903 <sub>0.014</sub>
220	570.90 <sub>0.53</sub>	7.155 <sub>0.097</sub>	4.667 <sub>0.082</sub>	15.283 <sub>0.049</sub>	0.929 <sub>0.021</sub>

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

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
380	441.0 <sub>7.9</sub>	82.2 <sub>3.1</sub>	38.39 <sub>0.90</sub>	10.96 <sub>0.34</sub>	0.592 <sub>0.026</sub>
370	472.7 <sub>5.0</sub>	62.7 <sub>2.7</sub>	31.64 <sub>0.73</sub>	12.83 <sub>0.31</sub>	0.657 <sub>0.033</sub>
360	498.3 <sub>2.8</sub>	48.6 <sub>1.9</sub>	25.84 <sub>0.57</sub>	14.34 <sub>0.24</sub>	0.711 <sub>0.032</sub>
350	520.1 <sub>2.4</sub>	38.1 <sub>1.3</sub>	20.88 <sub>0.45</sub>	15.58 <sub>0.19</sub>	0.754 <sub>0.030</sub>
340	539.4 <sub>2.1</sub>	29.88 <sub>0.90</sub>	16.67 <sub>0.35</sub>	16.65 <sub>0.15</sub>	0.791 <sub>0.029</sub>
330	556.6 <sub>1.4</sub>	23.31 <sub>0.72</sub>	13.13 <sub>0.27</sub>	17.58 <sub>0.11</sub>	0.822 <sub>0.031</sub>
320	572.1 <sub>1.3</sub>	18.02 <sub>0.60</sub>	10.18 <sub>0.19</sub>	18.41 <sub>0.11</sub>	0.850 <sub>0.032</sub>
310	587.6 <sub>1.3</sub>	13.76 <sub>0.47</sub>	7.76 <sub>0.12</sub>	19.20 <sub>0.12</sub>	0.876 <sub>0.033</sub>
300	603.3 <sub>1.5</sub>	10.35 <sub>0.32</sub>	5.799 <sub>0.068</sub>	19.97 <sub>0.13</sub>	0.900 <sub>0.030</sub>
290	617.9 <sub>2.2</sub>	7.65 <sub>0.20</sub>	4.240 <sub>0.040</sub>	20.67 <sub>0.15</sub>	0.921 <sub>0.025</sub>

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

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
410	445.1 <sub>5.3</sub>	76 <sub>12</sub>	29.5 <sub>1.0</sub>	12.82 <sub>0.72</sub>	0.620 <sub>0.097</sub>
400	472.3 <sub>3.4</sub>	59.2 <sub>6.8</sub>	24.64 <sub>0.50</sub>	14.61 <sub>0.60</sub>	0.677 <sub>0.079</sub>
390	495.0 <sub>2.6</sub>	47.1 <sub>2.3</sub>	20.38 <sub>0.30</sub>	16.08 <sub>0.32</sub>	0.722 <sub>0.037</sub>
380	515.5 <sub>2.0</sub>	37.54 <sub>0.86</sub>	16.69 <sub>0.23</sub>	17.37 <sub>0.16</sub>	0.761 <sub>0.020</sub>
370	534.5 <sub>1.3</sub>	29.90 <sub>0.70</sub>	13.51 <sub>0.18</sub>	18.53 <sub>0.13</sub>	0.795 <sub>0.021</sub>
360	552.0 <sub>1.6</sub>	23.69 <sub>0.62</sub>	10.81 <sub>0.13</sub>	19.57 <sub>0.16</sub>	0.824 <sub>0.024</sub>
350	567.8 <sub>1.9</sub>	18.62 <sub>0.51</sub>	8.524 <sub>0.086</sub>	20.50 <sub>0.18</sub>	0.851 <sub>0.025</sub>
340	582.2 <sub>1.1</sub>	14.49 <sub>0.38</sub>	6.623 <sub>0.060</sub>	21.34 <sub>0.13</sub>	0.874 <sub>0.024</sub>
330	595.8 <sub>1.1</sub>	11.15 <sub>0.24</sub>	5.061 <sub>0.049</sub>	22.112 <sub>0.082</sub>	0.895 <sub>0.021</sub>
320	610.6 <sub>2.8</sub>	8.45 <sub>0.14</sub>	3.795 <sub>0.049</sub>	22.905 <sub>0.095</sub>	0.913 <sub>0.019</sub>
310	624.6 <sub>1.8</sub>	6.284 <sub>0.087</sub>	2.782 <sub>0.051</sub>	23.650 <sub>0.059</sub>	0.929 <sub>0.021</sub>

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

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

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

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



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

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
470	445.8 <sub>3.1</sub>	83.4 <sub>6.2</sub>	27.7 <sub>1.2</sub>	14.09 <sub>0.22</sub>	0.578 <sub>0.049</sub>
460	473.8 <sub>1.9</sub>	65.6 <sub>5.4</sub>	23.43 <sub>0.88</sub>	16.27 <sub>0.30</sub>	0.636 <sub>0.057</sub>
450	496.8 <sub>1.0</sub>	52.5 <sub>3.7</sub>	19.73 <sub>0.64</sub>	18.06 <sub>0.28</sub>	0.685 <sub>0.053</sub>
440	516.64 <sub>0.73</sub>	42.4 <sub>2.3</sub>	16.50 <sub>0.48</sub>	19.56 <sub>0.22</sub>	0.725 <sub>0.045</sub>
430	534.83 <sub>0.74</sub>	34.3 <sub>1.7</sub>	13.69 <sub>0.36</sub>	20.89 <sub>0.19</sub>	0.761 <sub>0.042</sub>
420	551.57 <sub>0.81</sub>	27.7 <sub>1.4</sub>	11.26 <sub>0.25</sub>	22.08 <sub>0.19</sub>	0.792 <sub>0.044</sub>
410	566.89 <sub>0.86</sub>	22.3 <sub>1.2</sub>	9.17 <sub>0.16</sub>	23.16 <sub>0.22</sub>	0.821 <sub>0.048</sub>
400	581.3 <sub>1.1</sub>	17.9 <sub>1.0</sub>	7.394 <sub>0.080</sub>	24.15 <sub>0.26</sub>	0.847 <sub>0.049</sub>
390	595.3 <sub>1.6</sub>	14.24 <sub>0.71</sub>	5.890 <sub>0.039</sub>	25.09 <sub>0.28</sub>	0.869 <sub>0.043</sub>
380	608.6 <sub>1.7</sub>	11.23 <sub>0.40</sub>	4.631 <sub>0.052</sub>	25.95 <sub>0.25</sub>	0.889 <sub>0.034</sub>
370	621.0 <sub>1.3</sub>	8.76 <sub>0.19</sub>	3.587 <sub>0.066</sub>	26.75 <sub>0.19</sub>	0.907 <sub>0.026</sub>
360	632.99 <sub>0.96</sub>	6.75 <sub>0.16</sub>	2.735 <sub>0.069</sub>	27.52 <sub>0.12</sub>	0.922 <sub>0.031</sub>
350	644.7 <sub>1.0</sub>	5.12 <sub>0.20</sub>	2.049 <sub>0.065</sub>	28.249 <sub>0.10</sub>	0.937 <sub>0.047</sub>

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

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
490	423.3 <sub>3.5</sub>	87.3 <sub>2.1</sub>	25.38 <sub>0.68</sub>	14.25 <sub>0.14</sub>	0.586 <sub>0.021</sub>
480	453.3 <sub>2.0</sub>	69.9 <sub>1.5</sub>	21.70 <sub>0.60</sub>	16.54 <sub>0.12</sub>	0.639 <sub>0.022</sub>
470	477.4 <sub>1.3</sub>	56.51 <sub>0.96</sub>	18.44 <sub>0.56</sub>	18.448 <sub>0.089</sub>	0.686 <sub>0.024</sub>
460	497.3 <sub>1.4</sub>	46.06 <sub>0.95</sub>	15.56 <sub>0.51</sub>	20.041 <sub>0.074</sub>	0.726 <sub>0.028</sub>
450	514.8 <sub>1.3</sub>	37.6 <sub>1.3</sub>	13.04 <sub>0.44</sub>	21.428 <sub>0.10</sub>	0.761 <sub>0.037</sub>
440	531.5 <sub>1.2</sub>	30.7 <sub>1.7</sub>	10.84 <sub>0.35</sub>	22.71 <sub>0.16</sub>	0.792 <sub>0.050</sub>
430	547.4 <sub>1.2</sub>	25.0 <sub>1.7</sub>	8.93 <sub>0.24</sub>	23.91 <sub>0.22</sub>	0.820 <sub>0.061</sub>
420	561.77 <sub>0.87</sub>	20.3 <sub>1.5</sub>	7.28 <sub>0.13</sub>	24.98 <sub>0.23</sub>	0.845 <sub>0.063</sub>
410	575.17 <sub>0.62</sub>	16.34 <sub>0.99</sub>	5.875 <sub>0.050</sub>	25.97 <sub>0.20</sub>	0.867 <sub>0.053</sub>
400	588.08 <sub>0.75</sub>	13.04 <sub>0.55</sub>	4.682 <sub>0.027</sub>	26.90 <sub>0.15</sub>	0.887 <sub>0.038</sub>
390	599.80 <sub>0.63</sub>	10.31 <sub>0.28</sub>	3.684 <sub>0.047</sub>	27.75 <sub>0.11</sub>	0.905 <sub>0.027</sub>
380	610.32 <sub>0.79</sub>	8.06 <sub>0.17</sub>	2.858 <sub>0.061</sub>	28.507 <sub>0.080</sub>	0.922 <sub>0.027</sub>
370	621.3 <sub>2.9</sub>	6.23 <sub>0.13</sub>	2.185 <sub>0.072</sub>	29.267 <sub>0.086</sub>	0.937 <sub>0.037</sub>
360	634.3 <sub>3.1</sub>	4.74 <sub>0.11</sub>	1.640 <sub>0.083</sub>	30.118 <sub>0.078</sub>	0.950 <sub>0.053</sub>

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

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
500	438.2 <sub>2.9</sub>	85.9 <sub>4.0</sub>	24.95 <sub>0.26</sub>	14.93 <sub>0.36</sub>	0.574 <sub>0.027</sub>
490	464.9 <sub>1.8</sub>	67.7 <sub>2.5</sub>	21.31 <sub>0.16</sub>	17.31 <sub>0.29</sub>	0.635 <sub>0.024</sub>
480	486.7 <sub>1.5</sub>	54.7 <sub>1.3</sub>	18.11 <sub>0.11</sub>	19.18 <sub>0.19</sub>	0.682 <sub>0.017</sub>
470	505.2 <sub>1.7</sub>	44.67 <sub>0.74</sub>	15.302 <sub>0.087</sub>	20.71 <sub>0.14</sub>	0.720 <sub>0.013</sub>
460	522.5 <sub>2.3</sub>	36.61 <sub>0.52</sub>	12.839 <sub>0.074</sub>	22.09 <sub>0.14</sub>	0.753 <sub>0.012</sub>
450	539.3 <sub>2.5</sub>	29.96 <sub>0.40</sub>	10.686 <sub>0.062</sub>	23.39 <sub>0.15</sub>	0.783 <sub>0.011</sub>
440	555.2 <sub>1.8</sub>	24.43 <sub>0.31</sub>	8.815 <sub>0.050</sub>	24.60 <sub>0.11</sub>	0.810 <sub>0.011</sub>
430	569.62 <sub>0.68</sub>	19.82 <sub>0.28</sub>	7.201 <sub>0.040</sub>	25.678 <sub>0.066</sub>	0.835 <sub>0.013</sub>
420	583.3 <sub>1.4</sub>	15.98 <sub>0.26</sub>	5.821 <sub>0.034</sub>	26.69 <sub>0.11</sub>	0.857 <sub>0.015</sub>
410	597.0 <sub>1.4</sub>	12.77 <sub>0.22</sub>	4.651 <sub>0.035</sub>	27.67 <sub>0.12</sub>	0.877 <sub>0.017</sub>
400	609.9 <sub>1.1</sub>	10.11 <sub>0.16</sub>	3.669 <sub>0.039</sub>	28.59 <sub>0.11</sub>	0.896 <sub>0.017</sub>
390	621.7 <sub>1.4</sub>	7.92 <sub>0.14</sub>	2.857 <sub>0.045</sub>	29.42 <sub>0.14</sub>	0.914 <sub>0.021</sub>
380	633.2 <sub>1.2</sub>	6.12 <sub>0.16</sub>	2.190 <sub>0.050</sub>	30.23 <sub>0.16</sub>	0.930 <sub>0.032</sub>
370	644.01 <sub>0.40</sub>	4.67 <sub>0.18</sub>	1.653 <sub>0.059</sub>	30.98 <sub>0.19</sub>	0.944 <sub>0.049</sub>

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

$T^{\text{sat}}$ (K)	$\rho_{\text{liq}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$\rho_{\text{vap}}^{\text{sat}}$ (kg/m <sup>3</sup> )	$P_{\text{vap}}^{\text{sat}}$ (MPa)	$\Delta H_v$ (kJ/mol)	$Z_{\text{vap}}^{\text{sat}}$
520	427.5 <sub>6.0</sub>	82.9 <sub>6.4</sub>	22.18 <sub>0.71</sub>	16.05 <sub>0.64</sub>	0.595 <sub>0.050</sub>
510	454.3 <sub>2.5</sub>	66.9 <sub>4.8</sub>	19.06 <sub>0.55</sub>	18.37 <sub>0.49</sub>	0.646 <sub>0.050</sub>
500	476.5 <sub>1.4</sub>	54.5 <sub>3.3</sub>	16.29 <sub>0.41</sub>	20.34 <sub>0.35</sub>	0.691 <sub>0.045</sub>
490	495.7 <sub>1.4</sub>	44.8 <sub>2.4</sub>	13.84 <sub>0.30</sub>	22.02 <sub>0.25</sub>	0.730 <sub>0.042</sub>
480	512.9 <sub>1.6</sub>	36.9 <sub>1.8</sub>	11.68 <sub>0.20</sub>	23.51 <sub>0.18</sub>	0.764 <sub>0.040</sub>
470	528.7 <sub>2.0</sub>	30.3 <sub>1.4</sub>	9.79 <sub>0.12</sub>	24.85 <sub>0.13</sub>	0.794 <sub>0.037</sub>
460	543.2 <sub>1.9</sub>	24.91 <sub>0.95</sub>	8.138 <sub>0.072</sub>	26.066 <sub>0.092</sub>	0.821 <sub>0.032</sub>
450	556.9 <sub>1.5</sub>	20.37 <sub>0.57</sub>	6.705 <sub>0.058</sub>	27.199 <sub>0.070</sub>	0.846 <sub>0.025</sub>
440	570.2 <sub>1.0</sub>	16.57 <sub>0.25</sub>	5.472 <sub>0.063</sub>	28.279 <sub>0.062</sub>	0.868 <sub>0.016</sub>
430	583.08 <sub>0.58</sub>	13.38 <sub>0.11</sub>	4.419 <sub>0.062</sub>	29.301 <sub>0.062</sub>	0.888 <sub>0.015</sub>
420	595.19 <sub>0.32</sub>	10.71 <sub>0.23</sub>	3.526 <sub>0.055</sub>	30.253 <sub>0.097</sub>	0.907 <sub>0.024</sub>
410	606.63 <sub>0.36</sub>	8.50 <sub>0.30</sub>	2.779 <sub>0.046</sub>	31.14 <sub>0.16</sub>	0.923 <sub>0.037</sub>
400	617.58 <sub>0.39</sub>	6.66 <sub>0.33</sub>	2.160 <sub>0.048</sub>	31.98 <sub>0.23</sub>	0.938 <sub>0.050</sub>
390	628.63 <sub>0.36</sub>	5.16 <sub>0.31</sub>	1.654 <sub>0.061</sub>	32.81 <sub>0.31</sub>	0.950 <sub>0.067</sub>

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

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

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

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

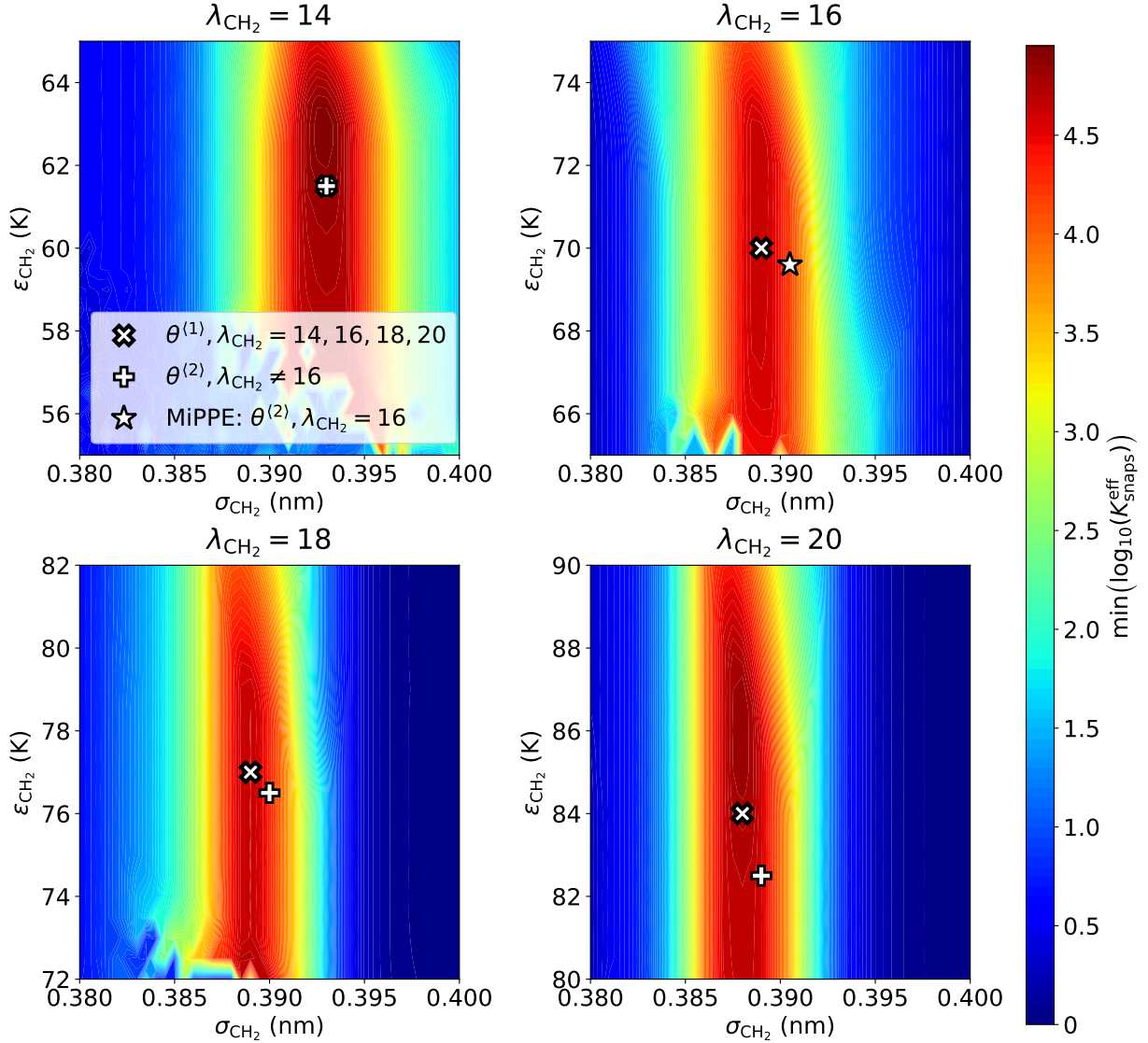


Figure SI.1: Minimum number of effective snapshots ( $\min(K_{\text{snaps}}^{\text{eff}})$ ) with respect to  $\epsilon_{\text{CH}_2}$  and  $\sigma_{\text{CH}_2}$  for cyclohexane. Optimization has converged as  $\min(K_{\text{snaps}}^{\text{eff}}) \gg 50$  for the optimal  $\epsilon_{\text{CH}_2}, \sigma_{\text{CH}_2}, \lambda_{\text{CH}_2}$  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  $\lambda_{\text{CH}_2}$