

Supporting Information

Thermodynamic Behavior of (Methylcyclopentane + Ethyl Acetate) Binary Liquid Mixture: Density at Several Temperatures and Vapor–Liquid Equilibrium at 25, 50 and 101.3 kPa

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Table S1. Coefficients of the polynomial function density (at 298.15 K) – composition ^a

Binary System	A	B	C	D	E	$\sigma_{x1}/\text{g}\cdot\text{cm}^{-3}$ ^b
EA (1) – mC6 (2)	-1049.02735	3612.65989	-4682.32813	2712.81112	-593.18169	0.0007
mC5 (1) – EA (2)	427.27672	-1456.26208	1870.79396	-1079.12505	237.12347	0.0005

^a The polynomial function is $x_1 = A \rho_m^4 + B \rho_m^3 + C \rho_m^2 + D \rho_m + E$ with x_1 the mole fraction of component 1 and ρ_m the density of the mixture at 298.15 K in $\text{g}\cdot\text{cm}^{-3}$

^b Standard deviation between experimental mixture mole fraction and calculated mole fraction

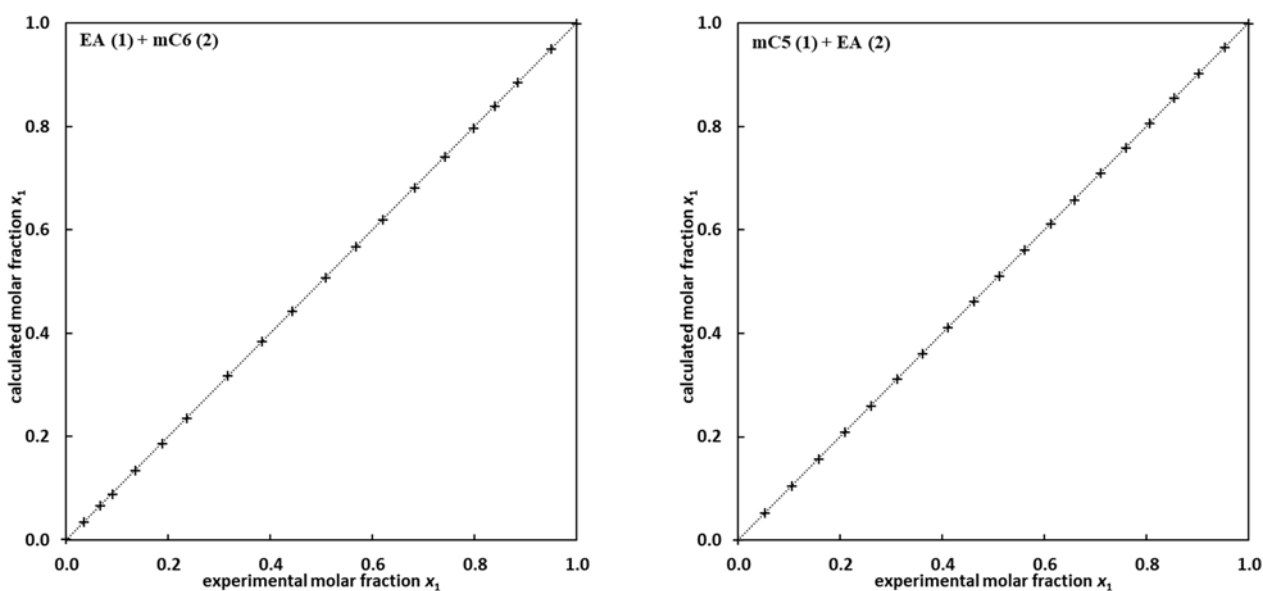


Figure S1. Calibration curve analysis of the binary systems EA + mC6 and mC5 + EA.

Table S2. Redlich-Kister parameters (eq. 7) for the correlation of the excess molar volumes ^a

Binary System	<i>T</i> /K	<i>a</i> ₀	<i>a</i> ₁	<i>a</i> ₂	<i>a</i> ₃	$\sigma_{VE}/\text{cm}^3\cdot\text{mol}^{-1}$ ^b
EA (1) – mC6 (2)	288.15	3.519	-0.093	0.355	-0.163	0.004
EA (1) – mC6 (2)	293.15	3.612	-0.084	0.337	-0.194	0.004
EA (1) – mC6 (2)	298.15	3.709	-0.084	0.341	-0.168	0.004
EA (1) – mC6 (2)	303.15	3.803	-0.067	0.342	-0.196	0.004
EA (1) – mC6 (2)	308.15	3.913	-0.077	0.344	-0.172	0.005
mC5 (1) – EA (2)	288.15	3.932	0.474	0.431	0.261	0.003
mC5 (1) – EA (2)	293.15	4.040	0.497	0.389	0.225	0.002
mC5 (1) – EA (2)	298.15	4.147	0.508	0.404	0.202	0.002
mC5 (1) – EA (2)	303.15	4.252	0.518	0.391	0.215	0.002
mC5 (1) – EA (2)	308.15	4.369	0.546	0.396	0.179	0.002

^a Parameters of eq. 7 with V_m^E in $\text{cm}^3\cdot\text{mol}^{-1}$

^b Standard deviation between experimental and calculated excess molar volumes

Table S3. Experimental Isobaric Vapor-Liquid Equilibrium Data and Densities, ρ , (at 298.15 K and atmospheric pressure) of the Liquid (L) and Condensed Vapor (CV) Phases for the Ethyl Acetate (1) – Methylcyclohexane (2) System at $p = 20$ kPa ^a

T /K	ρ_L /g·cm ⁻³	x_1 /mol·mol ⁻¹	ρ_{CV} /g·cm ⁻³	y_1 /mol·mol ⁻¹
319.11	0.76942	0.057	0.78754	0.259
316.53	0.77278	0.097	0.79827	0.362
314.72	0.77618	0.137	0.80586	0.429
312.95	0.78083	0.188	0.81379	0.494
311.77	0.78541	0.237	0.81918	0.537
310.61	0.79153	0.298	0.82465	0.578
309.83	0.79737	0.354	0.82892	0.609
308.49	0.81256	0.484	0.83701	0.666
308.14	0.81881	0.534	0.84016	0.687
307.78	0.82844	0.606	0.84422	0.714
307.46	0.83902	0.680	0.84939	0.748
307.39	0.84234	0.702	0.85092	0.757
307.30	0.85114	0.759	0.85533	0.785
307.25	0.85688	0.795	0.85864	0.805
307.24	0.86322	0.833	0.86257	0.829
307.30	0.87121	0.879	0.86849	0.863
307.37	0.87565	0.903	0.87245	0.886
307.57	0.88294	0.942	0.87953	0.924
307.73	0.88703	0.963	0.88407	0.948

^a Standard uncertainties u are $u(p) = 0.3$ kPa, $u(T) = 0.07$ K, $u(\rho) = 0.00014$ g·cm⁻³ and $u(x) = u(y) = 0.002$ mol·mol⁻¹. ρ , density of the liquid (L) and condensed vapor (CV) phases at 298.15 K used to determine x_1 and y_1 .

Table S4. Experimental Isobaric Vapor-Liquid Equilibrium Data and Densities, ρ , (at 298.15 K and atmospheric pressure) of the Liquid (L) and Condensed Vapor (CV) Phases for the Methylcyclopentane (1) – Ethyl Acetate (2) System at $p = 25, 50$ and 101.3 kPa ^a

T /K	ρ_L /g·cm ⁻³	x_1 /mol·mol ⁻¹	ρ_{CV} /g·cm ⁻³	y_1 /mol·mol ⁻¹
$p = 25$ kPa				
311.55	0.88919	0.025	0.87664	0.087
309.90	0.88304	0.055	0.86024	0.173
308.53	0.87656	0.088	0.84732	0.245
307.26	0.86903	0.127	0.83555	0.313
306.04	0.85998	0.175	0.82516	0.376
305.33	0.85297	0.213	0.81927	0.412
304.37	0.84203	0.275	0.81123	0.463
303.85	0.83440	0.320	0.80629	0.496
302.74	0.80964	0.474	0.79370	0.582
302.50	0.80093	0.532	0.78985	0.609
302.37	0.79262	0.589	0.78621	0.635
302.28	0.78524	0.642	0.78271	0.661
302.27	0.77822	0.695	0.77928	0.687
302.35	0.77223	0.742	0.77593	0.713
302.49	0.76713	0.783	0.77242	0.741
303.00	0.75817	0.860	0.76504	0.801
303.20	0.75524	0.886	0.76249	0.822
303.81	0.75037	0.930	0.75624	0.877
304.51	0.74698	0.962	0.75077	0.927
$p = 50$ kPa				
326.96	0.88092	0.066	0.86061	0.171
326.70	0.88016	0.070	0.85859	0.182
325.68	0.87466	0.097	0.84931	0.234
324.81	0.86910	0.126	0.84171	0.277
324.00	0.86340	0.156	0.83394	0.323
323.08	0.85560	0.199	0.82613	0.370
322.24	0.84673	0.248	0.81822	0.419
321.53	0.83674	0.306	0.81184	0.459
320.97	0.82745	0.362	0.80624	0.496
320.16	0.80790	0.485	0.79591	0.566
319.94	0.79961	0.541	0.79183	0.595
319.85	0.79360	0.582	0.78890	0.616
319.82	0.78842	0.619	0.78637	0.634
319.81	0.77976	0.683	0.78160	0.670
319.99	0.76957	0.763	0.77546	0.717

320.10	0.76624	0.791	0.77307	0.735
320.33	0.76212	0.825	0.76981	0.762
320.63	0.75847	0.857	0.76607	0.792
320.89	0.75570	0.882	0.76307	0.817
321.66	0.75068	0.927	0.75662	0.873

$p = 101.3 \text{ kPa}$

348.46	0.88767	0.033	0.87699	0.085
346.70	0.87951	0.073	0.86006	0.174
345.72	0.87399	0.101	0.85105	0.224
344.82	0.86714	0.137	0.84272	0.271
343.65	0.85827	0.184	0.83248	0.331
342.76	0.84961	0.232	0.82439	0.380
341.85	0.83795	0.299	0.81590	0.433
341.33	0.82961	0.349	0.81030	0.469
340.63	0.81375	0.447	0.80162	0.527
340.38	0.80652	0.494	0.79774	0.553
340.27	0.80045	0.535	0.79440	0.577
340.22	0.79351	0.583	0.79094	0.601
340.21	0.78485	0.645	0.78642	0.634
340.25	0.77830	0.695	0.78240	0.664
340.32	0.77364	0.731	0.77947	0.686
340.44	0.76940	0.765	0.77626	0.710
340.72	0.76238	0.823	0.77063	0.755
341.66	0.75616	0.878	0.76398	0.810
341.99	0.75365	0.900	0.76090	0.836

^a Standard uncertainties u are $u(p) = 0.3 \text{ kPa}$, $u(T) = 0.07 \text{ K}$, $u(\rho) = 0.00060 \text{ g}\cdot\text{cm}^{-3}$ and $u(x) = u(y) = 0.009 \text{ mol}\cdot\text{mol}^{-1}$. ρ , density of the liquid (L) and condensed vapor (CV) phases at 298.15 K used to determine x_1 and y_1 .

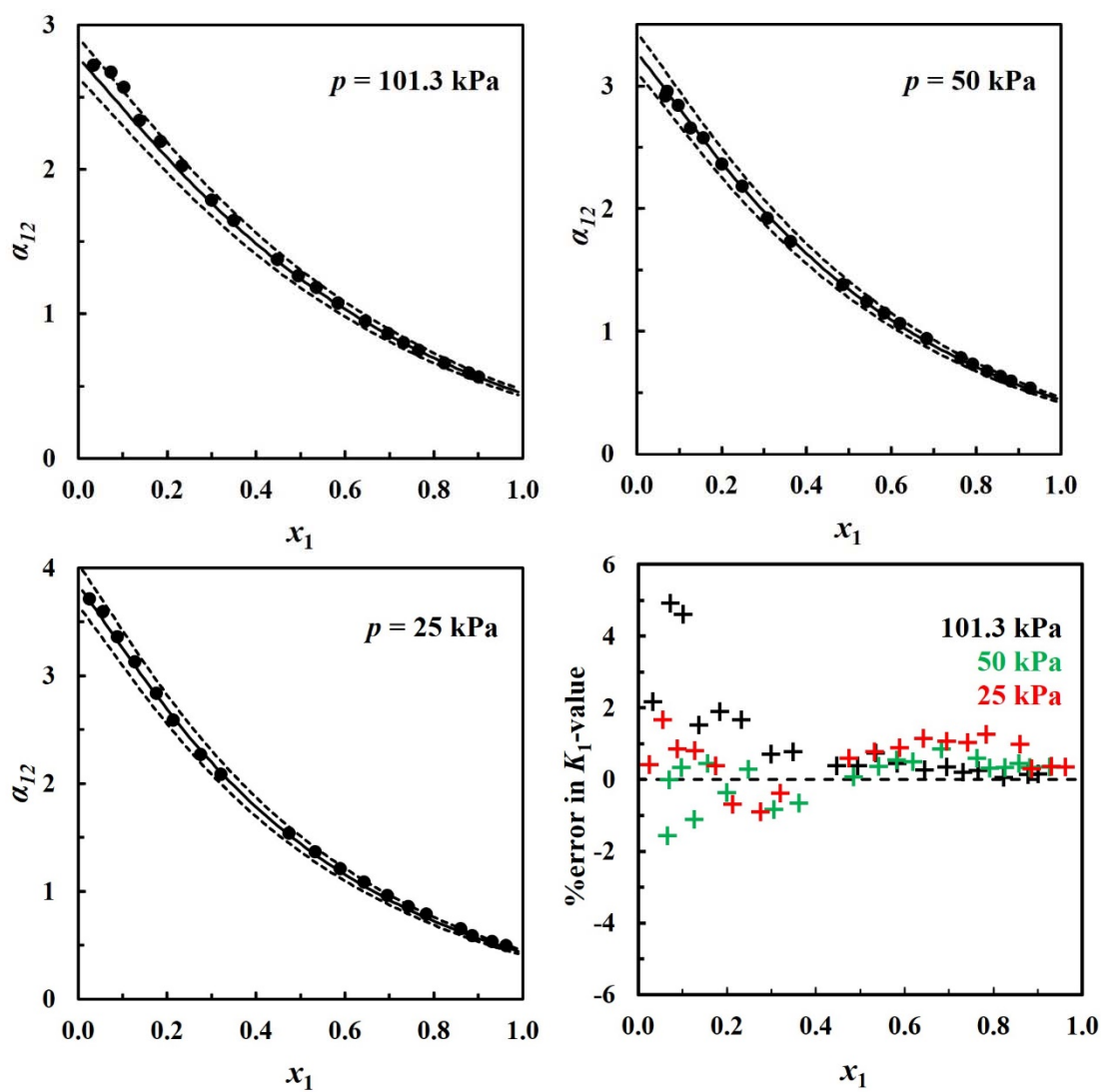


Figure S2. Experimental relative volatilities (α_{12}) of the mC5 (1) + EA (2) binary system compared to NRTL model results at 101.3, 50 and 25 kPa. Dashed lines are $\pm 5\%$ deviations. Bottom right chart: percent errors of NRTL model K_1 -values (mC5 absolute volatilities).

Example of density uncertainty calculations for the binary system EA + mC6 at 288.15 K

Pure substances:

$$x_{\text{purity,EA}} = x_{\text{purity,mC6}} = 0.999$$

$$\rho_{\text{EA}}(288.15 \text{ K}) = 0.90658 \text{ g}\cdot\text{cm}^{-3} \text{ and } \rho_{\text{mC6}}(288.15 \text{ K}) = 0.77364 \text{ g}\cdot\text{cm}^{-3}$$

$\xi = 0.1$ (postulated difference between the pure substances and their impurities)

$$u(\rho_{EA}) = \sqrt{\left(\frac{u(\rho)}{\sqrt{3}}\right)^2 + (\rho_i \xi (1 - x_{\text{purity},i}))^2}$$

$$u(\rho_{EA}) = \sqrt{\left(\frac{0.00005}{\sqrt{3}}\right)^2 + (0.90658 \times 0.1 \times (1 - 0.999))^2} = 0.000095 \approx \mathbf{0.0001 \text{ g}\cdot\text{cm}^{-3}}$$

$$u(\rho_{mC6}) = \sqrt{\left(\frac{0.00005}{\sqrt{3}}\right)^2 + (0.77634 \times 0.1 \times (1 - 0.999))^2} = 0.000083 \approx \mathbf{0.0001 \text{ g}\cdot\text{cm}^{-3}}$$

Binary mixture:

$x_1 = x_{\text{EA}} = 0.0901$; gravimetrically prepared mixture with $m_1 = 0.6710 \text{ g}$ and $m_2 = 7.5514 \text{ g}$.

$$\rho_m(288.15 \text{ K}) = 0.78101 \text{ g}\cdot\text{cm}^{-3}$$

$$u(x_1) = x_1(1 - x_1) \sqrt{\left(\frac{u(m_1)}{m_1}\right)^2 + \left(\frac{u(m_2)}{m_2}\right)^2}$$

$$u(x_1) = 0.0901(1 - 0.0901) \sqrt{\left(\frac{0.0002}{0.6710}\right)^2 + \left(\frac{0.0002}{7.5514}\right)^2} = 0.000025$$

and

$$u(\rho_m) = \sqrt{u(\rho_1)^2 + u(\rho_2)^2 + u(x_1)^2}$$

$$u(\rho_m) = \sqrt{0.0001^2 + 0.0001^2 + 0.000025^2} \approx \mathbf{0.00014 \text{ g}\cdot\text{cm}^{-3}}$$