

Density, Excess Molar Volume and Vapor–Liquid Equilibrium Measurements at 101.3 kPa for Binary Mixtures Containing Ethyl Acetate and a Branched Alkane: Experimental Data and Modeling

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Table S1. Comparison of the density at $T = 293.15$ K and 303.15 K and $P = 101$ kPa, ρ , of the pure components with literature values. ^a

Compound	$\rho^{293.15\text{ K}} / \text{g}\cdot\text{cm}^{-3}$		$\rho^{303.15\text{ K}} / \text{g}\cdot\text{cm}^{-3}$	
	This work	Literature	This work	Literature
ethyl acetate (EA)	0.90049	0.9005 [1]	0.88829	0.8882 [1]
		0.90057 [2]		0.88835 [2]
3-methylpentane	0.66427	0.66428 [3]	0.65511	0.65507 [3]
		0.66443 [4]		0.65555 [4]
2,3-dimethylbutane	0.66209	0.66158 [1]	0.65286	0.65231 [1]
		0.66181 [5]		0.65232 [5]

^a Standard uncertainties u are $u(\rho) = 0.00005$ $\text{g}\cdot\text{cm}^{-3}$, $u(T_{\rho\text{ meas}}) = 0.03$ K, $u(P_{\rho\text{ meas}}) = 3$ kPa

Table S2. Coefficients of the Antoine expression employed in this work. ^a

Component	A	B	C
ethyl acetate	15.0294	3271.98	35.8136
hexane	14.2616	2950.15	35.8736
3-methylpentane	14.2177	2903.16	33.8691
2,3-dimethylbutane	14.1575	2848.31	32.4016

^a The Antoine expression used is $\ln P_i^{\circ} = A - \frac{B}{T-C}$ with P in kPa and T in K.

Table S3. Coefficients of the polynomial equation density - composition. ^a

Binary system	A	B	C	D	E	F
hexane (1) – EA (2)	-247.484872	1004.480655	-1637.264321	1344.856131	-562.246451	97.335521
3-methylpentane (1) – EA (2)	-221.013283	906.640955	-1494.064113	1241.322249	-525.486554	92.282052
2,3-dimethylbutane (1) – EA (2)	-162.214185	667.364888	-1104.679897	924.330914	-396.275100	71.162386

^a The polynomial function is $x_1 = A\rho_m^5 + B\rho_m^4 + C\rho_m^3 + D\rho_m^2 + E\rho_m + F$ with x_1 the mole fraction of component 1 and ρ_m the density of the mixture at 298.15 K, expressed in $\text{g}\cdot\text{cm}^{-3}$.

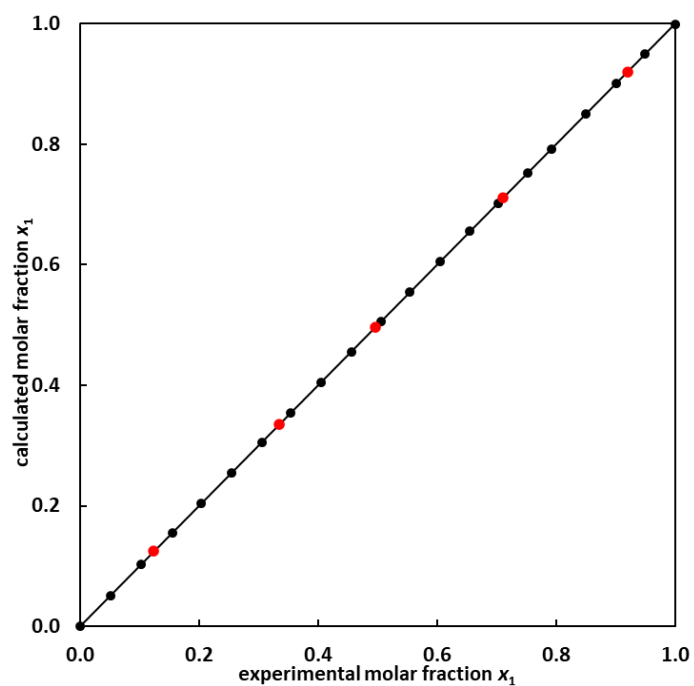


Figure S1. Calibration curve analysis of the binary system hexane (1) – ethyl acetate (2). •: experimental points used for the establishment of the calibration curve. •: mixtures of known compositions prepared and measured to check the accuracy of the method and to evaluate the uncertainty of the analysis ($u(x_1) = 0.001$).

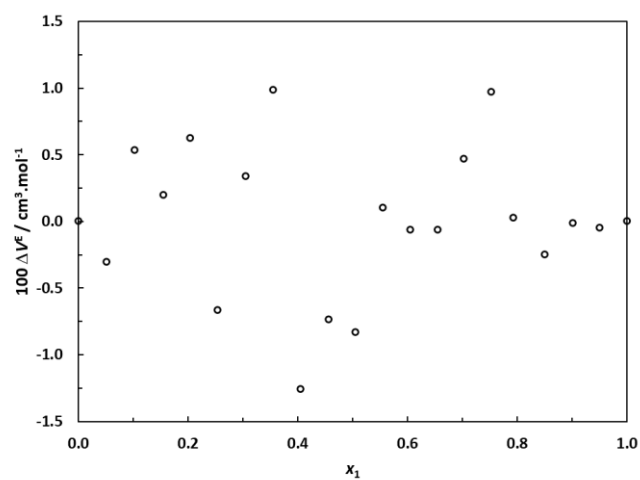


Figure S2. Residual distribution plot for the excess molar volume of the binary system hexane (1) – ethyl acetate (2) at 298.15 K resulting from Equation (2) with coefficients given in Table 6.

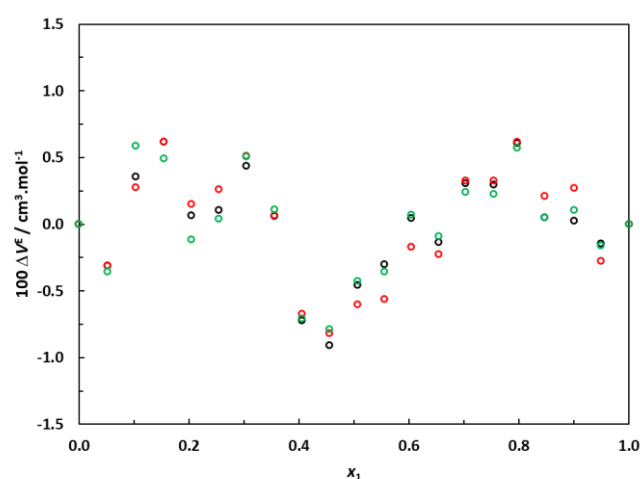


Figure S3. Residual distribution plot for the excess molar volume of the binary system 3-methylpentane (1) – ethyl acetate (2) at 293.15 K, 298.15 K and 303.15 K resulting from Equation (2) with coefficients given in Table 6.

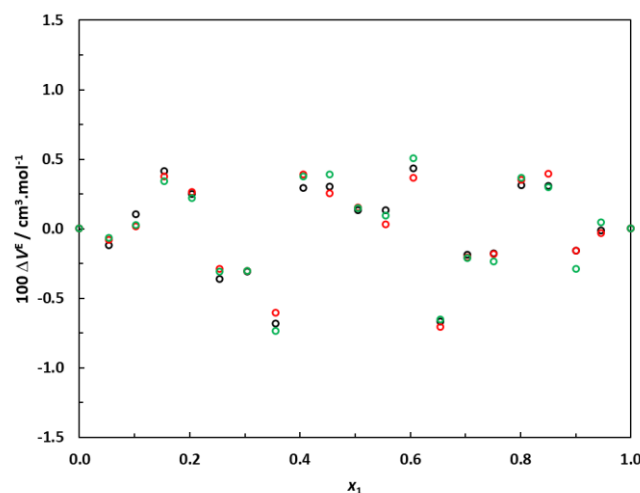


Figure S4. Residual distribution plot for the excess molar volume of the binary system 2,3-dimethylbutane (1) – ethyl acetate (2) at 293.15 K, 298.15 K and 303.15 K resulting from Equation (2) with coefficients given in Table 6.

References

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