

Supporting Information for  
Density, Viscosity, Speed of Sound, Bulk Modulus, and Surface Tension of Binary  
Mixtures of N-Heptane + 2,2,4-Trimethylpentane at (293.15 to 338.15) K and 0.1  
MPa

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The excess molar volumes for 2,2,4-trimethylpentane in n-heptane mixtures as calculated from eq 3 in the main text are given in Tables S1.

**Table S1. Excess Molar Volumes ( $\text{cm}^3 \cdot \text{mol}^{-1}$ ) of Mixtures of 2,2,4-Trimethylpentane (1) + n-Heptane from  $T = (293 \text{ to } 333) \text{ K}$  and  $0.1 \text{ MPa}^a$**

$T/\text{K}$	$X_1=$ 0.00	$X_1=$ 0.1000	$X_1=$ 0.2001	$X_1=$ 0.2999	$X_1=$ 0.4001	$X_1=$ 0.5001	$X_1=$ 0.6000	$X_1=$ 0.6999	$X_1=$ 0.8000	$X_1=$ 0.9000	$X_1=$ 1.00
293.15	0.00	-0.02	-0.02	-0.03	-0.04	-0.04	-0.04	-0.03	-0.02	-0.01	0.00
298.15	0.00	-0.022	-0.03	-0.03	-0.04	-0.05	-0.05	-0.04	-0.03	-0.02	0.00
303.15	0.00	-0.02	-0.02	-0.03	-0.04	-0.05	-0.05	-0.03	-0.03	-0.01	0.00
308.15	0.00	-0.02	-0.03	-0.04	-0.05	-0.05	-0.05	-0.04	-0.03	-0.02	0.00
313.15	0.00	-0.023	-0.03	-0.04	-0.05	-0.05	-0.05	-0.04	-0.03	-0.01	0.00
318.15	0.00	-0.02	-0.03	-0.04	-0.05	-0.06	-0.06	-0.04	-0.03	-0.02	0.00
323.15	0.00	-0.02	-0.03	-0.04	-0.05	-0.06	-0.05	-0.04	-0.03	-0.01	0.00
328.15	0.00	-0.02	-0.03	-0.04	-0.05	-0.06	-0.06	-0.04	-0.04	-0.02	0.00
333.15	0.00	-0.02	-0.03	-0.04	-0.05	-0.06	-0.06	-0.04	-0.03	-0.01	0.00
338.15	0.00	-0.03	-0.03	-0.04	-0.05	-0.06	-0.06	-0.04	-0.04	-0.01	0.00

It is important to note that excess molar volumes have a large error associated with them of approximately  $0.014 \text{ cm}^3 \cdot \text{mol}^{-1}$  as shown in Figure S1. Given below is the propagation of error for the excess molar volume of  $X_1 = 0.5001$  at 298.15 K using errors in the molar mass, mass of substances making the mixture, and measured density.

$$V_m^E = \frac{M_1 X_1 + M_2 X_2}{\rho_m} - \frac{M_1 X_1}{\rho_1} - \frac{M_2 X_2}{\rho_2} = \frac{M_1 X_1}{\rho_m} + \frac{M_2 X_2}{\rho_m} - \frac{M_1 X_1}{\rho_1} - \frac{M_2 X_2}{\rho_2}$$

$$e_{V_e} = \sqrt{\left(e_{(M_1 X_1 / \rho_{mix})}\right)^2 + \left(e_{(M_2 X_2 / \rho_{mix})}\right)^2 + \left(e_{(M_1 X_1 / \rho_1)}\right)^2 + \left(e_{(X_2 M_2 / \rho_2)}\right)^2}$$

Each of the four terms is calculated on the following pages.

**Term 1:**  $\%e_{(M_1X_1/\rho_{mix})} = \sqrt{(\%e_{M_1})^2 + (\%e_{X_1})^2 + (\%e_{\rho_{mix}})^2}$

For molar mass error, from Harris<sup>4</sup>

2,2,4-trimethylpentane: 8 carbons and 18 hydrogens

$$M_1 = 114.22852 \text{ g/mol}$$

$$e_{(M_1)} = \sqrt{\left(\frac{8 \cdot 0.0008}{\sqrt{3}}\right)^2 + \left(\frac{18 \cdot 0.00007}{\sqrt{3}}\right)^2} = 3.766 \times 10^{-3} \quad \%e_{M_1} = \frac{e_{(M_1)}}{M_1} \cdot 100 = \underline{\underline{3.297 \times 10^{-3}}}$$

n-heptane: 7 carbons and 16 hydrogens

$$M_2 = 100.20194 \text{ g/mol}$$

$$e_{(M_2)} = \sqrt{\left(\frac{7 \cdot 0.0008}{\sqrt{3}}\right)^2 + \left(\frac{16 \cdot 0.00007}{\sqrt{3}}\right)^2} = 3.297 \times 10^{-3} \quad \%e_{M_2} = \frac{e_{(M_2)}}{M_2} \cdot 100 = \underline{\underline{3.291 \times 10^{-3}}}$$

$$X_1 = \frac{m_1 / M_1}{(m_1 / M_1 + m_2 / M_2)}$$

Using  $X=0.5001$  mole fraction data  
For 0.0004 g error on balance

Mass of 2,2,4-trimethylpentane : 14.8263 g  
Mass of n-heptane : 13.0018 g

error for  $m_1/M_1$   $\%e_{(m_1/M_1)} = \sqrt{\%e_{m_1}^2 + \%e_{M_1}^2}$

$$\%e_{(m_1/M_1)} = \sqrt{(3.297 \cdot 10^{-3})^2 + (0.0004 \cdot 100 / 14.8263)^2} = 4.26015 \times 10^{-3}$$

$$e_{(m_1/M_1)} = [(4.26015 \times 10^{-3}) / (100)] (14.8263 \text{ g} / 114.22852 \text{ g/mol}) = 5.529 \times 10^{-6}$$

error for  $m_2/M_2$   $\%e_{(m_2/M_2)} = \sqrt{\%e_{m_2}^2 + \%e_{M_2}^2}$

$$\%e_{(m_2/M_2)} = \sqrt{(3.291 \cdot 10^{-3})^2 + (0.0004 \cdot 100 / 13.0018)^2} = 4.5051 \times 10^{-3}$$

$$e_{(m_2/M_2)} = [(4.5051 \times 10^{-3}) / (100)] (13.0018 \text{ g} / 100.20194 \text{ g/mol}) = 5.846 \times 10^{-6}$$

Error for  $(m_1/M_2 + m_2/M_2)$   $e_{(m_1/M_2 + m_2/M_2)} = \sqrt{e_{(m_1/M_2)}^2 + e_{(m_2/M_2)}^2}$

$$e_{(m_1/M_2 + m_2/M_2)} = \sqrt{(5.529 \times 10^{-6})^2 + (5.846 \times 10^{-6})^2} = 8.046 \times 10^{-6}$$

$$m_1/M_2 + m_2/M_2 = 0.25955$$

$$\%e_{(m_1/M_2 + m_2/M_2)} = 8.046 \times 10^{-6} \cdot 100 / 0.25955 = 3.1002 \times 10^{-3}$$

$$\%e_{X_1} = \sqrt{\%e_{(m_1/M_1)}^2 + \%e_{(m_1/M_2 + m_2/M_2)}^2} = \sqrt{(4.26015 \cdot 10^{-3})^2 + (3.1002 \cdot 10^{-3})^2} = \underline{\underline{5.269 \times 10^{-3}}}$$

$$\%e_{(\rho_{mix})} = e_{(\rho_{mix})}(100) / \rho_{mix} = 0.00004 \cdot 100 / 0.68412 = \underline{\underline{5.84693 \times 10^{-3}}}$$

$$\%e_{(M_1X_1/\rho_{mix})} = \sqrt{(\%e_{M_1})^2 + (\%e_{X_1})^2 + (\%e_{\rho_{mix}})^2} = \sqrt{(3.297 \cdot 10^{-3})^2 + (5.269 \cdot 10^{-3})^2 + (5.84693 \cdot 10^{-3})^2}$$

$$= \underline{\underline{8.5334 \times 10^{-3}}}$$

$$e_{(M_1X_1/\rho_{mix})} = (8.5334 \times 10^{-3})(114.22852 \text{ g/mol})(0.5001) / (100 \cdot 0.68412) = \underline{\underline{7.1256 \times 10^{-3}}} \text{ term 1}$$

**Term 2:**  $\%e_{(M_2X_2 / \rho_{mix})} = \sqrt{(\%e_{M_2})^2 + (\%e_{X_2})^2 + (\%e_{\rho_{mix}})^2}$

$$\%e_{X_2} = \sqrt{\%e_{(m_2/M_2)}^2 + \%e_{(m_1/M_1) + (m_2/M_2)}^2} = \sqrt{(4.5051 \cdot 10^{-3})^2 + (3.1002 \cdot 10^{-3})^2} = 5.469 \times 10^{-3}$$

$$\%e_{(M_2X_2 / \rho_{mix})} = \sqrt{(\%e_{M_2})^2 + (\%e_{X_2})^2 + (\%e_{\rho_{mix}})^2} = \sqrt{(3.291 \cdot 10^{-3})^2 + (5.469 \cdot 10^{-3})^2 + (5.84693 \cdot 10^{-3})^2} \\ = 8.6561 \times 10^{-3}$$

$$e_{(M_2X_2/\rho_{mix})} = (8.6561 \times 10^{-3})(100.20194 \text{ g/mol})(0.4999)/(100 \cdot 0.68412) = \underline{\underline{6.3379 \times 10^{-3} \text{ term 2}}}$$

**Term 3:**  $\%e_{(M_1X_1 / \rho_1)} = \sqrt{(\%e_{M_1})^2 + (\%e_{X_1})^2 + (\%e_{\rho_1})^2}$

$$\%e_{(\rho_1)} = e_{(\rho_1)}(100)/\rho_1 = 0.00004 * 100/0.68361 = 5.8513 \times 10^{-3}$$

$$\%e_{(M_1X_1 / \rho_1)} = \sqrt{(\%e_{M_1})^2 + (\%e_{X_1})^2 + (\%e_{\rho_1})^2} = \sqrt{(3.297 \cdot 10^{-3})^2 + (5.269 \cdot 10^{-3})^2 + (5.8513 \cdot 10^{-3})^2} \\ = 8.5364 \times 10^{-3}$$

$$e_{(M_1X_1/\rho_1)} = (8.5364 \times 10^{-3})(114.22852 \text{ g/mol})(0.5001)/(100 \cdot 0.68361) = \underline{\underline{7.1334 \times 10^{-3} \text{ term 3}}}$$

**Term 4:**  $\%e_{(M_2X_2 / \rho_2)} = \sqrt{(\%e_{M_2})^2 + (\%e_{X_2})^2 + (\%e_{\rho_2})^2}$

$$\%e_{(\rho_2)} = e_{(\rho_2)}(100)/\rho_1 = 0.00004 * 100/0.67961 = 5.8857 \times 10^{-3}$$

$$\%e_{(M_2X_2 / \rho_2)} = \sqrt{(\%e_{M_2})^2 + (\%e_{X_2})^2 + (\%e_{\rho_2})^2} = \sqrt{(3.291 \cdot 10^{-3})^2 + (5.469 \cdot 10^{-3})^2 + (5.8857 \cdot 10^{-3})^2} \\ = 8.6823 \times 10^{-3}$$

$$e_{(M_2X_2/\rho_2)} = (8.6823 \times 10^{-3})(100.20194 \text{ g/mol})(0.4999)/(100 \cdot 0.67961) = \underline{\underline{6.3993 \times 10^{-3} \text{ term 4}}}$$

$$e_{V_e} = \sqrt{(e_{(M_1X_1 / \rho_{mix})})^2 + (e_{(M_2X_2 / \rho_{mix})})^2 + (e_{(M_1X_1 / \rho_1)})^2 + (e_{(X_2 M_2 / \rho_2)})^2}$$

$$e_{V_e} = \sqrt{(7.1256 \cdot 10^{-3})^2 + (6.3379 \cdot 10^{-3})^2 + (7.1334 \cdot 10^{-3})^2 + (6.3993 \cdot 10^{-3})^2}$$

$$= \underline{\underline{0.0135 \text{ (final answer)}}}$$

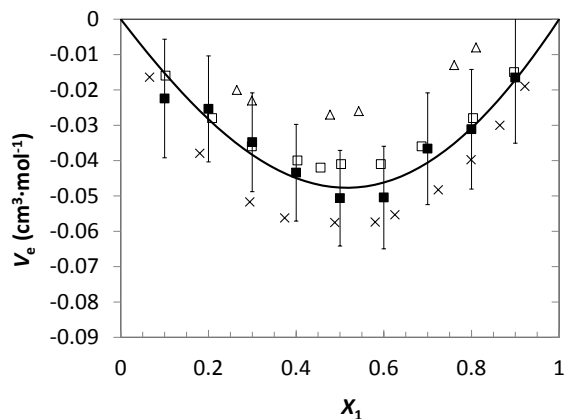


Figure S1: Excess molar volume of 2,2,4-trimethylpentane ( $X_1$ ) + n-heptane mixtures as calculated by eq 3 in the main text at 298.15 K for ■, this study; x, ref 1; □, ref 2; and Δ, ref 3. The line shown is the fit to eq 1 with the coefficients in Table S2.

The excess volumes for a few mixtures were fit using a Redlich-Kister type expression

$$V^E = X_1 X_2 \sum_{j=0}^{j-1} A_j (X_1 - X_2)^j \quad (1)$$

where  $A_j$  are adjustable parameters,  $j$  is the order of the polynomial, and  $X_1$  and  $X_2$  are the mole fraction of the 2,2,4-trimethylpentane and n-heptane, respectively. The standard error for the fit ( $\sigma$ ) was determined by eq 2 in the main text of the article, where  $P_{\text{measured}}$  is the calculated excess volume and  $P_{\text{fit}}$  is the fitted excess volume. Since there is not much variation in excess molar volume with temperature, the fits were only conducted at two temperatures for each set of mixtures. The fits are given in Table S2. The fits are good as shown in Figures S1. Also shown in Figure S1, the excess molar volumes reported herein fall within values reported by other researchers.<sup>1-3</sup>

**Table S2. Parameters for Redlich-Kister equation and the Standard Errors for Excess Molar Volumes of 2,2,4-Trimethylpentane + n-Heptane Mixtures at Select Temperatures and 0.1 MPa**

$T/K$	$A_1$ $\text{cm}^3 \cdot \text{mol}^{-1}$	$A_2$ $\text{cm}^3 \cdot \text{mol}^{-1}$	$A_3$ $\text{cm}^3 \cdot \text{mol}^{-1}$	$\sigma \times 10^3$ $\text{cm}^3 \cdot \text{mol}^{-1}$
298.15	-0.1906	-0.0121	-0.0163	4.1
328.15	-0.2305	-0.0268	0.0225	5.0

The kinematic viscosity deviations for 2,2,4-trimethylpentane in n-heptane mixtures as calculated from eq 6 in the main text are given in Tables S3.

**Table S3. Kinematic Viscosity Deviation ( $\text{mm}\cdot\text{s}^{-1}$ ) of 2,2,4-Trimethylpentane (1) in (2,2,4-Trimethylpentane + N-heptane) Mixtures from  $T = (293 \text{ to } 333) \text{ K}$  and  $0.1\text{MPa}^{\text{a}}$**

$T/ \text{K}$	$X_1=$ 0.1000	$X_1=$ 0.2001	$X_1=$ 0.2999	$X_1=$ 0.4001	$X_1=$ 0.5001	$X_1=$ 0.6000	$X_1=$ 0.6999	$X_1=$ 0.8000	$X_1=$ 0.9000
293.15	-0.005	-0.008	-0.011	-0.013	-0.013	-0.013	-0.011	-0.009	-0.005
298.15	-0.005	-0.008	-0.010	-0.012	-0.011	-0.011	-0.010	-0.009	-0.005
303.15	-0.004	-0.007	-0.009	-0.010	-0.011	-0.011	-0.009	-0.007	-0.004
308.15	-0.003	-0.006	-0.008	-0.009	-0.009	-0.009	-0.008	-0.007	-0.003
318.15	-0.002 <sup>b</sup>	-0.005	-0.006	-0.007	-0.008	-0.008	-0.007	-0.006	-0.003
323.15	-0.002 <sup>b</sup>	-0.005	-0.006	-0.007	-0.008	-0.007	-0.007	-0.006	-0.003 <sup>b</sup>
328.15	0.001 <sup>b</sup>	-0.002 <sup>b</sup>	-0.004	-0.005	-0.005	-0.005	-0.004	-0.004	-0.003 <sup>b</sup>
333.15	0.000 <sup>b</sup>	-0.002 <sup>b</sup>	-0.003 <sup>b</sup>	-0.004 <sup>b</sup>	-0.008 <sup>b</sup>	-0.006 <sup>b</sup>	-0.006 <sup>b</sup>	-0.004 <sup>b</sup>	-0.002 <sup>b</sup>

<sup>a</sup>  $x_1$  is the mole fraction of 2,2,4-trimethylpentane in the (2,2,4-trimethylpentane + n-heptane) mixture. Standard uncertainties  $u$  are  $u(T) = 0.01 \text{ K}$  and combined expanded uncertainties  $U_c$  is  $U(x_1) = 0.0001$  (level of confidence = 0.95,  $k \approx 2$ ).

<sup>b</sup>The error in these calculated values is larger than the values themselves.

## References

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- (2) Lepori, L.; Gianni, P.; Matteoli, E. The effect of the molecular size and shape on the volume behavior of binary liquid mixtures. Branched and cyclic alkanes in heptane at 298.15 K. *J. Solution Chem.* **2013**, *42*, 1263–1304.
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