Electronic Supplementary Information

Isobaric Vapor-Liquid Equilibrium prediction from Excess Molar Enthalpy using cubic Equations of State and PC-SAFT

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Content:

S1. Departure function Derivation

The general departure function, as shown in the main manuscript in equation 5, shows to be a deviation between the behavior of a real fluid and an ideal gas (ig). The ideal gas state is a state where ideality is obeyed. Hence, departure from ideality means in essence, in the coming sections, the deviation from ideal gas behavior. This is first derived for pure components, and using the mixing rule, also the departure function for mixtures can be calculated. The relation between these will result in the excess properties.

S1.1. Internal Energy

The non-ideal behavior of a fluid, or the departure from ideality, can be described by following a thermodynamic pathway. A pathway of a function, in this case the internal energy, is always relative to the ideal gas situation. Firstly, the temperature, pressure and volume are kept constant in the internal energy (U). In the second term, the variation in the volume between the non-ideal (V) and ideal gas situation (V^{ig}) is subtracted.

$$U_{dep} = (U - U^{ig}) = (U - U^{ig})_{TV} - \int_{V}^{V^{ig}} \left(\frac{\partial U}{\partial V}\right)_{T}^{ig} dV \tag{S1}$$

Also, the first right-hand-side term can be written as an integral, which reaches from infinity to the volume of the non-ideal fluid;

$$U_{dep} = (U - U^{ig}) = \int_{\infty}^{V} \left(\left(\frac{\partial U}{\partial V}\right)_{T} - \left(\frac{\partial U}{\partial V}\right)_{T}^{ig}\right) dV - \int_{V}^{V^{ig}} \left(\frac{\partial U}{\partial V}\right)_{T}^{ig} dV \tag{S2}$$

The internal energy of an ideal gas is not volume dependent, thus the $\left(\frac{\partial U}{\partial V}\right)_{T}^{ig}$ falls out of the equations, resulting:

$$U_{dep} = (U - U^{ig}) = \int_{\infty}^{V} \left(\frac{\partial U}{\partial V}\right)_{T} dV \tag{S3}$$

For non-ideal fluids, the volume dependency of the internal energy can be analysed as follows;

$$\left(\frac{\partial U}{\partial V}\right)_{T} = \left(\frac{\partial S}{\partial V}\right)_{T}\left(\frac{\partial U}{\partial S}\right)_{T} + \left(\frac{\partial U}{\partial V}\right)\left(\frac{\partial T}{\partial T}\right) \tag{S4}$$

With one of the Maxwell relations; $\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$ and the known relations of $\left(\frac{\partial U}{\partial S}\right)_T = T$ and $\left(\frac{\partial U}{\partial V}\right) = -P$

$$\left(\frac{\partial U}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V \left(\frac{\partial U}{\partial S}\right)_T + \left(\frac{\partial U}{\partial V}\right)\left(\frac{\partial T}{\partial T}\right) \tag{S5}$$

$$\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P \tag{S6}$$

$$U_{dep} = (U - U^{ig}) = \int_{\infty}^{V} \left(T\left(\frac{\partial P}{\partial T}\right)_V - P\right) dV \tag{S7}$$

For convenience, the departure function needs to be rewritten to molar density and the compressibility factor, resp. $\rho = \frac{1}{V}$ and Z.

Firstly, converting the equation to the compressibility variable. Knowing that the result has to be in the form of $\left(\frac{\partial Z}{\partial T}\right)_V$, via integration by substitution. The following correlation is obtained;

$$T\left(\frac{\partial Z}{\partial T}\right)_V = T\left(\left(\frac{\partial P}{\partial T}\right)_V \left(\frac{\partial Z}{\partial P}\right)_V + \left(\frac{\partial Z}{\partial T}\right)_V \left(\frac{\partial T}{\partial T}\right)_V\right) \tag{S8}$$

$$T\left(\frac{\partial Z}{\partial T}\right)_V = T\left(\frac{V}{RT}\left(\frac{\partial P}{\partial T}\right)_V - \frac{PV}{RT^2}\right) \tag{S9}$$

$$T\left(\frac{\partial Z}{\partial T}\right)_V = \frac{V}{R}\left(\frac{\partial P}{\partial T}\right)_V - Z \tag{S10}$$

$$\frac{RT^2}{V}\left(\frac{\partial Z}{\partial T}\right)_V + \frac{RTZ}{V} = T\left(\frac{\partial P}{\partial T}\right)_V \tag{S11}$$

$$\frac{RT^2}{V}\left(\frac{\partial Z}{\partial T}\right)_V + P = T\left(\frac{\partial P}{\partial T}\right)_V \tag{S12}$$

Putting this back in to the departure function:

$$U_{dep} = (U - U^{ig}) = \int_{\infty}^{V} \left(\frac{RT^2}{V} \left(\frac{\partial Z}{\partial T} \right)_V + P - P \right) dV \tag{S13}$$

$$U_{dep} = (U - U^{ig}) = RT \int_{\infty}^{V} \left(\frac{T}{V} \left(\frac{\partial Z}{\partial T} \right)_V \right) dV \tag{S14}$$

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66 Now, the transformation from the volume to density via integration by substitution:

67 $$\rho = \frac{1}{V} \rightarrow -\frac{1}{\rho^2} d\rho = dV$$

$$U_{dep} = (U - U^{ig}) = -RT \int_{0}^{\rho} \frac{\left(T\rho \left(\frac{\partial Z}{\partial T} \right)_V \right) d\rho}{\rho^2} \tag{S15}$$

$$U_{dep} = (U - U^{ig}) = -RT \int_{0}^{\rho} T \left(\frac{\partial Z}{\partial T} \right)_{\rho} \frac{d\rho}{\rho} \tag{S16}$$

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69 **S1.2. Entropy**

70 The derivation of the entropy description is likewise also a similar thermodynamic pathway of
71 a function and relative to the ideal gas situation. Firstly, the temperature, pressure and volume
72 are kept constant in the entropic description (S). In the second term, the variation in the volume
73 between the non-ideal (V) and ideal gas situation (V^{ig}) is subtracted.

$$S_{dep} = (S - S^{ig}) = (S - S^{ig})_{TV} - \int_{V}^{V^{ig}} \left(\frac{\partial S}{\partial V} \right)_T^{ig} dV \tag{S17}$$

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75 Also, the first right-hand-side term can be written as an integral, which reaches from infinity to
76 the volume of the non-ideal fluid;

$$S_{dep} = (S - S^{ig}) = \int_{\infty}^{V} \left(\left(\frac{\partial S}{\partial V} \right)_T - \left(\frac{\partial S}{\partial V} \right)_T^{ig} \right) dV - \int_{V}^{V^{ig}} \left(\frac{\partial S}{\partial V} \right)_T^{ig} dV \tag{S18}$$

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Following one of the Maxwell relations; $\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$, the entropy term (S) can be removed from the relation and replaced by a function of measurable quantities:

$$S_{dep} = (S - S^{ig}) = \int_{\infty}^{V} \left(\left(\frac{\partial P}{\partial T}\right)_V - \left(\frac{\partial P}{\partial T}\right)_V^{ig} \right) dV - \int_{V}^{V^{ig}} \left(\frac{\partial P}{\partial T}\right)_V^{ig} dV \quad \text{(S19)}$$

First solving the ideal gas terms, knowing that $P = \frac{RT}{V} \rightarrow \left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{V}$, gives us the temperature variation of the ideal gas pressure. Also the last term, can be rewritten to exclude an integral function:

$$S_{dep} = (S - S^{ig}) = \int_{\infty}^{V} \left(\left(\frac{\partial P}{\partial T}\right)_V - \frac{R}{V} \right) dV - \int_{V}^{V^{ig}} \frac{R}{V} dV \quad \text{(S20)}$$

$$S_{dep} = (S - S^{ig}) = \int_{\infty}^{V} \left(\left(\frac{\partial P}{\partial T}\right)_V - \frac{R}{V} \right) dV - Rln\left(\frac{V}{V^{ig}}\right) \quad \text{(S21)}$$

Furthermore, the $\frac{V}{V^{ig}}$ term, can be rewritten via $V = \frac{ZRT}{P}$ for an ideal gas Z =1, to $\frac{V}{V^{ig}} = Z$:

$$S_{dep} = (S - S^{ig}) = \int_{\infty}^{V} \left(\left(\frac{\partial P}{\partial T}\right)_V - \frac{R}{V} \right) dV - Rln(Z) \quad \text{(S22)}$$

$$S_{dep} = (S - S^{ig}) = R\left(\int_{\infty}^{V} \left(\frac{1}{R}\left(\frac{\partial P}{\partial T}\right)_V - \frac{1}{V} \right) dV - ln(Z) \right) \quad \text{(S23)}$$

For convenience, the departure function is likewise rewritten to density and the compressibility factor, resp. $\rho = \frac{1}{V}$ and Z.

Firstly, rewriting the equation to include the compressibility factor. Knowing that the result has to be in the form of $\left(\frac{\partial Z}{\partial T}\right)_V$, via integration by substitution. The following correlation is obtained;

$$T\left(\frac{\partial Z}{\partial T}\right)_V = T\left(\left(\frac{\partial P}{\partial T}\right)_V \left(\frac{\partial Z}{\partial P}\right)_V + \left(\frac{\partial Z}{\partial T}\right)_V \left(\frac{\partial T}{\partial T}\right)_V \right) \quad \text{(S24)}$$

$$T\left(\frac{\partial Z}{\partial T}\right)_V = T\left(\frac{V}{RT}\left(\frac{\partial P}{\partial T}\right)_V - \frac{PV}{RT^2} \right) \quad \text{(S25)}$$

$$T\left(\frac{\partial Z}{\partial T}\right)_V = \frac{V}{R}\left(\frac{\partial P}{\partial T}\right)_V - Z \quad \text{(S26)}$$

$$\frac{T}{V}\left(\frac{\partial Z}{\partial T}\right)_V + \frac{Z}{V} = \frac{1}{R}\left(\frac{\partial P}{\partial T}\right)_V \quad \text{(S27)}$$

Putting this result back into the departure function gives:

$$S_{dep} = (S - S^{ig}) = R\int_{\infty}^{V}\left(\frac{T}{V}\left(\frac{\partial Z}{\partial T}\right)_{V} + \frac{Z}{V} - \frac{1}{V}\right)dV - ln(Z) \tag{S28}$$

Now, the transformation from the volume to density via integration by substitution;

$$\rho = \frac{1}{V} \rightarrow -\frac{1}{\rho^2}d\rho = dV$$

$$S_{dep} = (S - S^{ig}) = R\int_{0}^{\rho} -\frac{\left(T\rho\left(\frac{\partial Z}{\partial T}\right)_{\rho} + Z\rho - \rho\right)d\rho}{\rho^2} - ln(Z) \tag{S29}$$

$$S_{dep} = (S - S^{ig}) = R\int_{0}^{\rho}\left(-T\left(\frac{\partial Z}{\partial T}\right)_{\rho} - (Z-1)\right)\frac{d\rho}{\rho} - ln(Z) \tag{S30}$$

S1.3. Enthalpy

Knowing the fact that the enthalpy is related to the internal energy in the following manner;

$$H = U + PV \tag{S31}$$

The departure function for enthalpy holds for;

$$H_{dep} = U_{dep} + (PV)_{dep} \tag{S32}$$

$$\frac{H - H^{ig}}{RT} = \frac{U - U^{ig}}{RT} + \frac{PV - (PV)^{ig}}{RT} \tag{S33}$$

As the ideal gas law is $PV = RT$, the relation can be rewritten as:

$$\frac{H - H^{ig}}{RT} = \frac{U - U^{ig}}{RT} + \frac{PV - RT}{RT} \tag{S34}$$

Then substituting the result for the internal energy gives the departure function of the enthalpy;

$$H_{dep} = H - H^{ig} = RT\left(\int_{0}^{\rho} -T\left(\frac{\partial Z}{\partial T}\right)_{\rho}\frac{d\rho}{\rho} + (Z-1)\right) \tag{S35}$$

S2. Generalization of cubic Equations of State

Table S1: Overview of seven two-parameter cubic Equation of States and there corresponding parameters.

Two-Parameter Cubic Equation of State		a	b	α
Van der Waals [1]	$P=\frac{RT}{V_m-b}-\frac{a}{V_m^2}$	$\frac{27R^2Tc^2}{64P_c}$	$0.125\frac{RTc}{P_c}$	(-)
Redlich-Kwong [2]	$P=\frac{RT}{V_m-b}-\frac{\alpha a}{V_m(V_m+b)}$	$0.42748\frac{R^2Tc^{2.5}}{P_c}$	$0.08664\frac{RTc}{P_c}$	$\alpha=\frac{1}{\sqrt{T}}$
Soave-Redlich-Kwong [3]		$0.42748\frac{R^2Tc^2}{P_c}$		$\alpha=\left[1+\left(1-\sqrt{\frac{T}{T_c}}\right)(0.48+1.574\omega-0.176\omega^2)\right]^2$
Peng-Robinson [4]	$P=\frac{RT}{V_m-b}-\frac{\alpha a}{V_m(V_m+b)+b(V_m-b)}$	$0.45724\frac{R^2Tc^2}{P_c}$	$0.0778\frac{RTc}{P_c}$	$\alpha=\left[1+\left(1-\sqrt{\frac{T}{T_c}}\right)(0.37464+1.54226\omega-0.26992\omega^2)\right]^2$
Peng-Robinson-Stryjek-Vera [5]				$\alpha=\left[1+m_i\left(1-\sqrt{\frac{T_i}{T_c}}\right)\right]^2$ $m_i=\ k_{0i}+k_{1i}\left(1-\sqrt{\frac{T}{T_c}}\right)\left(0.7-\frac{T_i}{T_c}\right)$ $k_{0i}=\ 0.378893+1.4897153\omega_i-0.1713848\omega_i^2+0.01965$ $k_{1i}=specific\ for\ each\ pure\ subtance$
Twu-Sim-Tassone [6]	$P=\frac{RT}{V_m-b}-\frac{\alpha a}{(V_m+3b)(V_m-0.5b)}$	$0.470507\frac{R^2Tc^2}{P_c}$	$0.0740740\frac{RTc}{P_c}$	$\alpha=T_r^{N(M-1)}e^{L\left(1-T_r^{NM}\right)}$ $N,M,L=specific\ for\ each\ pure\ subtance$
Nasrifir-Moshfeghian	$P=\frac{RT}{V_m-\beta b}-\frac{\alpha a}{V_m^2+2\beta bV_m-2\beta b^2}$	$0.497926\frac{R^2Tc^2}{P_c}$	$0.094451\frac{RTc}{P_c}$	$\alpha=\left[1+m_\alpha\left(1-\sqrt{\frac{T-T_{pt}}{T_c-T_{pt}}}\right)\right]^2$ $\beta=\left[1+m_\beta\left(1-\frac{T-T_{pt}}{T_c-T_{pt}}\right)\right]$

				$m_\alpha = \sqrt{\frac{a_{pt}}{a}} - 1$	$m_\beta = \frac{b_{pt}}{b} - 1$
				$\frac{a_{pt}}{b_{pt}RT_{pt}} = 29.7056$ $\frac{T_{pt}}{T_c} = 0.2498 + 0.3359\omega + 0.1037\omega^2$ $\frac{b_{pt}}{b_c} = 1 - 0.1519\omega - 3.9462\omega^2 + 7.0538\omega^3$	

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106 *Table S2: Overview of 4 three-parameter cubic Equations of State and there corresponding parameters.*

Three-Parameter Cubic Equation of State		a	b	c	α
Patel-Teja [7]	$P = \frac{RT}{V_m - b} - \frac{\alpha a}{V_m(V_m + b) + c(V_m - b)}$	$\frac{\Omega_a R^2 T_c^2}{P_c}$	$\frac{\Omega_b RT_c}{P_c}$	$\frac{\Omega_c RT_c}{P_c}$	$\alpha = \left[1 + F\left(1 - \sqrt{\frac{T_i}{T_c}}\right)\right]^2$ $\Omega_a = 3\gamma_c^3 + 3(1 - 2\gamma_c)\Omega_b + \Omega_b^2 + 1 - 3\gamma_c$ $\Omega_b^3 + (2 - 3\gamma_c)\Omega_b^2 + 3\gamma_c^2\Omega_b - \gamma_c^3 = 0$ $\Omega_c = 1 - 3\gamma_c$ Ω_b is the smallest positive root of the cubic equation. $non - polar: \begin{cases} F = 0.45213 + 1.3098\omega_i - 0.295937\omega_i^2 \\ \gamma_c = 0.329032 - 0.076799\omega_i + 0.211947\omega \end{cases}$ Otherwise, F and γ_c are adjustable parameters

Patel-Teja-Valderrama [8]	$P=\frac{RT}{V_m-b}-\frac{\alpha a}{V_m(V_m+b)+c(V_m-b)}$	$\frac{\Omega_a R^2 T_c^2}{P_c}$	$\frac{\Omega_b R T_c}{P_c}$	$\frac{\Omega_c R T_c}{P_c}$	$\alpha=\left[1+F\left(1-\sqrt{\frac{T_i}{T_c}}\right)\right]^2$ $\Omega_a=0.66121-0.76105Z_c$ $\Omega_b=0.02207+0.20868Z_c$ $\Omega_c=0.57765-1.87080Z_c$ $F=0.46283+3.58230(\omega Z_c)+8.19417(\omega Z_c)^2$
Esmaeilzadeh-Roshanfekr [9]	$P=\frac{RT}{V_m-b}-\frac{\alpha a}{V_m(V_m+c)+c(V_m-c)}$	$\frac{\Omega_a R^2 T_c^2}{P_c}$	$\frac{\Omega_b R T_c}{P_c}$	$\frac{\Omega_c R T_c}{P_c}$	$\alpha=\left[m_1+m_2\left(1-\sqrt{\frac{T_i}{T_c}}\right)\right]^2$ $\Omega_a=3\xi_c^2+\Omega_c^2+2\Omega_b\Omega_c+2\Omega_c$ $\Omega_b=2\Omega_c-1+3\xi_c$ $\Omega_c^3+\left(3\xi_c-\frac{5}{8}\right)\Omega_c^2+\left(3\xi_c^2-\frac{3}{4}\xi_c\right)\Omega_c+\left(\xi_c^3-\frac{3}{8}\xi_c^2\right)=0$ Ω_c is the smallest positive root of the cubic equation. $\begin{cases}\xi_c=0.3284438-0.0690264\omega_i+0.0078711\omega_i^2\\ m_1=0.999035-0.01061842\omega_i-0.0081174\omega_i^2\\ m_2=0.4400108+1.5297151\omega_i-0.4710752\omega_i^2\end{cases}$
Harmens-Knapp [10]	$P=\frac{RT}{V_m-b}-\frac{\alpha a}{V_m^2+cbV_m-(c-1)b^2}$	$\frac{\Omega_a R^2 T_c^2}{P_c}$	$\frac{\Omega_b R T_c}{P_c}$	$1+\frac{1-3\xi_c}{\beta\xi_c}$	$\Omega_a=1-3\xi_c+3\xi_c^2+\beta\xi_c(3-6\xi_c+\beta\xi_c)$ $\Omega_b=\beta\xi_c$ $\xi_c=0.3211-0.080\omega+0.0384\omega^2$ $\beta=0.10770+0.76405\xi_c-1.24282\xi_c^2+0.96210\xi_c^3$

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108 *Table S3: Overview of a four-parameter cubic Equation of State and there corresponding parameters.*

Four-Parameter Cubic Equation of State		a	b	c	D	α
Trebble-Bishnoi (1987) [11]	$P = \frac{RT}{V_m - b} - \frac{\alpha a}{{V_m}^2 + (b+c)V_m - bc - d^2}$	$\frac{\Omega_a R^2 T_c^2}{P_c}$	$\frac{\Omega_b R T_c}{P_c}$	$\frac{\Omega_c R T_c}{P_c}$	$\frac{\Omega_d R T_c}{P_c}$	$\Omega_a = 2\Omega_b\Omega_c + \Omega_b + \Omega_c + \Omega_b^2 + \Omega_d^2 + 3$ $\Omega_b^3 + (2 - 3\xi_c)\Omega_b^2 + 3\xi_c^2\Omega_b - (\Omega_d^2 + \xi_c^3$ $\Omega_c = -3\xi_c + 1$ $\Omega_d = 0.341V_c - 0.005$ $\xi_c = 1.075Z_c$ Ω_b is the smallest positive root of the cubic equation

S2.1 Mixing Rules

Table S4: The eight mixing rules

cubic Equation of State (cEoS)	a	b
1-parameter Van der Waals[1] (VdW1)	$\sum_i \sum_i x_i x_j \left(\sqrt{a_i a_j}(1 - K_{ij})\right)$	$\sum_i x_i b_i$
2-parameter Van der Waals[1] (VdW2)	$\sum_i \sum_i x_i x_j \left(\sqrt{a_i a_j}(1 - K_{ij})\right)$	$\sum_i \frac{\sum_i x_i x_j (b_i + b_j)(1 - L_{ij})}{2}$
Adachi-Sugie[12](AS)	$\sum_i \sum_i x_i x_j \sqrt{a_i a_j}(1 - K_{ij} + L_{ij}(x_i - x_j))$	$\sum_i x_i b_i$
Panagiotopoulos-Reid[13] (PR)	$\sum_i \sum_i x_i x_j \sqrt{a_i a_j}(1 - K_{ij} + (K_{ij} - K_{ji})x_i)$	
Stryjek-Vera Margules-type[5] (SVm)	$\sum_i \sum_i x_i x_j \sqrt{a_i a_j}(1 - K_{ij} x_i + K_{ji} x_j)$	
Stryjek-Vera van Laar-type[5] (SVvL)	$\sum_i \sum_i x_i x_j \sqrt{a_i a_j}\left(1 - \frac{K_{ij} K_{ji}}{K_{ij} x_i + K_{ji} x_j}\right)$	
Sandoval[14]	$\sum_i \sum_i x_i x_j \sqrt{a_i a_j}\left(1 - (K_{ij} x_i + L_{ij} x_j) - \frac{(K_{ij} + L_{ij})(1 - x_i - x_j)}{2}\right)$	
Huron-Vidal[15] (HV)[a]	$b \sum_i x_i \left(\frac{a_i}{b_i} - \frac{1}{\sqrt{2}} \sum_i x_i \frac{\sum_j x_j G_{ji} \tau_{ji}}{\sum_k x_k G_{ki}}\right)$	

[a] $\tau_{ji} = b_j \exp\left(-\alpha_{ji} \frac{G_{ji}}{RT}\right)$, where α_{ji} and G_{ji} are additional fitting parameters.

S3. Fitting Results in Manuscript

Table S5: Overview of the results behind manuscript figure 8, including the BIPs (K_{ij} and L_{ij}) of the Peng-Robinson Equation of State with the 2-parameter Stryjek-Vera Margules-type mixing rule.

		Absolute deviation in Concentration profile			Absolute deviation in Temperature profile			Average K_{ij}	Average L_{ij}
Compound1	Compound2	minimum	average	maximum	minimum	average	maximum		
n-Ethanol	n-Acetone	0.0000	0.0324	0.0848	0.0425	0.3994	1.8375	0.0129	-0.0355
Methanol	Diethylamine	0.0000	0.0724	0.2513	0.2267	8.0944	19.2590	-0.1910	0.2345
Methanol	Triethylamine	0.0095	0.1224	0.2557	1.5413	13.2027	19.4974	-0.1991	0.2197
Methanol	n,n-dimethylformamide	0.0000	0.0130	0.0388	0.4512	1.9311	4.2875	-0.1452	0.1554
n-Ethanol	n,n-dimethylformamide	0.0000	0.0508	0.2965	0.0817	6.5713	26.3288	-0.1194	0.1283
n-Propanol	n,n-dimethylformamide	0.0000	0.0211	0.0645	0.0610	4.0079	7.8493	-0.1029	0.1124
Methanol	Chloroform	0.0000	0.0915	0.1772	0.6367	7.1598	10.8025	-0.1039	0.0885
n-Ethanol	Chloroform	0.0000	0.0507	0.1165	0.5060	3.9806	8.8068	-0.0893	-0.0552
n-Propanol	Chloroform	0.0002	0.0229	0.0708	0.0121	1.7201	4.0682	-0.0713	-0.0591
2-propanol	Chloroform	0.0034	0.0315	0.0886	0.1024	1.4904	3.6091	-0.0607	-0.0652
Methanol	Tetrachloromethane	0.0000	0.1568	0.3354	0.2226	9.9484	16.4146	-0.0788	-0.0241
n-Ethanol	Tetrachloromethane	0.0000	0.0920	0.2000	0.4434	7.0912	12.1281	-0.0775	-0.0192
n-Propanol	Tetrachloromethane	0.0000	0.0678	0.1947	0.0137	5.0244	11.3710	-0.0698	-0.0207
2-propanol	Tetrachloromethane	0.0000	0.0651	0.1930	0.1142	5.3076	8.6944	-0.0625	-0.0224
Methanol	Methyl Acetate	0.0000	0.0332	0.0916	0.2132	1.9946	4.4669	-0.0518	-0.0218
Methanol	n-Ethyl Acetate	0.0000	0.0416	0.0985	0.1727	3.0277	4.5569	-0.0527	-0.0205
Methanol	n-Butyl Acetate	0.0000	0.0781	0.2895	0.0632	6.2210	14.2498	-0.0558	-0.0174
n-Ethanol	n-Ethyl Formate	0.0000	0.0263	0.0772	0.5746	3.2162	5.5533	0.0068	-0.0460
n-Ethanol	Methyl Acetate	0.0000	0.0274	0.1101	0.0035	0.8524	6.1392	0.0066	-0.0466
n-Ethanol	n-Ethyl Acetate	0.0000	0.0404	0.1723	0.0002	1.5618	4.5455	-0.0001	-0.0451
n-Ethanol	n-Hexane	0.0000	0.1278	0.3508	0.4520	9.1374	16.7711	-0.0251	-0.0304
n-Ethanol	n-Heptane	0.0000	0.1451	0.4624	0.9177	11.0089	18.9126	-0.0463	-0.0123

n-Ethanol	n-Octane	0.0178	0.1144	0.3968	2.2616	14.4294	29.0797	-0.0613	0.0027
		Absolute deviation in Concentration profile			Absolute deviation in Temperature profile			Average K_{ij}	Average L_{ij}
Compound1	Compound2	minimum	average	maximum	minimum	Compound1	Compound2	minimum	average
Methanol	n-Benzene	0.0000	0.1253	0.3601	0.2132	9.1588	16.2863	-0.0630	0.0005
Methanol	n-Toluene	0.0000	0.1024	0.3060	0.0746	8.8634	16.4563	-0.0654	0.0003
n-Ethanol	n-Benzene	0.0000	0.0835	0.1752	0.3681	6.2600	9.3025	-0.0664	-0.0061
n-Ethanol	n-Toluene	0.0000	0.0626	0.1846	0.2525	5.3255	10.2214	-0.0650	-0.0103
Methanol	Tetrahydrofuran	0.0078	0.0577	0.0945	2.6507	4.5583	5.7393	-0.0666	-0.0087
n-Ethanol	Diethyl Ether	0.0000	0.1008	0.2968	0.6179	7.8574	19.1117	-0.0675	-0.0066
n-Ethanol	Diisopropyl Ether	0.0113	0.0964	0.2012	1.4832	8.1601	11.7151	-0.0698	-0.0036
n-Methanol	n-Acetone	0.0000	0.0197	0.1099	0.2207	1.6563	3.4644	-0.0673	-0.0034
n-Methanol	2-Butanone	0.0015	0.0358	0.0663	1.1023	3.5835	8.2950	-0.0673	-0.0025
n-Ethanol	n-Acetone	0.0000	0.0326	0.0852	0.0345	0.3981	1.8376	-0.0648	-0.0035
n-Ethanol	2-Butanone	0.0000	0.0134	0.0310	0.1905	1.1970	2.0072	-0.0622	-0.0043
n-Methanol	Acetonitrile	0.0000	0.0210	0.0518	0.1722	1.3356	2.3770	-0.0609	-0.0051
n-Ethanol	Acetonitrile	0.0000	0.0172	0.0361	0.0424	0.6351	1.8411	0.0338	-0.0713
n-Methanol	n-Butanol	0.0000	0.0334	0.1747	0.0633	1.8072	8.3746	-0.0070	-0.0078
n-Ethanol	n-Propanol	0.0000	0.0090	0.0313	0.4181	1.5297	2.2876	-0.0063	-0.0054
n-Hexane	n-Benzene	0.0000	0.0153	0.0438	0.0057	0.6451	2.1763	0.0036	-0.0087
n-Hexane	n-Toluene	0.0000	0.0166	0.0722	0.0148	1.4843	3.3289	0.0057	-0.0098
n-Hexane	m-Xylene	0.0000	0.0154	0.0692	0.2129	1.0803	3.2500	0.0067	-0.0103
n-Hexane	o-Xylene	0.0000	0.0211	0.0590	0.4008	1.8817	4.1603	0.0075	-0.0107
n-Hexane	Chloroform	0.0000	0.0317	0.0626	0.4360	2.2844	4.5384	0.0137	-0.0034
n-Hexane	Tetrachloromethane	0.0031	0.0126	0.0230	0.0027	0.4315	0.8178	0.0131	-0.0041
n-Heptane	Chloroform	0.0025	0.0186	0.0349	0.0195	0.3558	1.2792	0.0131	-0.0035
n-Heptane	Tetrachloromethane	0.0027	0.0221	0.0526	0.1253	1.1803	2.2444	0.0124	-0.0039
n-Heptane	Propionic acid	0.0000	0.1400	0.4290	0.2229	9.2107	26.2293	0.0106	0.0056
n-Hexane	Methyl Formate	0.0000	0.0152	0.0386	0.3868	1.4169	2.7915	0.0144	0.0042

n-Hexane	n-Ethyl Formate	0.0000	0.0080	0.0266	0.2411	0.8047	1.2427	0.0183	0.0010
		Absolute deviation in Concentration profile			Absolute deviation in Temperature profile			Average K_{ij}	Average L_{ij}
Compound1	Compound2	minimum	average	maximum	minimum	Compound1	Compound2	minimum	average
n-Hexane	Propyl Formate	0.0000	0.0164	0.0432	0.0078	0.5643	1.4498	0.0214	-0.0016
n-Hexane	Butyl Formate	0.0000	0.0218	0.0588	0.0637	1.8476	4.2461	0.0229	-0.0027
n-Hexane	Tetrahydrofuran	0.0000	0.0102	0.0414	0.1057	0.7862	1.3627	0.0231	-0.0029
n-Heptane	Diisopropyl Ether	0.0013	0.0148	0.0369	0.2587	0.9788	1.6104	0.0228	-0.0032
n-Hexane	n-Acetone	0.0000	0.0160	0.0437	0.2186	1.9274	2.8904	0.0306	-0.0080
n-Heptane	n-Acetone	0.0078	0.0154	0.0312	0.3393	1.6873	2.6410	0.0340	-0.0097
n-Heptane	2-Butanone	0.0000	0.0156	0.0600	0.4910	2.0300	3.1958	0.0356	-0.0107
n-Benzene	n,n-dimethylformamide	0.0000	0.0269	0.0981	0.4471	3.5678	8.9065	0.0311	-0.0095
n-Toluene	n,n-dimethylformamide	0.0013	0.0329	0.1311	0.1788	3.5313	9.0256	0.0305	-0.0094
n-Benzene	Chloroform	0.0000	0.0123	0.0397	0.0394	1.5256	2.8579	0.0295	-0.0086
n-Benzene	Tetrachloromethane	0.0000	0.0034	0.0118	0.0160	0.3205	0.6665	0.0276	-0.0084
n-Toluene	Chloroform	0.0012	0.0648	0.1563	0.2213	2.8489	4.7546	0.0261	-0.0076
n-Benzene	Acetic Acid	0.0000	0.1136	0.3013	0.3341	9.5580	21.2786	0.0240	-0.0070
n-Benzene	Methyl Acetate	0.0003	0.0093	0.0309	0.0033	0.5773	1.5630	0.0235	-0.0069
n-Benzene	n-Ethyl Acetate	0.0017	0.0167	0.0350	0.0411	0.5497	1.3782	0.0232	-0.0069
n-Toluene	n-Ethyl Acetate	0.0000	0.0063	0.0223	0.0286	0.6010	1.2310	0.0227	-0.0068
n-Benzene	Diisopropyl Ether	0.0000	0.0195	0.0737	0.3860	1.4162	2.1458	0.0223	-0.0066
n-Toluene	n-Acetone	0.0004	0.0520	0.1036	0.4405	2.4374	4.6638	0.0215	-0.0063
n-Benzene	Acetonitrile	0.0000	0.0405	0.1023	0.4470	3.7443	5.6533	0.0213	-0.0070
n-Toluene	Acetonitrile	0.0000	0.0785	0.2319	0.6820	4.9335	12.5395	0.0212	-0.0075
Diethylamine	Triethylamine	0.0000	0.0372	0.0930	0.0812	2.0014	5.6325	0.0211	-0.0077
Chloroform	Tetrachloromethane	0.0000	0.0177	0.0393	0.0555	0.5090	1.1299	0.0188	-0.0069
Chloroform	Acetic Acid	0.0000	0.0596	0.2093	0.2278	10.2142	18.8320	0.0182	-0.0063
Tetrachloromethane	n-Ethyl Acetate	0.0000	0.0130	0.0690	0.4043	1.8574	2.8220	0.0165	-0.0052
Dichloromethane	n-Acetone	0.0000	0.0101	0.0263	0.7928	1.5916	2.7288	0.0128	-0.0008

Tetrachloromethane	Acetonitrile	0.0028	0.0948	0.1928	1.1799	6.4744	8.2922	0.0080	0.0024
		Absolute deviation in Concentration profile			Absolute deviation in Temperature profile			Average K_{ij}	Average L_{ij}
Compound1	Compound2	minimum	average	maximum	minimum	Compound1	Compound2	minimum	average
Acetic Acid	Propionic acid	0.0000	0.0438	0.0813	0.0246	0.6523	3.1293	0.0078	0.0023
Acetic Acid	n-Ethyl Acetate	0.0021	0.0282	0.0496	0.0178	0.6066	1.6451	0.0072	0.0024
n-Ethyl Acetate	n-Acetone	0.0000	0.0060	0.0251	0.3655	0.8179	1.2739	0.0064	0.0028
n-Ethyl Acetate	Acetonitrile	0.0000	0.0190	0.0388	0.7842	2.4926	3.5976	0.0063	0.0028
n-Acetone	2-Butanone	0.0000	0.0150	0.0692	0.0293	0.5968	1.3606	0.0062	0.0026
Nitromethane	n-Benzene	0.0075	0.0624	0.1322	6.0240	8.1754	10.3129	0.0074	0.0013
Dimethylsulfoxide	n-Propanol	0.0009	0.0937	0.4596	0.0093	15.1177	38.7239	0.0078	0.0003
Methylcyclohexane	n-Hexane	0.0000	0.0097	0.0294	0.0126	0.2366	0.5233	0.0078	-0.0001
n-Pyridine	n-Heptane	0.0310	0.1566	0.2891	2.9203	11.4107	18.5175	0.0078	-0.0009
n-Pyridine	n-Toluene	0.0016	0.0138	0.0405	0.1172	0.9119	1.8653	0.0075	-0.0009
n-Pyridine	n-Aniline	0.0000	0.0514	0.2284	0.3529	6.0640	16.5571	0.0067	-0.0004
n-Pyridine	n-Methanol	0.0093	0.0799	0.2335	1.1185	9.5795	20.7686	0.0055	0.0006
n-Pyridine	Chloroform	0.0004	0.0312	0.1645	0.7233	4.6853	10.4323	0.0043	0.0018
n-Pyridine	Acetic Acid	0.0000	0.0741	0.1695	0.1383	3.4344	20.1637	0.0027	0.0054
n-Pyridine	3-Methylpyridine	0.0008	0.0152	0.0463	0.0853	1.5524	2.8483	0.0027	0.0053
n-Pyridine	2-Methylpyridine	0.0000	0.0278	0.1110	0.2516	2.3918	8.1993	0.0027	0.0053
n-cyclohexane	n-Cyclohexene	0.0002	0.0240	0.0490	0.0097	1.0897	2.6826	0.0027	0.0052
water	Triethylamine	0.0152	0.2756	0.6141	0.7686	12.9331	26.2163	-0.0014	0.0104
n,n-dimethylformamide	Water	0.0000	0.0644	0.4531	0.4233	5.6348	19.9250	-0.0038	0.0117
n-Propanol	Water	0.0000	0.1401	0.3033	0.3793	8.8522	11.9839	-0.0128	0.0164
Formic acid	Water	0.0000	0.0450	0.2092	0.0226	2.5383	6.2168	-0.0127	0.0164
Acetic Acid	Water	0.0000	0.0230	0.1239	0.0419	2.9124	11.8026	-0.0187	0.0196
Tetrahydrofuran	Water	0.0000	0.3313	0.6512	0.7047	21.1229	32.0306	-0.0212	0.0189
n-Acetone	Water	0.0000	0.1548	0.6021	0.4670	12.4173	25.6447	-0.0227	0.0183

2-Butanone	Water	0.0000	0.1667	0.4954	0.3010	9.7188	23.7671	-0.0242	0.0171
		Absolute deviation in Concentration profile			Absolute deviation in Temperature profile			Average K_{ij} minimum	Average L_{ij} average
Compound1	Compound2	minimum	average	maximum	minimum	Compound1	Compound2		
Acetonitrile	Water	0.0000	0.0979	0.3726	0.7378	6.7935	16.2104	-0.0245	0.0166
Dimethylsulfoxide	Water	0.0000	0.1767	0.7282	0.7393	20.3717	66.8930	-0.0273	0.0169
Isoprene	2-methyl-2-butene	0.0000	0.0936	0.1727	2.6944	12.1448	22.6011	-0.0308	0.0170

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S4. Literature sources of Excess molar Enthalpy and isobaric Vapor-Liquid Equilibrium

The experimental excess molar enthalpy and isobaric Vapor-Liquid Equilibria used in the main manuscript and the references thereof are listed below;

Table S6: Overview of collected binary systems, the excess molar enthalpy and isobaric vapor-liquid equilibrium (VLE) thereof and the corresponding references.

Compound 1	Compound 2	Excess Molar Enthalpy	Isobaric VLE
		(references)	
Ethanol	Acetone	16	17-23
Ethanol	Acetic acid	24-26	27-28
Ethanol	Dipropylamine	n.a.	29
Methanol	Dipropylamine	n.a.	29
Methanol	n-Butylamine	30-35	36
Methanol	tert-Butylamine	34	37
Methanol	Diethylamine	30	36, 38-39
Methanol	Triethylamine	30, 40-41	36
Ethanol	Diethylamine	42	43
n-Propanol	n-Propylamine	44	45
n-Propanol	Dipropylamine	n.a.	45
2-Propanol	Dipropylamine	n.a.	29
Methanol	n,n-Dimethylformamide	46-50	51
Ethanol	n,n-Dimethylformamide	46, 49-50, 52-53	54-55
n-Propanol	n,n-Dimethylformamide	49-50, 56	57
2-Propanol	n,n-Dimethylacetamide	50, 56	58
Methanol	Dichloromethane	59	60-61
Ethanol	Dichloromethane	n.a.	62-63
Methanol	Chloroform	59, 64-66	67-69
Ethanol	Chloroform	64, 70	19, 71-73
n-Propanol	Chloroform	64, 66, 74-75	76
2-Propanol	Chloroform	74	77
Methanol	Tetrachloromethane	59, 78-82	83-84
Ethanol	Tetrachloromethane	40, 79, 85-89	90-91
n-Propanol	Tetrachloromethane	79, 92	93-97
2-Propanol	Tetrachloromethane	89, 92, 98-99	100-103
Methanol	Acetic acid	24, 81, 104	27, 105
Methanol	Propionic acid	24	106
Ethanol	Propionic acid	24	106
n-Propanol	Acetic acid	24, 107	27, 108
n-Propanol	Propionic acid	24	106, 109
2-Propanol	Acetic acid	n.a.	108
2-Propanol	Propionic acid	n.a.	106
Methanol	Methyl Formate	110-111	112
Methanol	Methyl Acetate	113-116	117-124
Methanol	Ethyl Acetate	125-126	67, 127-132
Methanol	Propyl Acetate	133	134-135
Methanol	Butyl Acetate	136-139	140-141
Ethanol	Ethyl Formate	110, 142-143	144
Ethanol	Propyl Formate	110	145
Ethanol	Butyl Formate	110	146

Compound 1	Compound 2	Excess Molar Enthalpy	Isobaric VLE
		(references)	
Ethanol	Methyl Acetate	115-116, 147	118, 148-151
Ethanol	Ethyl Acetate	25, 126	17, 119-120, 129, 132, 152-164
Ethanol	Propyl Acetate	165	166-167
Ethanol	Butyl Acetate	139, 168	146, 169
Methanol	n-Pentane	n.a.	170
Methanol	n-Heptane	n.a.	171-172
Methanol	n-Octane	n.a.	172
Ethanol	n-Hexane	87, 173-174	175-176
Ethanol	n-Heptane	70, 173, 177-178	179-181
Ethanol	n-Octane	177-178, 182	183-184
Methanol	Benzene	78, 185-188	121, 172, 189-198
Methanol	Toluene	185, 187, 199-200	172, 201-205
Methanol	p-Xylene	206	172
Methanol	m-Xylene	207	172
Methanol	o-Xylene	207	208
Ethanol	Benzene	85, 87, 165, 186-187, 199, 209-214	190, 195, 215-220
Ethanol	Toluene	187, 221	216, 222-225
Ethanol	p-Xylene	n.a.	226-227
Ethanol	o-Xylene	207	208
Methanol	Diethyl ether	64, 228-229	230
Methanol	Tetrahydrofuran	231-232	233
Ethanol	Diethyl ether	229, 234-235	236-237
Ethanol	Diisopropyl ether	238-239	240-241
Ethanol	Dipropyl ether	242	n.a.
Ethanol	Tetrahydrofuran	243	223, 244-245
Methanol	Acetone	65, 246-247	17, 22, 68, 248-268
Methanol	2-Butanone	115, 269-270	271-273
Methanol	2-Pentanone	274	271
Ethanol	2-Butanone	242, 269-270	18, 275-277
Ethanol	2-Pentanone	274	18
Methanol	Acetonitrile	278	279-281
Methanol	Propionitrile	n.a.	279
Methanol	Butyronitrile	282	279
Ethanol	Acetonitrile	283-285	279
Ethanol	Propionitrile	n.a.	279
Ethanol	Butyronitrile	286-287	279
Methanol	Ethanol	288	22, 118, 289-292
Methanol	n-Propanol	288, 293	262, 294-298
Methanol	2-Propanol	299-300	37, 257, 262, 295, 301-305
Methanol	n-Butanol	188	140, 271, 296, 306
Ethanol	n-Propanol	182, 288	295
Ethanol	2-Propanol	300, 307-308	302, 309-310
Ethanol	n-Butanol	311	18, 312-314
Ethanol	2-Butanol	n.a.	18
Butylamine	n-Hexane	315-316	317
Butylamine	p-Xylene	318	319
Butylamine	Ethylbenzene	320	319

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Compound 1	Compound 2	Excess Molar Enthalpy	Isobaric VLE
		(references)	
n-Hexane	n-Heptane	321	322
n-Hexane	Benzene	212, 323-333	326, 334-340
n-Hexane	Toluene	325, 341-343	334, 339, 344-346
n-Hexane	p-Xylene	347	339
n-Hexane	m-Xylene	347-348	349
n-Hexane	o-Xylene	347, 350	349
n-Hexane	n,n-Dimethylformamide	351	352
n-Heptane	n,n-Dimethylformamide	353	354
n-Hexane	Dichloromethane	355	356
n-Hexane	Chloroform	355, 357-358	359
n-Hexane	Tetrachloromethane	355, 360-365	366
n-Heptane	Chloroform	70, 355, 358, 367-369	370
n-Heptane	Tetrachloromethane	173, 355, 360, 363, 365, 367, 371-372	366
n-Heptane	Propionic acid	373-376	377
n-Octane	Acetic acid	n.a.	378
n-Octane	Propionic acid	379	380-381
n-Octane	Butyric acid	n.a.	382
n-Octane	isoButyric acid	n.a.	382
n-Hexane	Methyl Formate	383-384	384
n-Hexane	Ethyl Formate	373, 384-386	384, 386
n-Hexane	Propyl Formate	383-384	384
n-Hexane	Butyl Formate	383-384	384
n-Hexane	Diethyl ether	n.a.	230, 346
n-Hexane	Tetrahydrofuran	387-391	346, 392
n-Heptane	Diisopropyl ether	393-397	398
n-Heptane	Tetrahydrofuran	390, 399-401	402
n-Hexane	Acetone	403-405	176, 406-407
n-Hexane	2-Butanone	403, 408	409
n-Heptane	Acetone	410-413	414
n-Heptane	2-Butanone	369, 410, 415-417	409, 418
Benzene	Toluene	325, 419-428	429-439
Benzene	Ethylbenzene	440-441	432, 442
Toluene	Ethylbenzene	440-441	442
Benzene	n,n-Dimethylformamide	351, 443-444	51, 352, 445
Toluene	n,n-Dimethylformamide	351, 444, 446-447	354, 448-450
Benzene	Chloroform	64, 419, 451-454	67, 72, 370, 455-456
Benzene	Tetrachloromethane	64, 78, 419, 457-461	366, 462-467
Toluene	Chloroform	368, 452	468
Toluene	Tetrachloromethane	422, 452, 469-470	191, 366, 467
Benzene	Acetic acid	373, 376, 471	248, 472-476
Benzene	Propionic acid	376	477
Toluene	Acetic acid	419	478-481
Benzene	Methyl acetate	482-483	67, 192, 484
Benzene	Ethyl acetate	64, 143, 483, 485-487	488-489
Benzene	Propyl acetate	n.a.	490

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Compound 1	Compound 2	Excess Molar Enthalpy	Isobaric VLE
		(references)	
Benzene	Butyl acetate	491	484, 492-493
Toluene	Methyl acetate	n.a.	494
Toluene	Ethyl acetate	487, 495	489, 496
Benzene	Diisopropyl ether	497-498	499
Toluene	Tetrahydrofuran	500-502	346, 503-505
Benzene	Acetone	411, 451, 506-509	95, 197, 456, 478, 510-511
Benzene	2-Butanone	408, 509	218, 418, 512-515
Toluene	Acetone	516-517	468
Toluene	2-Butanone	517-519	202, 418, 481, 520
Benzene	Acetonitrile	521-530	531-533
Toluene	Acetonitrile	516, 527, 534-536	531-534
Diethylamine	Dipropylamine	n.a.	537
Diethylamine	Diisopropylamine	n.a.	537
Diethylamine	Triethylamine	42, 538	539-540
Diethylamine	Chloroform	n.a.	541
Diisopropylamine	Chloroform	n.a.	537
Diethylamine	Ethyl acetate	n.a	542
Methylamine	n,n-Dimethylamine	n.a	543
n-Methylformamide	n-Methylacetamide	n.a	544
n,n-Dimethylformamide	Chloroform	n.a	545
n,n-Dimethylformamide	Acetic acid	n.a	546
n-Methylacetamide	Acetic acid	n.a	547
n,n-Dimethylacetamide	Acetic acid	548	549
n,n-Dimethylformamide	Methyl formate	n.a	550
n,n-Dimethylformamide	Ethyl acetate	551	55
n,n-Dimethylformamide	Dipropyl ether	n.a	57
n,n-Dimethylacetamide	Diisopropyl ether	n.a	58
n,n-Dimethylformamide	Acetone	47	54, 354, 552
n,n-Dimethylformamide	2-Butanone	553	450, 552
n,n-Dimethylacetamide	Acetone	n.a.	554
Dichloromethane	Chloroform	555	556
Dichloromethane	Tetrachloromethane	528, 555, 557-558	556, 559
Chloroform	Tetrachloromethane	64, 485, 555, 557	556
Dichloromethane	Acetic acid	n.a.	560
Dichloromethane	Butyric acid	n.a.	560
Chloroform	Acetic acid	561-563	564-565
Tetrachloromethane	Acetic acid	566	567
Tetrachloromethane	Propionic acid	n.a.	568-569
Dichloromethane	Ethyl acetate	570	571
Chloroform	Methyl acetate	572	67
Tetrachloromethane	Methyl acetate	570	492, 573
Tetrachloromethane	Ethyl acetate	570, 574-575	573
Chloroform	Dipropyl ether	576-578	579
Chloroform	Diisopropyl ether	576-578	580
Dichloromethane	Acetone	581-583	62, 584
Dichloromethane	2-Butanone	n.a.	585
Chloroform	Acetone	64-65, 411, 453, 586-593	23, 359, 456, 594-599
Tetrachloromethane	Acetonitrile	521, 524, 528, 530	531

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Compound 1	Compound 2	Excess Molar Enthalpy	Isobaric VLE
		(references)	
Acetic acid	Propionic acid	600-601	602-604
Propionic acid	Butyric acid	601	605
Acetic acid	Methyl acetate	373	105, 606-607
Acetic acid	Ethyl acetate	25, 608	156
Acetic acid	Propyl acetate	107	607
Acetic acid	Butyl acetate	609	610-612
Acetic acid	Diethyl ether	n.a.	613
Acetic acid	Dipropyl ether	n.a.	614
Acetic acid	Diisopropyl ether	n.a.	614
Acetic acid	Acetone	n.a.	478, 615-616
Acetic acid	2-Butanone	617	618-620
Acetic acid	Methyl isobutyl ketone	n.a.	478, 621
Methyl acetate	Ethyl Acetate	n.a.	150, 622
Methyl acetate	Butyl Acetate	n.a.	140
Ethyl acetate	Diisopropyl ether	n.a.	240, 623
Propyl acetate	Diisopropyl ether	n.a.	240
Propyl acetate	Dibutyl ether	n.a.	624
Methyl acetate	Acetone	n.a.	492
Methyl acetate	2-Butanone	n.a.	625-626
Ethyl acetate	Acetone	64, 627	407, 628-629
Methyl acetate	Acetonitrile	630	631
Ethyl acetate	Acetonitrile	630-631	632
Propyl acetate	Acetonitrile	631	631
Diethyl ether	tetrahydrofuran	231	346, 504
Dipropyl ether	Diisopropyl ether	n.a.	633
Diisopropyl ether	Dibutyl ether	n.a.	634
Diethyl ether	Acetone	64, 635	230, 636
Dipropyl ether	Acetone	n.a.	633
Diisopropyl ether	Acetone	n.a.	633
Acetone	2-Butanone	637	625-626, 638-639
Acetone	Methyl isobutyl ketone	n.a.	596
2-Butanone	Methyl isobutyl ketone	n.a.	640
Nitroethane	n-Heptane	n.a.	641
Nitropropane	n-Heptane	642	641
2-Nitropropane	n-Heptane	n.a.	641
2-Nitropropane	Benzene	521, 643-646	647
Nitromethane	Methanol	n.a.	648
Nitromethane	Ethanol	n.a.	43
Nitroethane	Methanol	n.a.	649
Nitroethane	Ethanol	n.a.	649
Nitromethane	Ethyl acetate	n.a.	650
Nitromethane	Propyl acetate	n.a.	650
Nitroethane	Ethyl acetate	n.a.	651
Nitroethane	Propyl acetate	n.a.	651
Dimethylsulfoxide	Ethylbenzene	652	653
Dimethylsulfoxide	n-Propanol	49, 654-656	657
Dimethylsulfoxide	Acetonitrile	658-660	661
Acetaldehyde	Benzene	662	478
Acetaldehyde	Toluene	n.a.	478
Butyraldehyde	Toluene	n.a.	663

Compound 1	Compound 2	Excess Molar Enthalpy	Isobaric VLE
		(references)	
Formaldehyde	Methanol	n.a.	664
Acetaldehyde	Methanol	n.a.	665
Acetaldehyde	Ethanol	n.a.	28, 666-667
Propaldehyde	Methanol	n.a.	260
Propaldehyde	Ethanol	n.a.	668
Propaldehyde	n-Propanol	n.a.	669
Propaldehyde	2-Methyl-1-propanol	n.a.	669
Acetaldehyde	Acetic acid	n.a.	28, 670-671
Acetaldehyde	Methyl formate	n.a.	672
Acetaldehyde	Methyl acetate	n.a.	673
Acetaldehyde	Diethyl ether	64	667
Acetaldehyde	Acetone	n.a.	674
Propaldehyde	Acetone	n.a.	675
Butyraldehyde	2-Butanone	n.a.	676
Thiophene	n-Heptane	677	678
Thiophene	n-Octane	677	679
3-Methylthiophene	n-Heptane	n.a.	680
Thiophene	Toluene	n.a.	449
3-Methylthiophene	Toluene	n.a.	680
Thiophene	n,n-Dimethylformamide	n.a.	445
Thiophene	n-Methylpyrrolidone	n.a.	445
Methylcyclohexane	n-Hexane	681-682	683
Methylcyclohexane	n-Heptane	682, 684-687	344, 688-690
Pyridine	n-Heptane	691-694	695
Pyridine	Cyclohexane	n.a.	696
Pyridine	Benzene	428, 440, 697-699	196, 700-701
Pyridine	Toluene	702-704	695, 701
2-Pyridine	Benzene	428, 699, 703, 705-707	708
Pyridine	Aniline	693, 709-710	711
Pyridine	Piperidine	712	713
Pyridine	n,n-Dimethylformamide	710	714
Pyridine	n,n-Dimethylacetamide	n.a.	715
Pyridine	Methanol	33, 48, 81, 716-717	648
Pyridine	Chloroform	563, 591, 718-720	721
Pyridine	Acetic acid	563, 691, 722-723	724-725
Pyridine	Ethyl acetate	n.a.	726-727
Pyridine	Propyl acetate	n.a.	726
Pyridine	Butyl acetate	n.a.	726
Pyridine	Acetone	n.a.	696
2-Pyridine	Acetonitrile	n.a.	728
Pyridine	3-methylpyridine	729	701, 730
Pyridine	2-methylpyridine	703, 729	701, 731
Aniline	Cyclohexylamine	n.a.	732
Triethylamine	Formic acid	n.a.	733
Triethylamine	Acetic acid	n.a.	734
Pyridine	Thiophene	n.a.	700-701, 735
Thiophene	Dimethyl sulfoxide	n.a.	735
Dimethyl sulfoxide	Pyridine	n.a.	735

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Compound 1	Compound 2	Excess Molar Enthalpy	Isobaric VLE
		(references)	
Water	Benzene	n.a.	736-737
Water	m-Xylene	n.a.	737
Water	Methylamine	n.a.	738
Water	Butylamine	n.a.	739
Water	Isobutylamine	n.a.	740
Water	Ethylamine	n.a.	741
Water	Propylamine	33	742
Water	Isopropylamine	n.a.	742-743
Water	Dimethylamine	744	738
Water	Diethylamine	745	739
Water	Trimethylamine	746	738
Water	Triethylamine	747-748	749-750
Water	n,n-Dimethylformamide	548, 751-755	54, 756-760
Water	n-Methylformamide	n.a.	544
Water	N,n-Dimethylacetamide	548, 744, 761	549, 762-763
Water	Methanol	n.a.	118, 129, 159, 219, 255, 291, 294, 301, 688, 764-776
Water	Ethanol	777-778	118, 129, 291, 309, 568, 688, 767, 771, 779-796
Water	n-Propanol	777, 797	17, 73, 132, 215, 294, 798-805
Water	2-Propanol	n.a.	257, 294, 301, 312, 736, 773, 806-818
Water	Dichloromethane	n.a.	819
Water	1,2-Dichloroethane	n.a.	820
Water	Formic acid	821-823	564, 824-833
Water	Acetic acid	609, 823, 834-839	156, 564, 610, 613, 615, 618, 620, 670, 828-830, 833, 840-855
Water	Propionic acid	856	380, 478, 828, 830, 833, 857-861
Water	Butyric acid	n.a.	859, 862
Water	Methyl formate	n.a.	863
Water	Methyl acetate	864	118, 123, 151, 865
Water	Ethyl acetate	864	159-160, 866-870
Water	Diethyl ether	871	613
Water	Diisopropyl ether	n.a.	614, 872
Water	Tetrahydrofuran	873-879	392, 880-886
Water	Acetone	246, 410, 506, 635, 887-889	17, 255, 257, 294, 594, 615, 638, 766, 808, 814, 890-894
Water	2-Butanone	889, 895-897	515, 638, 766, 866, 898-903
Water	Methyl isobutyl ketone	n.a.	904
Water	Acetonitrile	905	661, 906-913
Water	Propionitrile	897	909
Water	Dimethylsulfoxide	635, 914-917	661
Water	Formaldehyde	n.a.	918-921
Water	Acetaldehyde	922	667, 923
Water	Propaldehyde	922	669
water	Butyraldehyde	922	924
water	Pyridine	925	196, 926-928

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