Supporting Information

Phase behaviour of binary mixtures containing succinic acid or its esters

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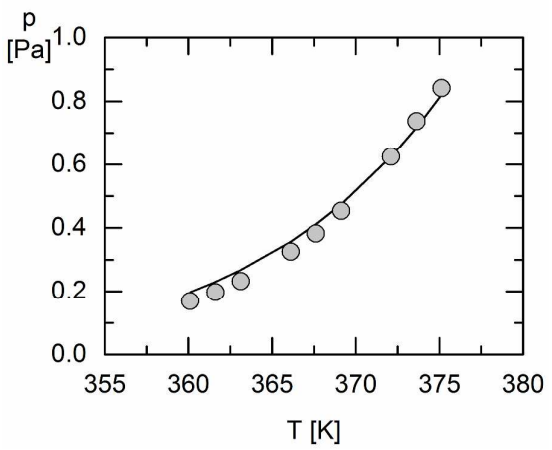

Figure S1. Sublimation pressures of SA. The circles are experimental data [1], line was modeled with PC-SAFT using the parameters from Table 2.

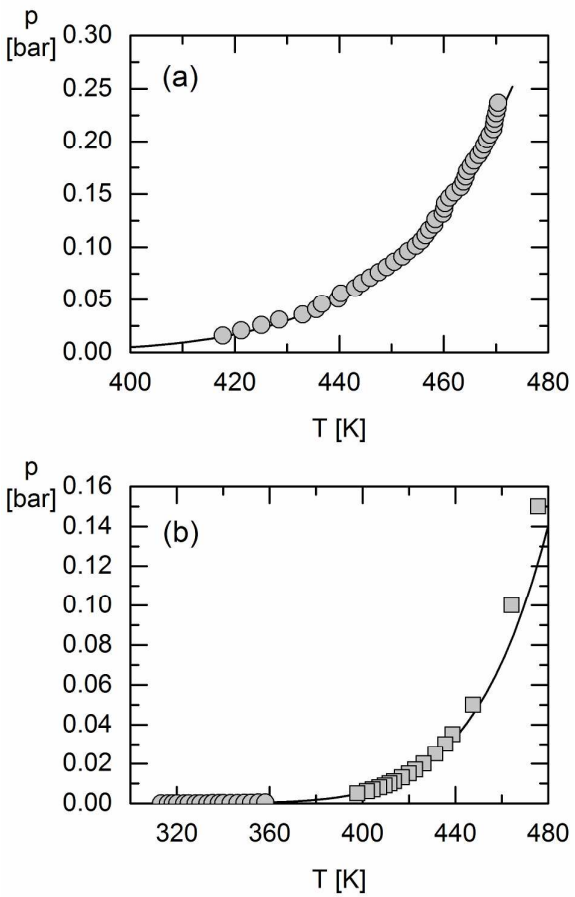

Figure S2. Vapor pressures of MES (a) [2] and of DBS (b) [3] (circles) and [4] (squares). Lines represent modeling results with PC-SAFT, using parameters from Table 2.

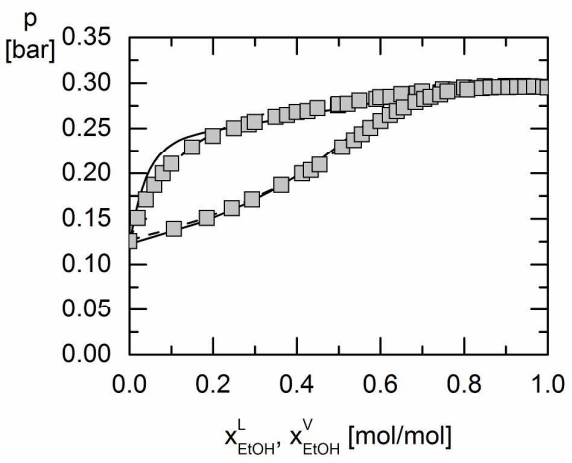

Figure S3. Isothermal VLE of the binary mixture EtOH and water at 323.15 K. Squares are experimental data retrieved from Kurihara et al. [5]. Solid line represents PC-SAFT calculation with the 2B association scheme for water with a binary interaction parameter of k_{ij} = -0.0382 [6] (ARD of 2.60 %). Dashed line represents PC-SAFT calculation with the 4C association scheme for water with a k_{ij} = 0.028 fitted in this work (ARD of 1.75 %).

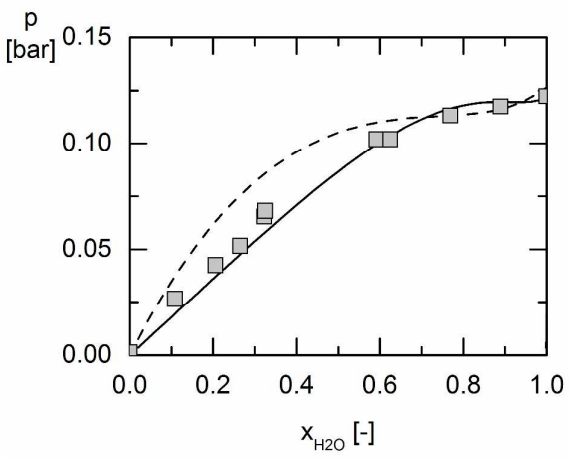

Figure S4. Isothermal VLE of the binary mixture MES and water at 323.15 K. Squares experimental data from [2]. Solid line represents PC-SAFT calculation with the 2B association scheme for water with a binary interaction parameter of k_{ij} = -0.066 (ARD of 9.62 %). Dashed line represents PC-SAFT calculation with the 4C association scheme for water with a k_{ij} = 0.015 (ARD of 21.93 %). Both k_{ij} are fitted in this work.

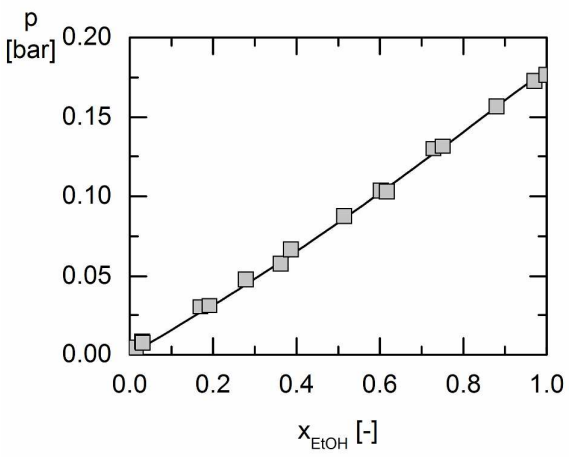

Figure S5. Isothermal VLE of the binary mixture MES and EtOH at 313.15 K. Squares experimental data from [2]. Line is PC-SAFT calculation with a binary interaction parameter of k_{ij} = -0.01 fitted in this work (ARD of 2.97 %).

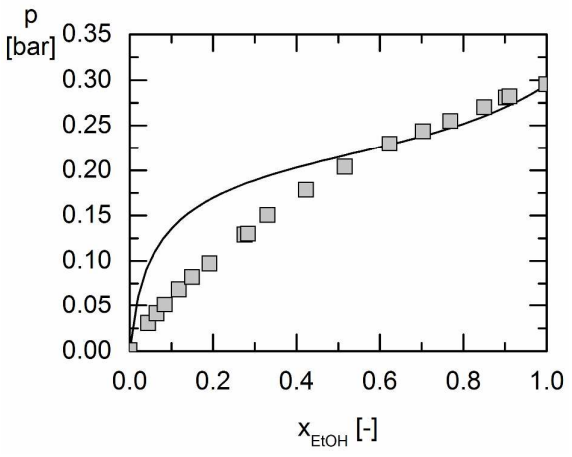

Figure S6. Isothermal VLE of the binary mixture DES and EtOH at 323.15 K. Squares experimental data from [7]. Line is PC-SAFT calculation with a binary interaction parameter of k_{ij} = 0 (ARD of 48.37 %).

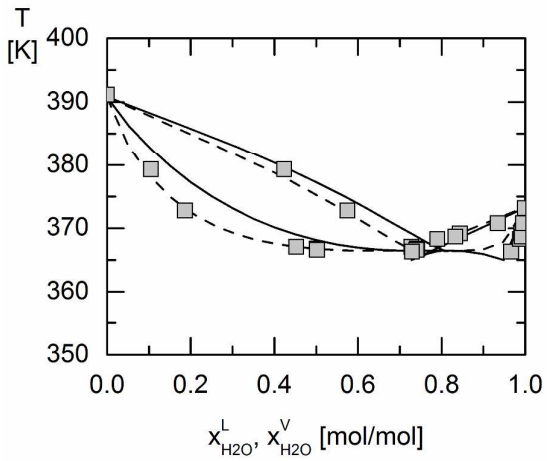

Figure S7. Isobaric VLE of the binary mixture 1-BuOH and water at 101.325 kPa. Squares represent experimental data retrieved from [8]. Solid line represents PC-SAFT calculation with the 2B association scheme for water with a temperature-dependent k_{ij} from [9]. Dashed line represents PC-SAFT calculation with the 4C associtaion scheme for water with a k_{ij} = 0.09 fitted in this work (ARD of 0.34 %).

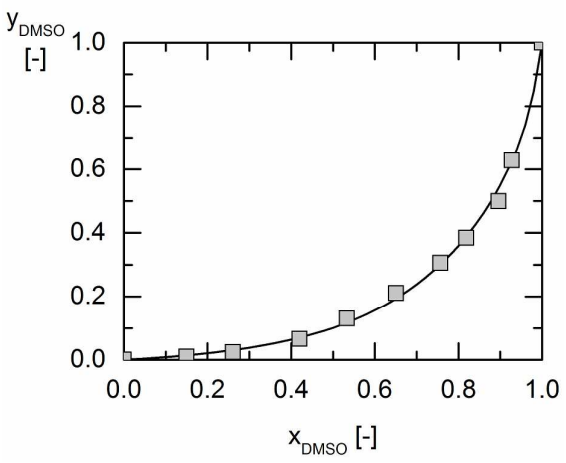

Figure S8. Isothermal VLE of the binary mixture DMSO and 1-BuOH at 393.35 K. Squares represent experimental data from [10]. Line represents PC-SAFT calculation with a binary interaction parameter of k_{ij} = -0.075 fitted in this work (ARD of 13.20 %).

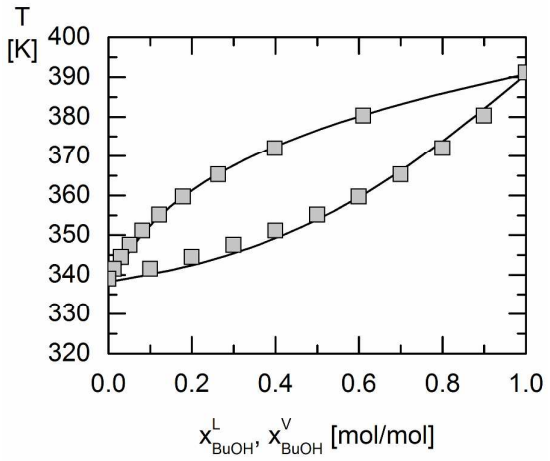

Figure S9. Isothermal VLE of the binary mixture 1-BuOH and THF at 101.325 kPa. Squares experimental data from [11]. Line represents PC-SAFT calculation with a binary interaction parameter of k_{ij} = -0.03 fitted in this work (ARD of 0.37 %).

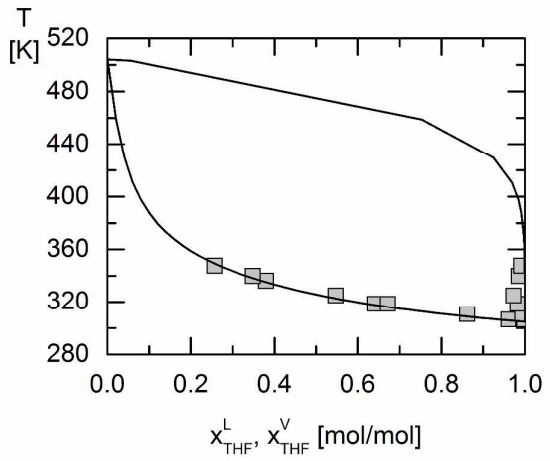

Figure S10. VLE of THF with DBS at 30 kPa, measured in this work (squares). The line was modeled with PC-SAFT with a k_{ij} = 0, resulting in an ARD of 0.46%. The measured data are summarized in table S 1.

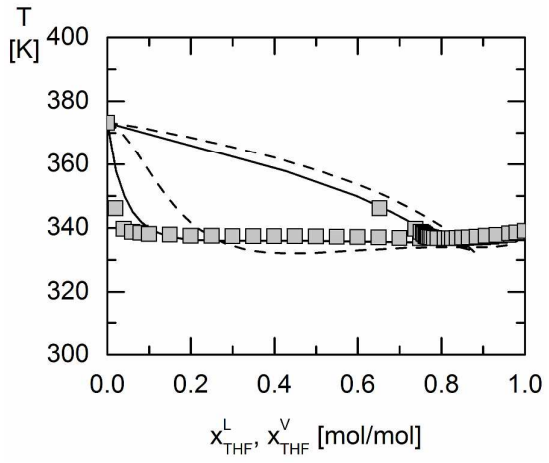

Figure S11. Isobaric VLE of the binary mixture THF and water at 101.325 kPa. Squares are experimental data retrieved from [12]. Solid line represents PC-SAFT calculation with the 2B asspciatoin scheme for water with a binary interaction parameter of k_{ij} = -0.05 (ARD of 0.64 %). Dashed line represents PC-SAFT calculation with the 4C association scheme for water with a k_{ij} = -0.04 (ARD of 2.01 %). Both k_{ij} were fitted in this work.

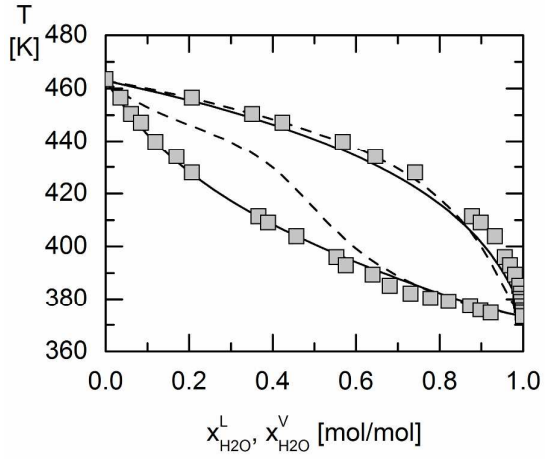

Figure S12. Isobaric VLE of the binary mixture DMSO and water at 101.325 kPa. Squares are experimental data retrieved from [13]. Solid line represents PC-SAFT calculation with the 2B association scheme for water with a temperature-dependent k_{ij} = -0.002212*T+0.75658 (T in Kelvin) (ARD of 0.44 %) Dashed line represents PC-SAFT calculation with the 4C association scheme for water with a k_{ij} = -0.00526473*T+1.970738 (T in Kelvin) (ARD of 1.89 %). Both k_{ij} were fitted in this work.

Table S1. Isobaric VLE of THF with DBS at 30 kPa measured in this work. Standard uncertainties are u(T) = (0.15 + 0.002 (T − 273.15)) K, u(x) = 0.0173. Superscript L=liquid phase, V=vapor phase.

T [K]	x_{THF}^{L}	x_{THF}^{V}
306.35	0.9613	0.9987
310.55	0.8622	0.9945
318.45	0.6409	0.9975
318.45	0.6718	0.9827
324.85	0.5477	0.9733
339.65	0.3484	0.9855
347.35	0.2577	0.9916

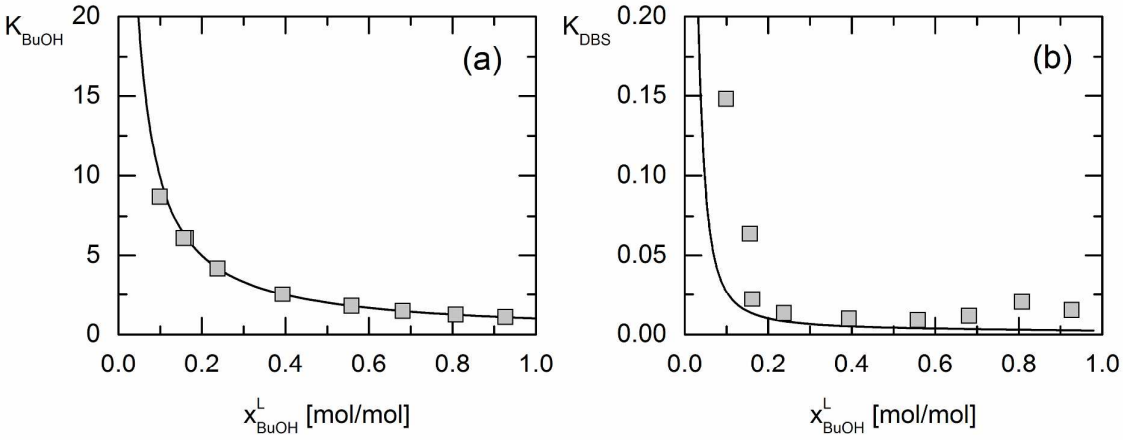

Figure S13. Binary isobaric VLE of 1-BuOH and DBS at 20 kPa. (a) KBuOH (b) KDBS. The K value in a binary mixture of a component i is defined as $K_i = y_i/x_i$. y_i is the mole fraction of i in the vapor phase and x_i in the liquid phase. Squares: experimental data (see Table 5), lines modeled with PC-SAFT with parameters summarized in Table 2 and 8. This experimental VLE is shown exemplarily and findings account similarly for all other binary VLE that were measured in this work and are not shown here explicitly.

Table S2. Summary over all binary interaction parameters that were fitted in this work. Average relative deviations (ARD) between calculated and experimental data are given as well as reference of experimental data. Note, that these binary interaction parameters are valid with the pure-component parameters in Table 2.

Substance i	Substance j	k_{ij}	ARD	Data Ref.
SLE				
SA	Water (2B)	$k_{ij} = -0.0002 \cdot T + 0.0126$	4.61 %	14, 15
	Water (4C)	$k_{ij} = -0.00055 \cdot T + 0.1068$	10.87 %	
SA	EtOH	$k_{ij} = 0.000047 \cdot T - 0.1774$	4.90 %	14
SA	1-BuOH	$k_{ij} = -0.105$	6.68 %	16
SA	ACN	$k_{ij} = 0.000643 \cdot T - 0.2208$	3.81 %	17
LLE				
DES	Water (2B)	$k_{ij} = 0.00025974 \cdot T - 0.14351$	2.52 %	18
	Water (4C)	$k_{ij} = 0.05$	45.84 %	
	Water (4C) with additional k_{ij}^{ws}	$k_{ij} = 0.05$ *and* $k_{ij}^{ws} = -0.5$	2.41 %	
DBS	Water (2B)	$k_{ij} = 0.000625 \cdot T - 0.23072$	4.66 %	This work
	Water (4C)	$k_{ij} = 0.05$	37.09 %	
	Water (4C) with additional k_{ij}^{ws}	$k_{ij} = 0.05$ *and* $k_{ij}^{ws} = -0.25$	11.33 %	
VLE				
ACN	DES	0.01	0.98 %	This work
ACN	1-BuOH	0	0.61 %	19
ACN	Water (2B)	-0.036	0.83 %	13
	Water (4C)	-0.03	1.23 %	
ACN	DBS	0	1.24 %	This work
1-BuOH	DBS	-0.015	1.88 %	This work
EtOH	Water (4C)	0.028	1.75 %	5
MES	Water (2BT)	-0.066	9.62 %	2
	Water (4C)	0.015	21.93 %	
MES	EtOH	-0.01	2.97 %	2
DES	EtOH	0	48.37 %	7
1-BuOH	Water (4C)	0.09	0.34 %	8
1-BuOH	DMSO	-0.075	13.2 %	10
1-BuOH	THF	-0.03	0.37 %	11
THF	DBS	0	0.46 %	This work
THF	Water (2BT)	-0.05	0.64 %	12
	Water (4C)	-0.04	2.01 %	
DMSO	Water (2BT)	$k_{ij} = -0.002212 \cdot T + 0.75658$	0.44 %	13
	Water (4C)	$k_{ij} = -0.00526473 \cdot T + 1.970738$	1.89 %	

Table S3. LLE of binary water/DBS mixture at different temperatures and atmospheric pressure. Standard uncertainty of temperature: u(T) = (0.15 + 0.002 (T − 273.15)) K. u(x) = 0.021.

T [K]	x_{H2O}^{aq}	x_{H2O}^{org}
313.15	0.9989	0.1045
323.15	0.9991	0.1144
333.15	0.9995	0.1074
353.15	0.9972	0.1432

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