Supporting Information

Investigation of Molecular Interactions in Binary Mixtures of *n*-Butyl acetate and (C_6 −C_{10}) 1-Alkanol: PC-SAFT Model

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Table S1: Excess molar volumes, V_m^E and viscosity deviations $\Delta\eta$ for binary mixtures as a mole fraction x_1 of *n*-Butyl acetate [a]

n-Butyl acetate + 1-Hexanol							
V_m^E /($cm^3 \cdot mol^{-1}$)							
x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0811	0.065	0.084	0.109	0.128	0.159	0.181	0.213
0.1602	0.113	0.142	0.183	0.217	0.282	0.316	0.366
0.2398	0.151	0.183	0.239	0.284	0.373	0.418	0.484
0.3507	0.187	0.225	0.289	0.352	0.458	0.511	0.601
0.4402	0.202	0.241	0.308	0.381	0.493	0.553	0.643
0.5596	0.198	0.237	0.301	0.376	0.484	0.545	0.635
0.6504	0.181	0.219	0.284	0.346	0.443	0.507	0.589
0.7398	0.153	0.185	0.248	0.293	0.378	0.437	0.493
0.8507	0.099	0.122	0.175	0.208	0.257	0.300	0.341
0.9397	0.051	0.061	0.089	0.106	0.137	0.153	0.165
$\Delta\eta$ /(mPa·s)							
0.0811	-0.295	-0.281	-0.261	-0.233	-0.221	-0.197	-0.161
0.1602	-0.492	-0.461	-0.416	-0.382	-0.361	-0.324	-0.272
0.2398	-0.621	-0.583	-0.531	-0.487	-0.447	-0.407	-0.347
0.3507	-0.702	-0.651	-0.601	-0.553	-0.502	-0.449	-0.389
0.4402	-0.695	-0.643	-0.586	-0.547	-0.485	-0.439	-0.386
0.5596	-0.616	-0.574	-0.524	-0.491	-0.424	-0.374	-0.334
0.6504	-0.512	-0.481	-0.441	-0.409	-0.346	-0.301	-0.274
0.7398	-0.392	-0.369	-0.343	-0.316	-0.256	-0.215	-0.197
0.8507	-0.221	-0.208	-0.197	-0.181	-0.141	-0.118	-0.105
0.9397	-0.087	-0.081	-0.072	-0.068	-0.057	-0.042	-0.034

Table S1: Continued

n -Butyl acetate + 1-Heptanol							
V_m^E /($cm^3 \cdot mol^{-1}$)							
x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0819	0.075	0.095	0.121	0.141	0.181	0.205	0.239
0.1604	0.134	0.159	0.205	0.241	0.318	0.366	0.407
0.2399	0.181	0.208	0.267	0.315	0.417	0.485	0.545
0.3497	0.217	0.256	0.324	0.387	0.499	0.593	0.665
0.4399	0.234	0.273	0.342	0.415	0.546	0.638	0.716
0.5743	0.227	0.268	0.334	0.407	0.535	0.624	0.699
0.6496	0.209	0.249	0.318	0.379	0.504	0.581	0.651
0.7391	0.176	0.208	0.274	0.323	0.435	0.501	0.564
0.8491	0.118	0.139	0.193	0.224	0.301	0.346	0.391
0.9385	0.059	0.071	0.104	0.121	0.163	0.174	0.198
$\Delta\eta$ /(mPa·s)							
0.0819	-0.343	-0.321	-0.301	-0.274	-0.258	-0.236	-0.206
0.1604	-0.557	-0.527	-0.489	-0.445	-0.416	-0.377	-0.336
0.2399	-0.708	-0.672	-0.629	-0.569	-0.524	-0.482	-0.432
0.3497	-0.793	-0.763	-0.708	-0.648	-0.589	-0.536	-0.484
0.4399	-0.788	-0.755	-0.698	-0.641	-0.577	-0.529	-0.479
0.5743	-0.689	-0.661	-0.612	-0.561	-0.491	-0.441	-0.407
0.6496	-0.595	-0.569	-0.521	-0.476	-0.421	-0.369	-0.341
0.7391	-0.456	-0.433	-0.401	-0.365	-0.311	-0.274	-0.255
0.8491	-0.269	-0.249	-0.228	-0.205	-0.173	-0.147	-0.133
0.9385	-0.109	-0.098	-0.087	-0.081	-0.067	-0.057	-0.046

n -Butyl acetate + 1-Octanol							
V_m^E /($cm^3 \cdot mol^{-1}$)							
x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0809	0.084	0.106	0.134	0.152	0.201	0.231	0.261
0.1595	0.148	0.177	0.231	0.253	0.344	0.398	0.446
0.2399	0.202	0.234	0.296	0.332	0.455	0.531	0.593
0.3499	0.247	0.286	0.353	0.407	0.561	0.645	0.732
0.4399	0.265	0.305	0.376	0.443	0.598	0.692	0.789
0.5626	0.261	0.298	0.372	0.439	0.587	0.677	0.778
0.6499	0.241	0.275	0.348	0.413	0.543	0.633	0.714
0.7401	0.203	0.232	0.303	0.352	0.465	0.541	0.614
0.8499	0.135	0.157	0.215	0.241	0.326	0.375	0.422
0.9395	0.068	0.079	0.114	0.133	0.181	0.192	0.217
$\Delta\eta$ /(mPa·s)							
0.0809	-0.385	-0.368	-0.351	-0.315	-0.295	-0.264	-0.231
0.1595	-0.628	-0.607	-0.569	-0.509	-0.465	-0.421	-0.374
0.2399	-0.803	-0.762	-0.721	-0.656	-0.596	-0.533	-0.474
0.3499	-0.906	-0.87	-0.816	-0.746	-0.674	-0.597	-0.543
0.4399	-0.899	-0.861	-0.809	-0.739	-0.669	-0.587	-0.539
0.5626	-0.817	-0.787	-0.734	-0.653	-0.582	-0.518	-0.474
0.6499	-0.707	-0.674	-0.638	-0.546	-0.495	-0.431	-0.398
0.7401	-0.549	-0.523	-0.497	-0.421	-0.372	-0.331	-0.298
0.8499	-0.307	-0.289	-0.276	-0.231	-0.211	-0.191	-0.169
0.9395	-0.125	-0.109	-0.101	-0.091	-0.085	-0.073	-0.063

n -Butyl acetate + 1-Nonanol							
V_m^E /($cm^3 \cdot mol^{-1}$)							
x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0812	0.097	0.119	0.151	0.164	0.223	0.253	0.286
0.1601	0.167	0.196	0.244	0.274	0.381	0.431	0.495
0.2399	0.221	0.254	0.316	0.363	0.497	0.574	0.661
0.3499	0.271	0.309	0.381	0.444	0.604	0.716	0.803
0.4399	0.291	0.332	0.405	0.475	0.641	0.776	0.863
0.5599	0.288	0.327	0.397	0.465	0.633	0.762	0.843
0.6501	0.264	0.302	0.369	0.434	0.582	0.712	0.784
0.7399	0.224	0.258	0.321	0.375	0.503	0.616	0.667
0.8499	0.149	0.176	0.231	0.267	0.361	0.421	0.472
0.9452	0.071	0.085	0.121	0.136	0.193	0.205	0.238
$\Delta\eta$ /(mPa·s)							
0.0812	-0.457	-0.409	-0.387	-0.343	-0.321	-0.285	-0.252
0.1601	-0.748	-0.675	-0.629	-0.561	-0.531	-0.469	-0.416
0.2399	-0.964	-0.841	-0.795	-0.723	-0.667	-0.596	-0.527
0.3499	-1.080	-0.966	-0.905	-0.823	-0.753	-0.674	-0.602
0.4399	-1.065	-0.957	-0.889	-0.819	-0.748	-0.665	-0.598
0.5599	-0.971	-0.885	-0.816	-0.741	-0.656	-0.592	-0.541
0.6501	-0.823	-0.753	-0.701	-0.625	-0.546	-0.502	-0.457
0.7399	-0.623	-0.587	-0.541	-0.481	-0.412	-0.381	-0.349
0.8499	-0.361	-0.341	-0.317	-0.281	-0.234	-0.218	-0.202
0.9452	-0.141	-0.124	-0.116	-0.105	-0.087	-0.077	-0.071

n -Butyl acetate + 1-Decanol							
V_m^E /($cm^3 \cdot mol^{-1}$)							
x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0809	0.108	0.129	0.162	0.173	0.246	0.269	0.318
0.1599	0.187	0.215	0.272	0.293	0.416	0.473	0.561
0.2401	0.248	0.282	0.354	0.392	0.544	0.641	0.751
0.3499	0.302	0.344	0.419	0.477	0.644	0.799	0.916
0.4401	0.326	0.371	0.442	0.512	0.692	0.857	0.981
0.5598	0.322	0.364	0.435	0.497	0.684	0.845	0.971
0.6499	0.296	0.338	0.403	0.459	0.644	0.783	0.915
0.7401	0.249	0.286	0.351	0.396	0.561	0.677	0.776
0.8499	0.168	0.197	0.251	0.283	0.402	0.476	0.531
0.9399	0.084	0.101	0.139	0.158	0.226	0.253	0.284
$\Delta\eta$ /(mPa·s)							
0.0809	-0.515	-0.457	-0.412	-0.372	-0.346	-0.318	-0.281
0.1599	-0.826	-0.737	-0.682	-0.615	-0.565	-0.509	-0.455
0.2401	-1.066	-0.929	-0.859	-0.781	-0.715	-0.641	-0.586
0.3499	-1.216	-1.053	-0.973	-0.889	-0.806	-0.732	-0.673
0.4401	-1.211	-1.038	-0.964	-0.881	-0.795	-0.723	-0.669
0.5598	-1.091	-0.965	-0.895	-0.801	-0.724	-0.663	-0.609
0.6499	-0.908	-0.823	-0.763	-0.686	-0.604	-0.564	-0.522
0.7401	-0.691	-0.633	-0.604	-0.531	-0.469	-0.435	-0.402
0.8499	-0.402	-0.377	-0.356	-0.321	-0.276	-0.257	-0.238
0.9399	-0.171	-0.151	-0.141	-0.134	-0.113	-0.104	-0.094

[a]x_1 is the mole fraction of *n* -Butyl acetate in the (*n* -Butyl acetate + 1-alkanol) solutions. Standard uncertainties u are (T) = 0.02 K, u(x) = 0.001, u(p) = 10 kPa, the expanded uncertainty is $U(\rho)$ = 0.01 $g \cdot cm^{-3}$ for density and for viscosity the relative expanded uncertainty $U_r(\eta)$ = 0.05 (0.95 level of confidence).

Table S2: Parameters A_k and Standard Deviations σ, for Binary mixtures at various temperatures

		T/K =	A_0	A_1	A_2	σ
n-Butyl acetate + 1-Hexanol	V_m^E /($cm^3 \cdot mol^{-1}$)	293.15	0.807	0.035	0.033	0.003
		298.15	0.946	0.052	0.113	0.003
		303.15	1.228	0.007	0.316	0.003
		308.15	1.516	0.009	0.228	0.006
		313.15	1.946	0.053	0.235	0.008
		318.15	2.212	0.003	0.333	0.006
		323.15	2.581	0.06	0.262	0.006
	$\Delta\eta$ /(mPa·s)	293.15	-2.657	-1.383	-0.139	0.002
		298.15	-2.469	-1.284	-0.025	0.004
		303.15	-2.26	-1.15	-0.21	0.006
		308.15	-2.103	-1.04	-0.104	0.003
		313.15	-1.842	-1.132	-0.161	0.003
		318.15	-1.644	-1.095	-0.073	0.002
		323.15	-1.462	-0.871	-0.066	0.002
n -Butyl acetate + 1-Heptanol	V_m^E /($cm^3 \cdot mol^{-1}$)	293.15	0.935	0.057	0.063	0.003
		298.15	1.097	0.059	0.106	0.003
		303.15	1.371	0.018	0.338	0.005
		308.15	1.659	0.028	0.269	0.007
		313.15	2.178	0.016	0.417	0.008
		318.15	2.556	0.027	0.330	0.007
		323.15	2.861	0.026	0.425	0.008
	$\Delta\eta$ /(mPa·s)	293.15	-3.024	-1.496	-0.272	0.004
		298.15	-2.097	-1.439	-0.112	0.003
		303.15	-2.689	-1.368	-0.119	0.005
		308.15	-2.464	-1.245	-0.055	0.004
		313.15	-2.196	-1.266	-0.115	0.004
		318.15	-1.988	-1.224	-0.056	0.004
		323.15	-1.821	-1.062	-0.051	0.003

Table S2 Continued

		T/K =	A_0	A_1	A_2	σ
n -Butyl acetate + 1-Octanol	V_m^E /($cm^3 \cdot mol^{-1}$)	293.15	1.066	0.035	0.064	0.003
		298.15	1.217	0.070	0.155	0.003
		303.15	1.504	0.021	0.435	0.005
		308.15	1.773	0.026	0.318	0.008
		313.15	2.383	0.031	0.444	0.01
		318.15	2.765	0.049	0.454	0.008
		323.15	3.151	0.038	0.410	0.01
	$\Delta\eta$ /(mPa·s)	293.15	-3505	-1.58	-0.252	0.01
		298.15	-3.364	-1.54	-0.163	0.01
		303.15	-3.157	-1.437	-0.219	0.01
		308.15	-2.832	-1.445	-0.07	0.006
		313.15	-2.543	-1.343	-0.157	0.007
		318.15	-2.24	-1.213	-0.23	0.005
		323.15	-2.058	-1.072	-0.041	0.004
n -Butyl acetate + 1-Nonanol	V_m^E /($cm^3 \cdot mol^{-1}$)	293.15	1.167	0.043	0.112	0.003
		298.15	1.324	0.050	0.239	0.005
		303.15	1.605	0.031	0.497	0.009
		308.15	1.889	0.004	0.430	0.01
		313.15	2.551	0.036	0.655	0.01
		318.15	3.100	0.055	0.415	0.01
		323.15	3.431	0.048	0.620	0.01
	$\Delta\eta$ /(mPa·s)	293.15	-4.137	-1.975	-0.3	0.01
		298.15	-3.739	-1.622	-0.296	0.01
		303.15	-3.472	-1.56	-0.34	0.009
		308.15	-3.164	-1.451	-0.153	0.005
		313.15	-2.84	-1.526	-0.164	0.003
		318.15	-2.558	-1.289	-0.155	0.004
		323.15	-2.312	-1.086	-0.1	0.004

Table S2 Continued

		T/K =	A_0	A_1	A_2	σ
n -Butyl acetate + 1-Decanol	V_m^E /($cm^3 \cdot mol^{-1}$)	293.15	1.305	0.050	0.127	0.003
		298.15	1.478	0.045	0.238	0.005
		303.15	1.759	0.062	0.554	0.009
		308.15	2.022	0.027	0.441	0.01
		313.15	2.759	0.029	0.866	0.01
		318.15	3.430	0.077	0.488	0.02
		323.15	3.951	0.009	0.590	0.01
	$\Delta\eta$ /(mPa·s)	293.15	-4..651	-2.229	-0.189	0.01
		298.15	-4.064	-1.8	-0.437	0.01
		303.15	-3.744	-1.601	-0.412	0.01
		308.15	-3.414	-1.503	-0.35	0.004
		313.15	-3.073	-1.48	-0.314	0.006
		318.15	-2.81	-1.273	-0.277	0.008
		323.15	-2.598	-1.124	-0.14	0.005

TABLE S3: Parameters of the Pure Components Used PC-SAFT equation.

Components	m_i	σ_i/Å	ϵ_i/k	$k^{A_iB_i}$	$\varepsilon^{A_iB_i}/k$
n -Butyl acetate	3.93	3.56	241		
1-hexanol	3.54	3.63	263	0.0061	2542
1-heptanol	4.41	3.58	250	0.0013	2866
1-octanol	4.32	3.73	267	0.0022	2738
1-nonanol	4.64	3.76	262	0.0015	2952
1-decanol	5.72	3.87	268	0.0013	2910

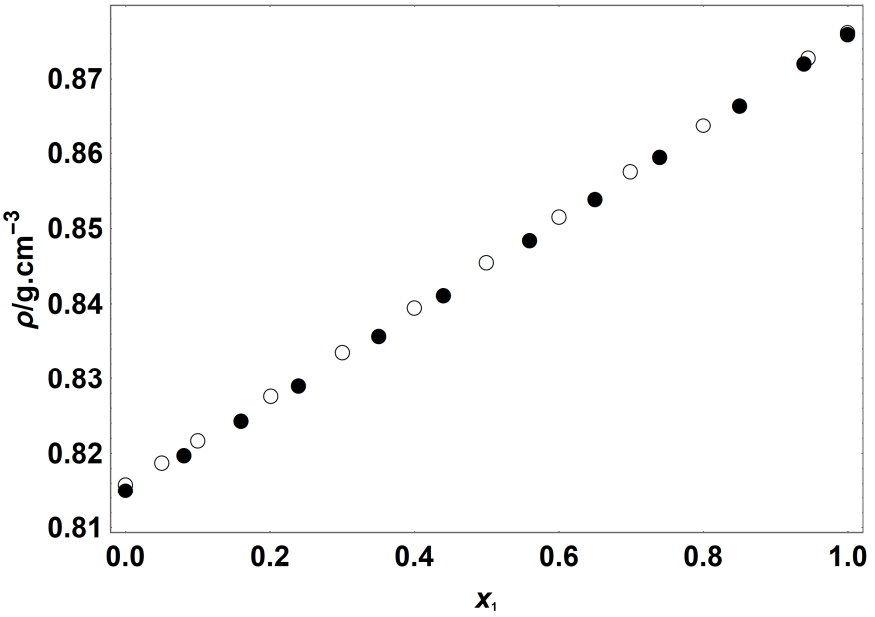

Fig. S1. Comparisons of our densities ρ (filled points) for *n* -Butyl acetate + 1-hexanol (●) and data of ref. 5 (empty points).

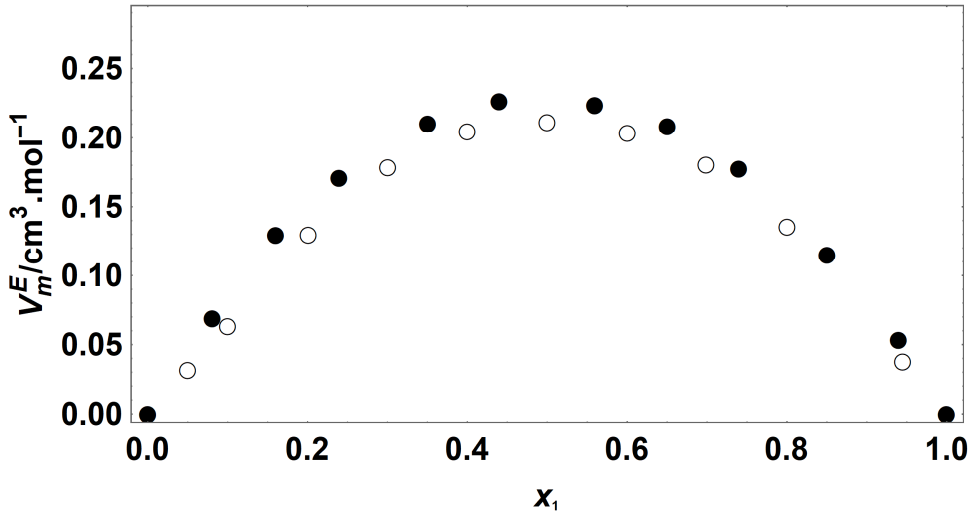

Fig. S2. Comparisons of our excess molar volumes V_m^E (filled points) for *n* -Butyl acetate + 1-hexanol (●) and data of ref. 5 (empty points).

REFERENCE

(1) Lee, H. K.; Park, S. Isothermal vapor-liquid equilibria, excess molar volume and the deviation of refractive indices for binary mixtures of 1-butanol, 1- hexanol, 3-methyl-1-butanol and butyl acetate, *Fluid Phase Equilib*. **2017**, *436*, 47–54.