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SUPPLEMENTARY MATERIAL TO

Densities and viscosities for binary mixtures of *n*-heptane with alcohols at different temperatures

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TABLE S-I. Comparison of experimental densities (ρ) and viscosities (η) of pure liquids with literature values at different temperature and atmospheric pressure; uncertainties, u, are: $u(x)$ = = ±0.0001; $u(T)$ = ±0.05 K; $u(\rho)$ = ±0.05 kg.m^{-3}; $u(t)$ = ±0.01s; $u(\eta)$ = ±0.001 mPa s

Component	T / K	ρ / kg m^{-3}		η / mPa s	
		Experimental	Literature	Experimental	Literature
n-Heptane	288.15	688.20	687.9[1]	0.4427	–
	293.15	684.30	683.9[2]	0.4197	0.4169[6]
	298.15	680.00	679.48[3]	0.3934	0.3900[5]
	303.15	675.70	675.1[4]	0.3774	0.3785[6]
	308.15	671.40	670.9[5]	0.3582	0.3470[7]
Ethanol	288.15	795.80	–	1.3652	–
	293.15	789.50	789.45[8]	1.2206	1.1988[11]
	298.15	785.70	785.0[9]	1.1088	1.1050[9]
	303.15	781.60	781.0[10]	1.0056	1.0102[12]
	308.15	777.00	776.7[10]	0.9222	0.9037[11]
n-Propanol	288.15	808.41	–	2.4915	–
	293.15	804.40	804.28[13]	2.2304	2.1970[13]
	298.15	800.71	800.21[13]	1.9885	1.9700[9]
	303.15	796.71	796.42[13]	1.7641	1.7843[14]
	308.15	792.90	792.27[13]	1.5540	1.5460[14]
iso-Propanol	288.15	791.20	–	2.7622	–
	293.15	787.11	785.35[13]	2.4064	2.4140[13]
	298.15	783.20	782.70[15]	2.0546	2.0436[16]
	303.15	778.91	777.12[13]	1.7908	1.7850[13]
	308.15	774.51	772.88[13]	1.5605	1.5510[17]

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TABLE S-II. Densities (ρ) and viscosities (η) of the (*n*-heptane + alcohols) mixtures at different temperatures and atmospheric pressure

x	ρ / kg m^{-3}					η / mPa s				
	T / K									
	288.15	293.15	298.15	303.15	308.15	288.15	293.15	298.15	303.15	308.15
	n-Heptane + ethanol									
0.1005	770.87	764.80	760.84	756.43	751.70	1.0803	0.9853	0.9069	0.8186	0.7535
0.2020	751.33	745.76	741.64	737.40	732.87	0.8992	0.8256	0.7656	0.6950	0.6432
0.3022	736.60	731.34	727.22	722.84	718.25	0.7824	0.7149	0.6673	0.6164	0.5695
0.4016	725.02	720.14	716.01	711.49	706.93	0.6870	0.6285	0.5856	0.5429	0.5077
0.5079	715.08	710.58	706.41	701.84	697.37	0.5992	0.5670	0.5214	0.4865	0.4521
0.5967	708.24	703.81	699.64	695.07	690.62	0.5510	0.5160	0.4815	0.4506	0.4271
0.7041	701.43	697.06	692.83	688.47	684.00	0.5002	0.4658	0.4422	0.4154	0.3957
0.8008	696.14	691.94	687.63	683.35	678.97	0.4629	0.4428	0.4149	0.3953	0.3691
0.8935	691.89	687.76	683.40	679.12	674.67	0.4485	0.4230	0.4021	0.3827	0.3633
	n-Heptane + propan-1-ol									
0.1020	785.75	781.54	777.40	773.16	769.05	1.8182	1.6409	1.4771	1.3187	1.1889
0.2018	767.57	763.40	759.30	754.91	750.70	1.4201	1.2906	1.1663	1.0466	0.9659
0.2990	752.27	748.15	744.01	739.72	735.47	1.1367	1.0521	0.9499	0.8669	0.7776
0.4005	738.89	734.60	730.49	726.12	721.85	0.9138	0.8426	0.7687	0.7025	0.6444
0.5017	727.19	722.99	718.84	714.35	710.15	0.7616	0.6995	0.6453	0.5949	0.5454
0.6033	716.75	712.60	708.40	704.04	699,76	0.6327	0.5899	0.5511	0.5056	0.4781
0.7025	708.19	704.08	699.87	695.47	691.09	0.5474	0.5126	0.4886	0.4543	0.4308
0.8010	700.67	696.47	692.26	687.94	683.53	0.4997	0.4793	0.4419	0.4254	0.3988
0.8918	694.39	690.34	686.11	681.70	677.38	0.4744	0.4475	0.4174	0.3943	0.3783
	n-Heptane + propan-2-ol									
0.1003	772.03	767.65	763.67	759.16	754.60	1.8249	1.5964	1.4129	1.2300	1.0913
0.2009	756.15	752.02	747.94	743.53	738.83	1.3311	1.1776	1.0444	0.9270	0.8401
0.3009	742.52	738.36	734.19	729.84	725.32	1.0146	0.9242	0.8165	0.7388	0.6728
0.3980	731.65	727.47	723.08	718.63	714.21	0.8246	0.7437	0.6851	0.6200	0.5770
0.5002	721.62	717.13	712.92	708.42	703.97	0.6801	0.6223	0.5866	0.5333	0.4915
0.5961	713.33	708.85	704.65	700.17	695.74	0.5870	0.5479	0.5025	0.4679	0.4441
0.6981	705.59	701.17	696.97	692.49	688.08	0.5243	0.4930	0.4623	0.4351	0.4083
0.8014	698.89	694.59	690.12	685.66	681.21	0.4845	0.4607	0.4268	0.4137	0.3805
0.9084	692.49	688.42	684.05	679.59	675.25	0.4559	0.4360	0.4025	0.3897	0.3637

TABLE S-III. Excess molar volumes (V^E / 10^{-6} m^3 mol^{-1}) of the *n*-heptane + alcohols mixtures at different temperatures and atmospheric pressure; uncertainties, u, are: $u(x) = \pm 0.0001$; $u(T) = \pm 0.05$ K; $u(V^E) = \pm 5.5\times10^{-8}$ m^3 mol^{-1}

x	T / K				
	288.15	293.15	298.15	303.15	308.15
	n-Heptane + ethanol				
0.0000	0.000	0.000	0.000	0.000	0.000
0.1005	0.115	0.148	0.150	0.174	0.192
0.2020	0.265	0.291	0.306	0.313	0.320
0.3022	0.358	0.388	0.400	0.422	0.443
0.4016	0.415	0.431	0.440	0.481	0.505

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TABLE S-III. Continued

x	T / K				
	288.15	293.15	298.15	303.15	308.15
			n-Heptane + ethanol		
0.5079	0.424	0.432	0.443	0.493	0.509
0.5967	0.432	0.436	0.443	0.496	0.513
0.7041	0.377	0.395	0.408	0.426	0.451
0.8008	0.329	0.336	0.360	0.363	0.373
0.8935	0.241	0.251	0.284	0.285	0.313
1.0000	0.000	0.000	0.000	0.000	0.000
			n-Heptane + propan-1-ol		
0.0000	0.000	0.000	0.000	0.000	0.000
0.1020	0.080	0.102	0.137	0.156	0.177
0.2018	0.118	0.136	0.160	0.193	0.219
0.2990	0.180	0.194	0.218	0.236	0.261
0.4005	0.191	0.231	0.246	0.272	0.294
0.5017	0.221	0.249	0.265	0.306	0.315
0.6033	0.272	0.297	0.314	0.337	0.353
0.7025	0.242	0.262	0.278	0.305	0.334
0.8010	0.198	0.237	0.249	0.260	0.293
0.8918	0.163	0.174	0.185	0.213	0.223
1.0000	0.000	0.000	0.000	0.000	0.000
			n-Heptane + propan-2-ol		
0.0000	0.000	0.000	0.000	0.000	0.000
0.1003	0.111	0.143	0.146	0.170	0.190
0.2009	0.185	0.193	0.201	0.215	0.257
0.3009	0.276	0.291	0.309	0.316	0.339
0.3980	0.281	0.300	0.346	0.370	0.383
0.5002	0.287	0.359	0.377	0.410	0.432
0.5961	0.291	0.367	0.382	0.414	0.436
0.6981	0.277	0.349	0.362	0.397	0.417
0.8014	0.208	0.264	0.324	0.357	0.387
0.9084	0.171	0.186	0.227	0.261	0.270
1.0000	0.000	0.000	0.000	0.000	0.000

TABLE S-IV. Excess viscosities (η^E / mPa s) of the *n*-heptane + alcohols mixtures at different temperatures and atmospheric pressure; uncertainties, u, are: $u(x) = \pm 0.0001$; $u(T) = \pm 0.05$ K; $u(\eta^E) = \pm 4\times10^{-3}$ mPa s

x	T / K				
	288.15	293.15	298.15	303.15	308.15
			n-Heptane + ethanol		
0.0000	0.000	0.000	0.000	0.000	0.000
0.1005	–0.192	–0.155	–0.130	–0.124	–0.112
0.2020	–0.279	–0.233	–0.199	–0.184	–0.165
0.3022	–0.304	–0.264	–0.225	–0.199	–0.182
0.4016	–0.308	–0.270	–0.236	–0.210	–0.188
0.5079	–0.297	–0.247	–0.224	–0.200	–0.184

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TABLE S-IV. Continued

x	T / K				
	288.15	293.15	298.15	303.15	308.15
			n-Heptane + ethanol		
0.5967	–0.264	–0.227	–0.200	–0.180	–0.159
0.7041	–0.215	–0.191	–0.163	–0.148	–0.129
0.8008	–0.164	–0.136	–0.121	–0.107	–0.101
0.8935	–0.092	–0.082	–0.067	–0.062	–0.055
1.0000	0.000	0.000	0.000	0.000	0.000
			n-Heptane + propan-1-ol		
0.0000	0.000	0.000	0.000	0.000	0.000
0.1020	–0.464	–0.405	–0.349	–0.304	–0.242
0.2018	–0.658	–0.574	–0.500	–0.438	–0.347
0.2990	–0.742	–0.637	–0.562	–0.483	–0.419
0.4005	–0.757	–0.663	–0.581	–0.506	–0.431
0.5017	–0.702	–0.622	–0.543	–0.473	–0.409
0.6033	–0.623	–0.548	–0.475	–0.422	–0.354
0.7025	–0.505	–0.446	–0.379	–0.336	–0.283
0.8010	–0.351	–0.301	–0.269	–0.228	–0.197
0.8918	–0.190	–0.168	–0.148	–0.133	–0.109
1.0000	0.000	0.000	0.000	0.000	0.000
			n-Heptane + propan-2-ol		
0.0000	0.000	0.000	0.000	0.000	0.000
0.1003	–0.705	–0.611	–0.475	–0.419	–0.349
0.2009	–0.965	–0.830	–0.676	–0.580	–0.479
0.3009	–1.050	–0.884	–0.738	–0.627	–0.526
0.3980	–1.014	–0.872	–0.708	–0.608	–0.505
0.5002	–0.922	–0.790	–0.637	–0.550	–0.468
0.5961	–0.793	–0.674	–0.562	–0.480	–0.400
0.6981	–0.619	–0.526	–0.433	–0.369	–0.313
0.8014	–0.419	–0.354	–0.296	–0.244	–0.216
0.9084	–0.199	–0.166	–0.143	–0.117	–0.105
1.0000	0.000	0.000	0.000	0.000	0.000

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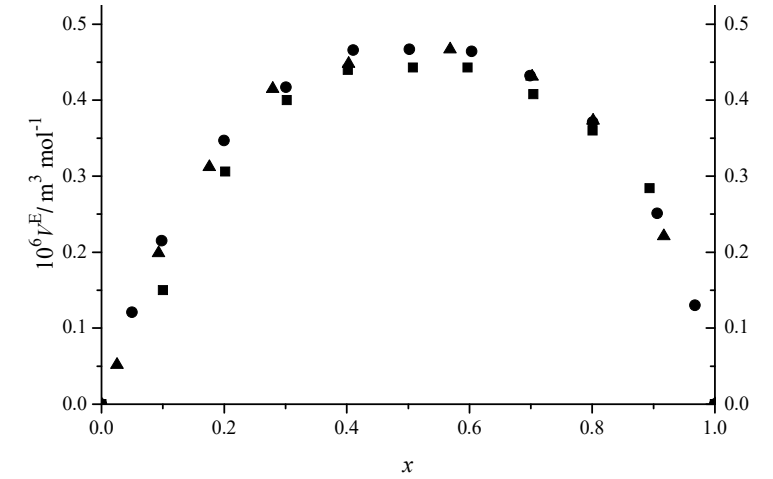

Fig. S-1. Excess molar volumes of (x) *n*-heptane + ethanol system at 298.15 K: ■) experimental; ●) Pereiro *et al.*[18] ▲) Orge *et al.*[19]

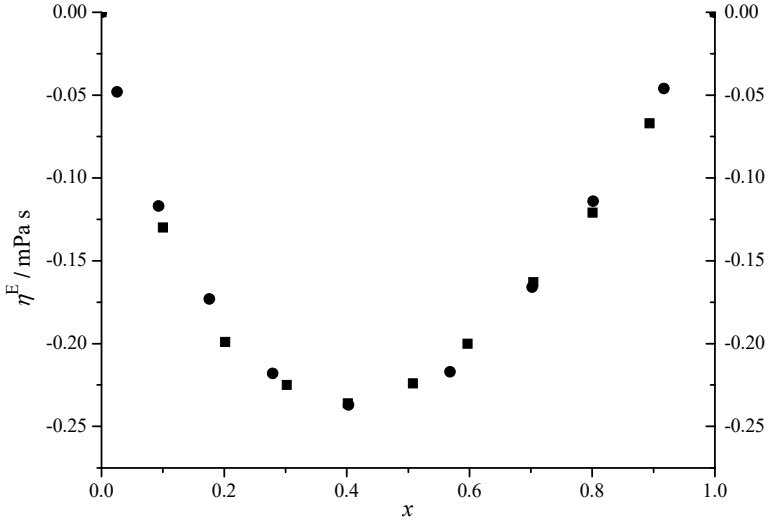

Fig. S-2. Excess viscosity of (x) *n*-heptane + ethanol system at 298.15 K: ■) experimental; ●) Orge *et al.*[19]

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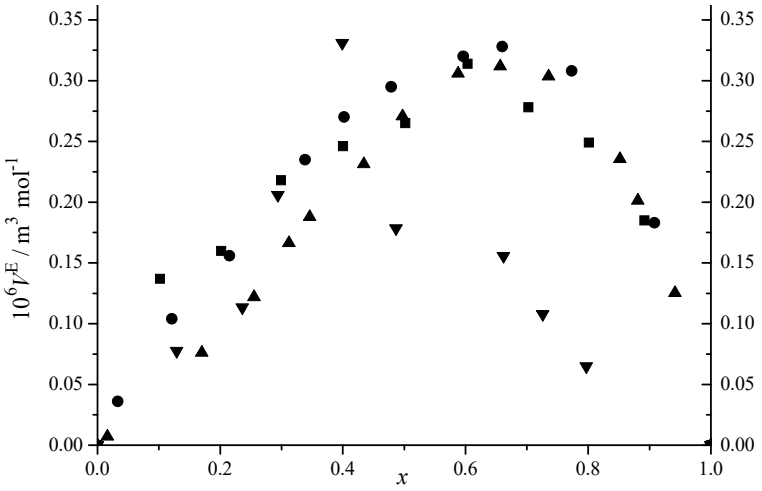

Fig. S-3. Excess molar volumes of *n*-heptane + propan-1-ol system at 298.15 K: ■) experimental; ●) Orge *et al*.[19] ▲) Jimenez *et al*.[20] ▼) Rajendran.[21]

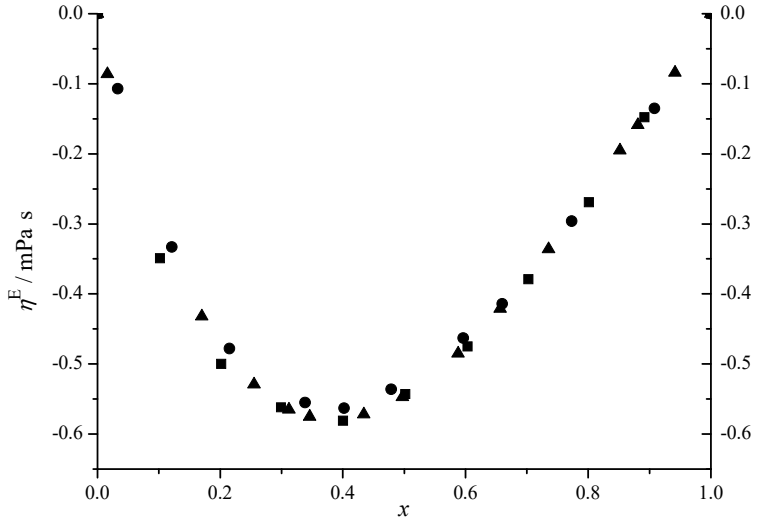

Fig. S-4. Excess viscosity of *n*-heptane + propan-1-ol system at 298.15 K: ■) experimental; ●) Orge *et al*.[19] ▲) Jimenez *et al*.[20]

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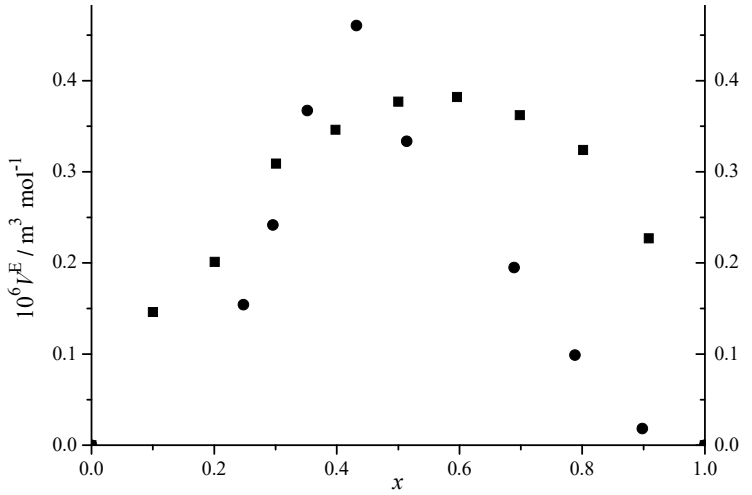

Fig. S-5. Excess molar volumes of *n*-heptane + propan-2-ol system at 298.15 K: ■) experimental; ●) Rajendran.[21]

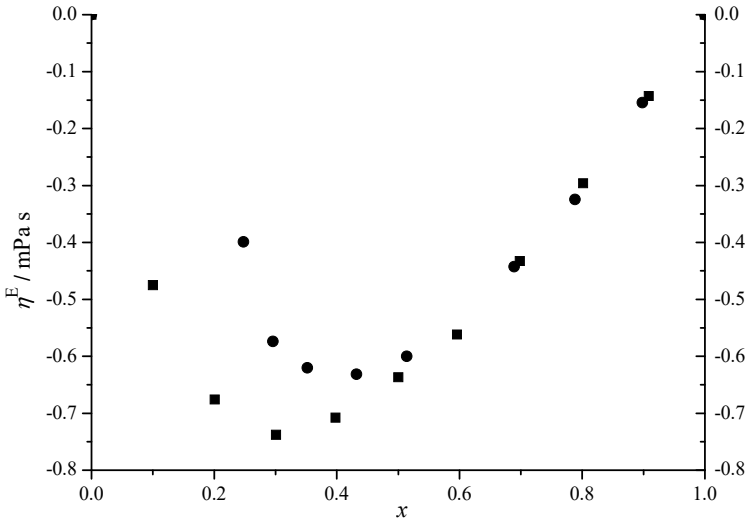

Fig. S-6. Excess viscosity of *n*-heptane + propan-1-ol system at 298.15 K: ■) experimental; (●) Rajendran.[21]

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TABLE S-V. Coefficients A_k and standard deviations, σ, for excess molar volume at different temperatures (all in m^3 mol^{-1})

T / K	$A_0\times10^6$	$A_1\times10^6$	$A_2\times10^6$	$A_3\times10^6$	$\sigma\times10^6$
			n-Heptane + ethanol		
288.15	1.72482	–0.04426	0.30956	1.24112	0.0078
293.15	1.76419	–0.11136	0.58527	1.12746	0.0062
298.15	1.79120	–0.17632	0.83641	1.51667	0.0067
303.15	1.97390	–0.08814	0.55322	1.13746	0.0132
308.15	2.04506	–0.11059	0.6910	1.27051	0.0187
			n-Heptane + propan-1-ol		
288.15	0.92022	0.49895	0.42104	–0.08171	0.0151
293.15	1.03145	0.52803	0.52025	–0.10929	0.0122
298.15	1.08665	0.54794	0.75585	–0.38737	0.0148
303.15	1.19777	0.52584	0.87876	–0.36976	0.0163
308.15	1.26477	0.55144	1.14112	–0.47573	0.0116
			n-Heptane + propan-2-ol		
288.15	1.17179	–0.10704	0.49217	0.81795	0.0156
293.15	1.39784	0.45763	0.46907	–0.17666	0.0184
298.15	1.48027	0.30581	0.74264	0.65875	0.0151
303.15	1.5811	0.4509	0.95112	0.56564	0.0204
308.15	1.65291	0.47941	1.22512	0.3723	0.0159

TABLE S-VI. Coefficients A_k and standard deviations, σ, for excess viscosities at different temperatures (all in mPa s)

T / K	A_0	A_1	A_2	A_3	σ
			n-Heptane + ethanol		
288.15	–1.17059	0.44174	–0.56711	0.43989	0.0036
293.15	–1.01004	0.41839	–0.42647	0.18487	0.0027
298.15	–0.89479	0.3403	–0.27042	0.17447	0.0018
303.15	–0.79589	0.27399	–0.30653	0.29205	0.0027
308.15	–0.71489	0.27151	–0.29219	0.20123	0.0035
			n-Heptane + propan-1-ol		
288.15	–2.82496	1.22654	–0.9919	1.09367	0.0059
293.15	–2.48186	1.00314	–0.79575	1.08458	0.0023
298.15	–2.16384	0.97194	–0.70223	0.6812	0.0056
303.15	–1.89223	0.78527	–0.59003	0.72463	0.0022
308.15	–1.62645	0.71789	–0.30942	0.30673	0.0063
			n-Heptane + propan-2-ol		
288.15	–3.65753	2.28763	–2.05348	1.63074	0.0105
293.15	–3.12076	1.91927	–1.75579	1.58995	0.0117
298.15	–2.56338	1.63908	–1.3988	0.90719	0.0054
303.15	–2.19627	1.36686	–1.17012	1.01654	0.0063
308.15	–1.84071	1.11945	–1.01897	0.75203	0.0061

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TABLE S-VII. Parameters of the pure components, coefficient of thermal expansion, α, isothermal compressibility k_T, reduced volume, $\tilde{v}$, characteristic volume, V^*, characteristic pressure, p^*, characteristic temperature, T^*, and reduced temperature, $\tilde{T}$, for Flory theory

Component	α / 10^{-3} K^{-1}	k_T / 10^{4} MPa^{-1}	$\tilde{v}$	V^* / 10^{-6} m^3 mol^{-1}	p^* / 10^{-6} J m^{-3}	T^* / K	$\tilde{T}$
293.15 K							
n-Heptane	1.24	14.38[22]	1.2909	113.4584	421.0756	4638.1	0.0632
Ethanol	1.19	11.05[23]	1.2815	45.5330	518.5073	4733.6	0.0619
Propan-1-ol	0.97	9.55[24]	1.2381	60.3438	456.4552	5281.1	0.0555
Propan-2-ol	1.07	10.81[24]	1.2583	60.6829	459.4142	5003.3	0.0586
298.15 K							
n-Heptane	1.24	14.606[25]	1.2948	113.8119	424.2082	4678.1	0.0637
Ethanol	1.19	11.53[26]	1.2854	45.6163	508.4346	4773.5	0.0624
Propan-1-ol	0.97	10.26[27]	1.2415	60.4575	434.4775	5320.4	0.0560
Propan-2-ol	1.07	11.30[26]	1.2619	60.8110	449.5515	5042.9	0.0591
303.15 K							
n-Heptane	1.24	16.3[23]	1.2987	114.1912	388.835	4718.2	0.0642
Ethanol	1.19	11.95[23]	1.2892	45.7197	501.7603	4813.5	0.0630
Propan-1-ol	0.97	10.57[24]	1.2449	60.5970	431.1326	5359.7	0.0566
Propan-2-ol	1.07	11.82[28]	1.2655	60.9737	439.4645	5082.5	0.0596
308.15 K							
n-Heptane	1.24	17.7[29]	1.3026	114.5799	366.1661	4758.4	0.0647
Ethanol	1.19	12.3[30]	1.2930	45.8555	498.4433	4853.5	0.0635
Propan-1-ol	0.97	11.08[11]	1.2482	60.7244	420.3194	5399.0	0.0571
Propan-2-ol	1.07	12.32[11]	1.2690	61.1482	430.9963	5122.2	0.0602

TABLE S-VIII. Parameters of the liquid mixtures for Flory and Prigogine–Flory–Patterson theories

T / K	φ_2	θ_2	$\tilde{v}$	$\tilde{T}$	χ_{12} / 10^{-6} J m^{-3}	ψ_1
n-Heptane + ethanol						
293.15	0.2864	0.2284	1.2938	0.0636	34.9794	0.6692
298.15	0.2861	0.2281	1.2977	0.0641	34.3676	0.6755
303.15	0.2859	0.2278	1.3022	0.0647	35.3985	0.6593
308.15	0.2858	0.2277	1.3062	0.0652	34.9129	0.6473
n-Heptane + propan-1-ol						
293.15	0.3472	0.3012	1.2755	0.0611	25.2022	0.6343
298.15	0.3469	0.3008	1.2794	0.0616	21.7395	0.6476
303.15	0.3467	0.3005	1.2835	0.0622	26.2681	0.6296
308.15	0.3464	0.3001	1.2874	0.0627	27.4530	0.6217
n-Heptane + propan-2-ol						
293.15	0.3485	0.3027	1.2835	0.0622	24.7486	0.6315
298.15	0.3482	0.3024	1.2876	0.0627	24.2387	0.6385
303.15	0.3481	0.3022	1.2917	0.0633	25.8128	0.6236
308.15	0.3480	0.3021	1.2956	0.0638	26.4277	0.6142

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TABLE S-IX. Experimental and calculated excess volumes (cm^3 mol^{-1}) at 0.5 mole fraction and calculated values of the three contributions to V^E

T / K	V^E_{exp}	V^E_{Flory}	V^E_{PFP}	$V^E_{int.}$	V^E_{FV}	V^E_{p*}	*ADD* / %	
							Flory	PFP
n-Heptane + ethanol								
293.15	0.4410	0.4374	0.4453	0.4805	0.0023	-0.0329	0.8	0.5
298.15	0.4478	0.4441	0.4521	0.4832	0.0023	-0.0288	0.8	0.9
303.15	0.4935	0.4890	0.4988	0.5429	0.0024	-0.0417	0.9	1.0
308.15	0.5113	0.5065	0.5172	0.5712	0.0025	-0.0515	0.9	1.1
n-Heptane + propan-1-ol								
293.15	0.2579	0.2567	0.2624	0.4304	0.0832	-0.0848	0.5	1.7
298.15	0.2717	0.2704	0.2756	0.3847	0.0838	-0.0253	0.5	1.4
303.15	0.2994	0.2979	0.3050	0.5044	0.0876	-0.1118	0.5	1.9
308.15	0.3162	0.3145	0.3228	0.5650	0.0903	-0.1519	0.5	2.1
n-Heptane + propan-2-ol								
293.15	0.3495	0.3474	0.3531	0.4419	0.0319	-0.0569	0.6	1.0
298.15	0.3701	0.3677	0.3737	0.4443	0.0324	-0.0382	0.6	1.0
303.15	0.3953	0.3926	0.4000	0.5161	0.0337	-0.0824	0.7	1.8
308.15	0.4132	0.4104	0.4189	0.5653	0.0347	-0.1117	0.7	1.4

TABLE S-X. Parameters for the semi-empirical relations of Grunberg–Nissan, Heric–Brewer, Joyban–Acree and McAllister and standard deviations at different temperatures

Equation	Parameters and σ	T / K				
		288.15	293.15	298.15	303.15	308.15
n-Heptane + ethanol						
Grunberg–Nissan	d	–1.03339	–0.98234	–0.92819	–0.93839	–0.92373
	σ	0.0159	0.0133	0.0225	0.0113	0.0140
Heric–Brewer	α_{12}	–0.73607	–0.68501	–0.63085	–0.64117	–0.62658
	α_{21}	–0.02572	–0.0298	–0.03183	–0.00191	–0.01579
	σ	0.0158	0.0130	0.0060	0.0097	0.0121
Jouyban–Acree	A_0	–280.2367	–273.37925	–269.89168	–274.10778	–272.5385
	A_1	–7.37491	13.79187	4.40707	–4.69605	16.13374
	A_2	–123.0185	–102.42284	–48.25045	–73.12746	–85.46377
	A_3	67.78576	0.76301	27.02307	82.8945	37.86172
	σ	0.0059	0.0066	0.0035	0.0046	0.0091
McAllister three-body model	η_{12}	0.47063	0.4411	0.41952	0.39759	0.37708
	η_{21}	0.68907	0.6426	0.59851	0.5457	0.50566
	σ	0.0158	0.0139	0.0189	0.0308	0.0121
McAllister four-body model	η_{1112}	0.42355	0.40301	0.39913	0.37311	0.35117
	η_{1122}	0.65931	0.60454	0.5245	0.50242	0.47761
	η_{2221}	0.74193	0.69182	0.67092	0.60061	0.55073
	σ	0.0070	0.0060	0.0035	0.0062	0.0085
n-Heptane + propan-1-ol						
Grunberg–Nissan	d	–1.33517	–1.30165	–1.26286	–1.27154	–1.2067
	σ	0.0139	0.0146	0.0076	0.0121	0.0087
	α_{12}	–1.20515	–1.17167	–1.13303	–1.14173	–1.07688

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TABLE S-X. Continued

Equation	Parameters and σ	T / K				
		288.15	293.15	298.15	303.15	308.15
		n-Heptane + propan-1-ol				
Heric–Brewer	α_{21}	–0.08064	–0.06412	–0.01719	–0.01409	–0.00629
	σ	0.0139	0.0151	0.0081	0.0129	0.0093
Jouyban–Acree	A_0	–379.36536	–380.59804	–372.73156	–384.13063	–379.38218
	A_1	–87.51838	–95.69916	–38.5322	–56.15547	–20.57744
	A_2	–36.79759	–6.70406	–26.25663	–9.42309	51.85301
	A_3	214.3258	252.40447	121.40922	177.40899	76.24936
	σ	0.0073	0.0078	0.0046	0.0106	0.0068
McAllister three-body model	η_{12}	0.49922	0.47214	0.44782	0.41777	0.39624
	η_{21}	0.93389	0.857	0.77478	0.70271	0.64677
	σ	0.0140	0.0151	0.0081	0.0129	0.0093
McAllister four-body model	η_{1112}	0.47098	0.45576	0.42505	0.40418	0.39999
	η_{1122}	0.71316	0.63831	0.60604	0.54545	0.47232
	η_{2221}	1.15803	1.08022	0.95958	0.8762	0.83254
	σ	0.0143	0.0163	0.0081	0.0139	0.0075
		n-Heptane + propan-2-ol				
Grunberg–Nissan	d	–1.97241	–1.91852	–1.80002	–1.7713	–1.68887
	σ	0.0352	0.0422	0.0386	0.0467	0.039
Heric–Brewer	α_{12}	–1.20515	–1.17167	–1.13303	–1.14173	–1.07688
	α_{12}	–1.84051	–1.78619	–1.66795	–1.63868	–1.55674
	α_{21}	0.42013	0.51062	0.45421	0.57211	0.46658
	σ	0.0102	0.0115	0.0136	0.0113	0.0130
Jouyban–Acree	A_0	–559.4203	–555.95426	–524.27459	–530.98393	–506.14069
	A_1	90.51183	101.91733	127.37596	133.57252	129.64263
	A_2	–59.39539	–40.92224	–83.51906	–36.70979	–96.64779
	A_3	110.94436	163.74655	43.07002	140.52597	61.97205
	σ	0.0045	0.0064	0.0109	0.0087	0.0073
McAllister three-body model	η_{12}	0.494	0.47786	0.44325	0.43256	0.39587
	η_{21}	0.68497	0.60645	0.56619	0.49471	0.47211
	σ	0.0102	0.0116	0.0136	0.0113	0.0130
McAllister four-body model	η_{1112}	0.45932	0.44854	0.40454	0.40695	0.36044
	η_{1122}	0.62563	0.56439	0.55435	0.48165	0.48448
	η_{2221}	0.92647	0.82876	0.73406	0.66329	0.59372
	σ	0.0079	0.0114	0.0102	0.0113	0.0075

TABLE S-XI. Values of $\Delta G^{\neq}$, $\Delta H^{\neq}$, $\Delta S^{\neq}$ and r for the binary mixtures

x	$\Delta G^{\neq}$ / J mol^{-1}					$\Delta H^{\neq}$	$\Delta S^{\neq}$	r
	T / K					J mol^{-1}	J mol^{-1} K^{-1}	
	288.15	293.15	298.15	303.15	308.15			
	n-Heptane + ethanol							
0.0000	12660.30	12644.09	12627.88	12611.67	12595.46	13594.50	3.24	0.9992
0.1005	12461.31	12461.22	12461.13	12461.05	12460.96	12466.34	0.02	0.9978
0.2020	12326.33	12340.18	12354.04	12367.89	12381.74	11528.04	–2.77	0.9971
0.3022	12245.13	12272.84	12300.54	12328.25	12355.95	10648.58	–5.54	0.9984

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TABLE S-XI. Continued

x	$\Delta G^{\neq}$ / J mol^{-1}					$\Delta H^{\neq}$ / J mol^{-1}	$\Delta S^{\neq}$ / J mol^{-1} K^{-1}	r
	T / K							
	288.15	293.15	298.15	303.15	308.15			
0.4016	12162.76	12197.21	12231.67	12266.12	12300.57	10177.15	–6.89	0.9983
0.5079	12094.13	12136.69	12179.26	12221.82	12264.39	9641.12	–8.51	0.9933
0.5967	12047.06	12106.89	12166.72	12226.54	12286.37	8599.30	–11.96	0.9984
0.7041	12000.25	12074.95	12149.66	12224.36	12299.07	7694.94	–14.94	0.9960
0.8008	12004.89	12084.22	12163.54	12242.87	12322.19	7433.39	–15.86	0.9890
0.8935	12053.60	12145.30	12236.99	12328.69	12420.39	6769.07	–18.34	0.9992
1.0000	12178.33	12269.74	12361.14	12452.55	12543.95	6910.59	–18.28	0.9948
n-Heptane + propan-1-ol								
0.0000	14730.52	14696.83	14663.13	14.629.43	14595.74	16672.46	6.74	0.9970
0.1020	14194.50	14181.02	14167.54	14154.06	14140.58	14971.27	2.69	0.9986
0.2018	13795.95	13798.36	13800.77	13803.18	13805.59	13657.12	–0.48	0.9979
0.2990	13466.32	13470.58	13474.84	13479.11	13483.37	13220.72	–0.85	0.9927
0.4005	13103.01	13119.76	13136.51	13153.26	13170.01	12137.60	–3.35	0.9985
0.5017	12820.76	12845.94	12871.12	12896.30	12921.47	11369.77	–5.03	0.9990
0.6033	12531.08	12580.81	12630.53	12680.26	12729.99	9665.25	–9.94	0.9954
0.7025	12318.84	12394.59	12470.33	12546.08	12621.82	7953.70	–15.15	0.9946
0.8010	12242.40	12324.62	12406.83	12489.05	12571.27	7504.20	–16.44	0.9813
0.8918	12214.68	12294.00	12373.33	12452.65	12531.97	7643.22	–15.86	0.9917
1.0000	12178.33	12269.74	12361.14	12452.55	12543.95	6910.59	–18.28	0.9948
n-Heptane + propan-1-ol								
0.0000	15018.63	14924.62	14830.61	14736.60	14642.59	20436.51	18.80	0.9993
0.1003	14234.64	14166.02	14097.40	14028.79	13960.17	18189.04	13.72	0.9993
0.2009	13664.96	13619.54	13574.12	13528.70	13483.28	16282.43	9.08	0.9990
0.3009	13210.61	13186.93	13163.25	13139.56	13115.88	14575.30	4.74	0.9971
0.3980	12854.01	12862.86	12871.70	12880.54	12889.39	12344.36	–1.77	0.9970
0.5002	12566.97	12595.02	12623.07	12651.12	12679.16	10950.53	–5.61	0.9923
0.5961	12347.29	12393.98	12440.66	12487.34	12534.02	9656.94	–9.34	0.9927
0.6981	12223.10	12291.17	12359.24	12427.31	12495.38	8300.32	–13.61	0.9994
0.8014	12172.33	12248.78	12325.23	12401.67	12478.12	7766.80	–15.29	0.9735
0.9084	12156.33	12239.05	12321.77	12404.48	12487.20	7389.39	–16.54	0.9784
1.0000	12178.33	12269.74	12361.14	12452.55	12543.95	6910.59	–18.28	0.9948

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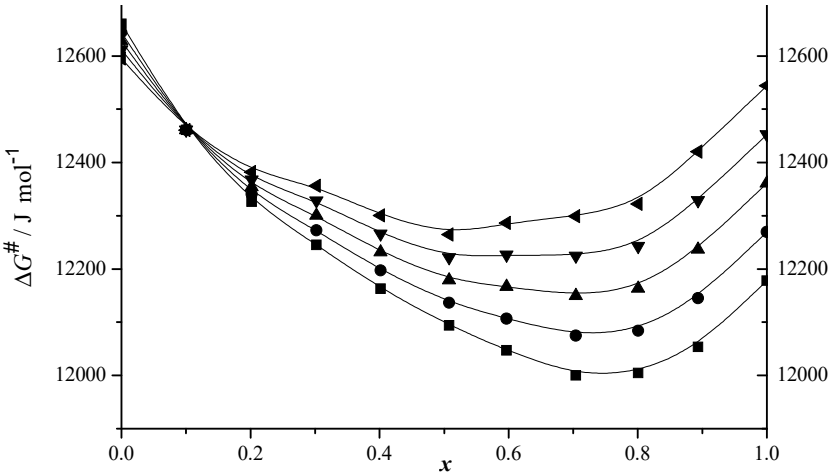

Fig. S-7. Gibbs energy change of activation versus *n*-heptane mole fraction of *n*-heptane + ethanol at: ■) 288.15, ●) 293.15, ▲) 298.15, ▼) 303.15 and ◀) 308.15 K.

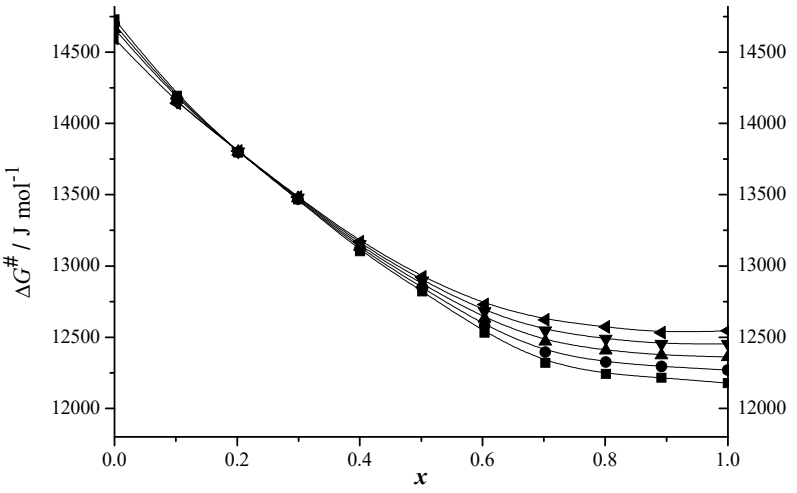

Fig. S-8. Gibbs energy change of activation versus *n*-heptane mole fraction of *n*-heptane + propan-1-ol at: ■) 288.15, ●) 293.15, ▲) 298.15, ▼) 303.15 and ◀) 308.15 K.

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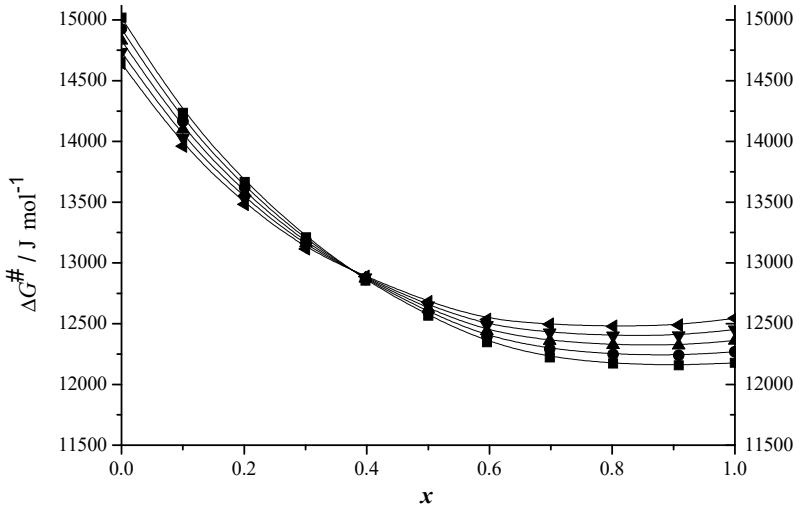

Fig. S-9. Gibbs energy change of activation versus *n*-heptane mole fraction of *n*-heptane + propan-2-ol at: ■) 288.15, ●) 293.15, ▲) 298.15, ▼) 303.15 and ◄) 308.15 K.

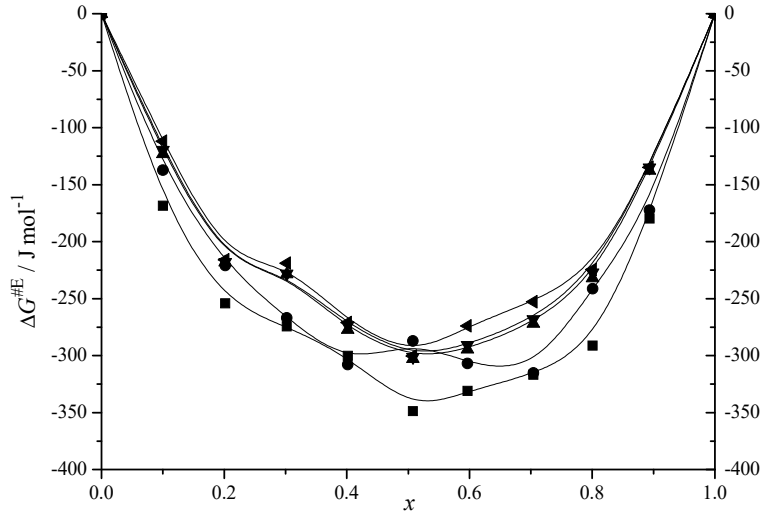

Fig. S-10. Excess Gibbs energy change of activation versus *n*-heptane mole fraction of *n*-heptane + ethanol at: ■) 288.15, ●) 293.15, ▲) 298.15, ▼) 303.15 and ◄) 308.15 K.

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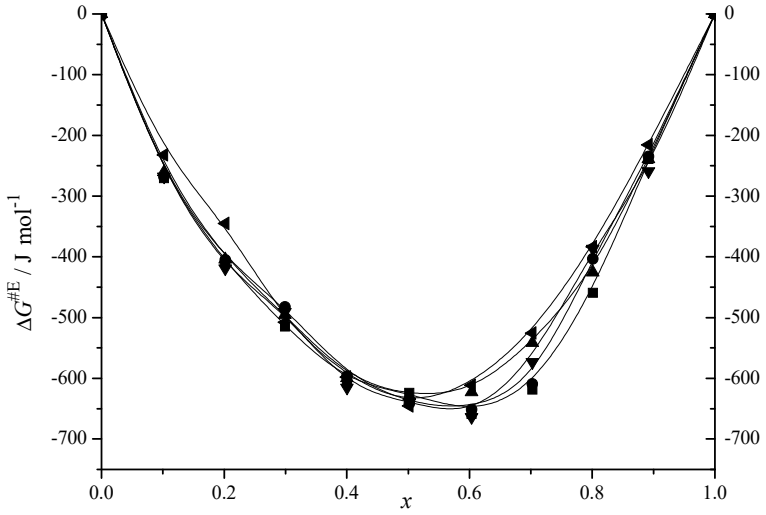

Fig. S-11. Excess Gibbs energy change of activation versus *n*-heptane mole fraction of *n*-heptane + propan-1-ol at: ■) 288.15, ●) 293.15, ▲) 298.15, ▼) 303.15 and ◀) 308.15 K.

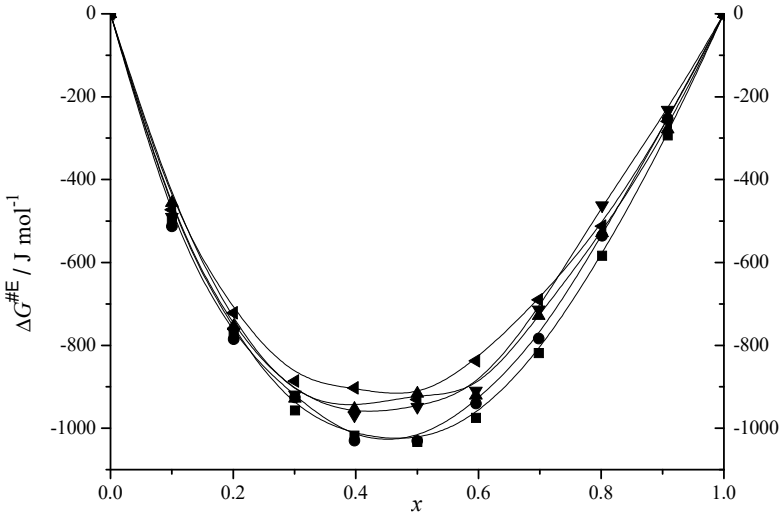

Fig. S-12. Excess Gibbs energy change of activation versus *n*-heptane mole fraction of *n*-heptane + propan-2-ol at: ■) 288.15, ●) 293.15, ▲) 298.15, ▼) 303.15 and ◀) 308.15 K.

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