

SUPPORTING INFORMATION

Liquid-liquid equilibria of ternary mixtures (1-heptanol, propanone, 2-butanone or 2-heptanone + γ -valerolactone + n-tetradecane)

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Binodal curve data points and physical properties measured at cloud point concentration

Table S-1. Experimental binodal curve data points for the system 1-heptanol (1) + GVL (2) + n-tetradecane (3) at 298.15 K and p = 94.2 kPa.¹⁶ *

w ₁	w ₂	w ₃	ρ (g.cm ⁻³)	s(ρ) ^a (10 ⁵ .g.cm ⁻³)	u _c (ρ) ^b (10 ⁵ .g.cm ⁻³)	U(ρ) ^c (10 ⁵ .g.cm ⁻³)
0.2612	0.2524	0.4864	0.83197	28	59	255
0.2599	0.2598	0.4803	0.83136	226	232	998
0.1801	0.1248	0.6951	0.79497	11	61	262
0.1775	0.1240	0.6985	0.79473	3	60	259
0.0976	0.0657	0.8368	0.77715	17	69	298
0.0997	0.0659	0.8344	0.77739	3	67	288
0.1426	0.0955	0.7618	0.78613	8	64	274
0.1385	0.0911	0.7705	0.78535	5	64	275
0.0507	0.0435	0.9058	0.76957	2	71	305
0.0526	0.0453	0.9021	0.77027	5	71	305
0.2102	0.1654	0.6244	0.80643	44	72	310
0.2119	0.1642	0.6239	0.80600	19	60	258
0.0976	0.8641	0.0383	1.00579	0	84	363
0.0968	0.8645	0.0387	1.00446	3	84	362
0.2541	0.5862	0.1597	0.92317	3	57	247
0.2543	0.5882	0.1575	0.92371	3	58	248
0.1861	0.7356	0.0782	0.96684	8	70	301
0.1866	0.7354	0.0781	0.96661	4	70	300
0.1451	0.7992	0.0557	0.98554	4	76	329
0.1438	0.8026	0.0536	0.98652	3	77	330
0.2249	0.6681	0.1070	0.94712	1	63	273
0.2248	0.6657	0.1095	0.94634	2	63	272
0.0516	0.9226	0.0258	1.02313	1	92	397
0.0500	0.9249	0.0251	1.02349	1	93	399

* Standard uncertainties u(T) = 0.05 K, u(w_i) = 0.0001, and u(p) = 0.5 kPa¹⁶; ^a s(ρ) – standard deviation from experimental triplicates; ^b u_c(ρ) – combined standard uncertainty; ^c U(ρ) – expanded uncertainty (2 degrees of freedom at 95% confidence interval).

Table S-2. Experimental binodal curve data points for the system propanone (4) + GVL (2) + n-tetradecane (3) at 298.15 K and p = 94.2 kPa.^{16*}

w ₄	w ₂	w ₃	ρ (g.cm ⁻³)	s(ρ) ^a (10 ⁵ .g.cm ⁻³)	u _c (ρ) ^b (10 ⁵ .g.cm ⁻³)	U(ρ) ^c (10 ⁵ .g.cm ⁻³)
0.0997	0.0249	0.8754	0.76330	2	68	291
0.0994	0.0237	0.8769	0.76316	2	68	291
0.1964	0.0247	0.7789	0.76430	10	63	269
0.1961	0.0254	0.7785	0.76441	9	62	268
0.2944	0.0251	0.6806	0.76624	6	57	247
0.2945	0.0250	0.6805	0.76616	0	57	246
0.3903	0.0277	0.5820	0.76999	8	55	236
0.3903	0.0276	0.5820	0.76912	1	54	233
0.4841	0.0356	0.4803	0.77334	1	53	228
0.4821	0.0349	0.4829	0.77309	1	53	228
0.5691	0.0541	0.3768	0.78043	2	54	231
0.5675	0.0549	0.3776	0.78060	0	54	230
0.0203	0.0188	0.9609	0.76223	9	74	319
0.0400	0.0200	0.9399	0.76243	9	73	312
0.0591	0.0215	0.9194	0.76271	9	71	306
0.0800	0.0222	0.8978	0.76277	9	70	300
0.1173	0.0219	0.8608	0.76289	9	67	289
0.1566	0.0219	0.8215	0.76318	9	65	279
0.1945	0.7733	0.0322	0.97806	5	75	321
0.1948	0.7734	0.0318	0.97800	2	75	321
0.2873	0.6679	0.0449	0.94729	1	66	284
0.2873	0.6682	0.0444	0.94755	3	66	285
0.3763	0.5632	0.0605	0.91756	4	61	263
0.3766	0.5635	0.0599	0.91748	8	61	265
0.4620	0.4569	0.0811	0.88893	6	59	253
0.4620	0.4566	0.0813	0.88854	4	59	252
0.1464	0.8269	0.0267	0.99334	1	80	344
0.2414	0.7210	0.0377	0.96241	1	70	301
0.3319	0.6166	0.0515	0.93200	1	63	272

* Standard uncertainties u(T) = 0.05 K, u(w_i) = 0.0001, and u(p) = 0.5 kPa¹⁶; ^a s(ρ) – standard deviation from experimental triplicates; ^b u_c(ρ) – combined standard uncertainty; ^c U(ρ) – expanded uncertainty (2 degrees of freedom at 95% confidence interval).

Table S-3. Experimental binodal curve data points for the system 2-butanone (5) + GVL (2) + n-tetradecane (3) at 298.15 K and p = 94.2 kPa.¹⁶ *

w ₅	w ₂	w ₃	ρ (g.cm ⁻³)	s(ρ) ^a (10 ⁵ .g.cm ⁻³)	u _c (ρ) ^b (10 ⁵ .g.cm ⁻³)	U(ρ) ^c (10 ⁵ .g.cm ⁻³)
0.1012	0.0429	0.8559	0.76938	1	67	289
0.1012	0.0432	0.8557	0.76950	1	67	289
0.1855	0.0823	0.7322	0.78150	2	61	262
0.1864	0.0831	0.7304	0.78095	4	61	261
0.2623	0.1307	0.6071	0.79484	1	55	237
0.2629	0.1296	0.6075	0.79488	3	55	238
0.3811	0.2380	0.3808	0.82755	2	50	215
0.3810	0.2381	0.3810	0.82746	3	50	215
0.3262	0.1874	0.4865	0.81168	2	51	221
0.3264	0.1871	0.4865	0.81156	1	51	221
0.0512	0.0288	0.9200	0.76511	1	71	306
0.0519	0.0274	0.9207	0.76500	2	71	306
0.0217	0.0238	0.9546	0.76340	1	73	315
0.0405	0.0251	0.9344	0.76438	0	72	310
0.0597	0.0294	0.9107	0.76581	0	71	303
0.0795	0.0374	0.8831	0.76770	2	69	296
0.0983	0.8701	0.0317	1.00861	5	86	368
0.0991	0.8699	0.0310	1.00830	3	85	367
0.1930	0.7639	0.0432	0.97702	1	73	316
0.1937	0.7639	0.0424	0.97705	2	73	316
0.2807	0.6498	0.0695	0.94473	2	64	276
0.2806	0.6509	0.0684	0.94464	4	64	276
0.3575	0.5346	0.1079	0.91205	4	58	248
0.3574	0.5348	0.1078	0.91228	2	58	248
0.0502	0.9255	0.0243	1.02491	1	93	400
0.0504	0.9261	0.0235	1.02433	4	93	400
0.4071	0.4053	0.1876	0.87548	1	53	226
0.4072	0.4049	0.1878	0.87520	2	53	226

* Standard uncertainties u(T) = 0.05 K, u(w_i) = 0.0001, and u(p) = 0.5 kPa¹⁶; ^a s(ρ) – standard deviation from experimental triplicates; ^b u_c(ρ) – combined standard uncertainty; ^c U(ρ) – expanded uncertainty (2 degrees of freedom at 95% confidence interval).

Table S-4. Experimental binodal curve data points for the system 2-heptanone (6) + GVL (2) + n-tetradecane (3) at 298.15 K and $p = 94.2$ kPa.^{16*}

w_6	w_2	w_3	ρ (g.cm ⁻³)	$s(\rho)^a$ (10 ⁵ .g.cm ⁻³)	$u_c(\rho)^b$ (10 ⁵ .g.cm ⁻³)	$U(\rho)^c$ (10 ⁵ .g.cm ⁻³)
0.1783	0.1125	0.7091	0.78930	6	60	260
0.1785	0.1142	0.7073	0.78981	6	60	260
0.0959	0.0511	0.8529	0.77430	6	68	293
0.0963	0.0533	0.8503	0.77287	17	69	299
0.2471	0.1787	0.5742	0.80934	0	55	235
0.2469	0.1796	0.5735	0.81025	25	60	259
0.2929	0.2714	0.4357	0.83601	0	51	218
0.2939	0.2672	0.4388	0.83509	6	51	220
0.0495	0.0327	0.9178	0.76678	0	71	306
0.0507	0.0322	0.9171	0.76703	0	71	306
0.1392	0.0793	0.7815	0.78109	15	66	282
0.1393	0.0790	0.7817	0.78061	6	64	276
0.0980	0.8695	0.0325	1.00768	0	85	366
0.0976	0.8701	0.0323	1.00786	0	85	367
0.0500	0.9247	0.0253	1.02444	6	93	400
0.0486	0.9267	0.0247	1.02478	0	93	400
0.1440	0.8104	0.0456	0.99042	6	78	336
0.1439	0.8118	0.0444	0.99065	6	78	337
0.2628	0.6105	0.1267	0.93213	6	60	258
0.2620	0.6095	0.1285	0.93275	0	60	257
0.1888	0.7480	0.0633	0.97210	0	71	307
0.1884	0.7491	0.0625	0.97333	0	72	308
0.3135	0.4691	0.2174	0.89123	0	52	224
0.3149	0.4706	0.2145	0.89205	0	52	225

* Standard uncertainties $u(T) = 0.05$ K, $u(w_i) = 0.0001$, and $u(p) = 0.5$ kPa¹⁶; ^a $s(\rho)$ – standard deviation from experimental triplicates; ^b $u_c(\rho)$ – combined standard uncertainty; ^c $U(\rho)$ – expanded uncertainty (2 degrees of freedom at 95% confidence interval).

Density of extract and raffinate phases

Table S-5. Density (ρ) physical property of extract and raffinate phases. System 1-heptanol (1) + GVL (2) + n-tetradecane (3) at 298.15 K and $p = 94.2 \text{ kPa}$.^{16*}

Initial mixture			Extract		Raffinate	
w_1	w_2	w_3	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)
0.0249	0.4502	0.5249	1.02247	99	0.76355	4
0.0490	0.4507	0.5003	1.01199	10	0.76510	2
0.0758	0.4486	0.4756	0.99864	2	0.76740	4
0.1005	0.4497	0.4499	0.98715	4	0.77011	3
0.1247	0.4517	0.4235	0.97705	2	0.77279	5
0.1502	0.4501	0.3997	0.96535	7	0.77673	5

* Standard uncertainties $u(T) = 0.05 \text{ K}$, $u(w_i) = 0.0001$, and $u(p) = 0.5 \text{ kPa}$.¹⁶

Table S-6. Density (ρ) physical property of extract and raffinate phases. System propanone (4) + GVL (2) + n-tetradecane (3) at 298.15 K and $p = 94.2 \text{ kPa}$.^{16*}

Initial mixture			Extract		Raffinate	
w_4	w_2	w_3	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)
0.0633	0.4498	0.4869	1.00564	5	0.76259	1
0.0999	0.4501	0.4500	0.98826	8	0.76297	5
0.1503	0.4489	0.4009	0.96684	3	0.76265	3
0.0198	0.4506	0.5296	1.02887	1	0.76234	2
0.2499	0.4500	0.3001	0.93377	2	0.76344	1
0.3000	0.4509	0.2492	0.92264	2	0.76329	3

* Standard uncertainties $u(T) = 0.05 \text{ K}$, $u(w_i) = 0.0001$, and $u(p) = 0.5 \text{ kPa}$.¹⁶

Table S-7. Density (ρ) physical property of extract and raffinate phases. System 2-butanone (5) + GVL (2) + n-tetradecane (3) at 298.15 K and $p = 94.2 \text{ kPa}^{16*}$.

Initial mixture			Extract		Raffinate	
w_5	w_2	w_3	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)
0.0996	0.4505	0.4499	0.99043	13	0.76487	1
0.0501	0.4500	0.4998	1.01395	1	0.76354	1
0.1487	0.4493	0.4020	0.96939	2	0.76604	1
0.2001	0.4500	0.3499	0.94963	7	0.76701	3
0.2498	0.4499	0.3004	0.93287	4	0.76730	30
0.2998	0.4495	0.2507	0.91805	3	0.77009	2
0.1250	0.4492	0.4257	0.97917	3	0.76507	4

* Standard uncertainties $u(T) = 0.05 \text{ K}$, $u(w_i) = 0.0001$, and $u(p) = 0.5 \text{ kPa}$.¹⁶

Table S-8. Density (ρ) physical property of extract and raffinate phases. System 2-heptanone (6) + GVL (2) + n-tetradecane (3) at 298.15 K and $p = 94.2 \text{ kPa}^{16*}$.

Initial mixture			Extract		Raffinate	
w_6	w_2	w_3	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)	ρ (g.cm^{-3})	$u(\rho)$ ($10^5 \cdot \text{g.cm}^{-3}$)
0.0499	0.4496	0.5005	1.01718	13	0.76505	1
0.1000	0.4499	0.4501	0.99555	1	0.76853	1
0.1500	0.4505	0.3995	0.97388	2	0.77268	1
0.0250	0.4498	0.5252	1.02946	7	0.76356	3
0.0750	0.4497	0.4753	1.00645	4	0.76816	30
0.1249	0.4501	0.4250	0.98400	3	0.77024	2
0.1749	0.4502	0.3749	0.96305	3	0.77502	4

* Standard uncertainties $u(T) = 0.05 \text{ K}$, $u(w_i) = 0.0001$, and $u(p) = 0.5 \text{ kPa}$.¹⁶

Extract and raffinate phase compositions – Liquid-Liquid Equilibrium

Table S-9. Phase compositions calculated through indirect method for the system 1-heptanol (1) + GVL (2) + n-tetradecane (3) at 298.15 K and p = 94.2 kPa^{16*}.

Initial mixture				GVL rich phase (extract)				n-tetradecane rich phase (raffinate)						
w ₁	w ₂	w ₃	w ₁	u(w ₁)	w ₂	u(w ₂)	w ₃	u(w ₃)	w ₁	u(w ₁)	w ₂	u(w ₂)	w ₃	u(w ₃)
0.0249	0.4502	0.5249	0.050	0.004	0.924	0.004	0.026	0.001	0.000	0.005	0.017	0.008	0.983	0.006
0.0490	0.4507	0.5003	0.083	0.003	0.883	0.003	0.034	0.000	0.010	0.005	0.024	0.008	0.966	0.006
0.0758	0.4486	0.4756	0.121	0.003	0.834	0.003	0.046	0.001	0.027	0.005	0.031	0.008	0.942	0.006
0.1005	0.4497	0.4499	0.150	0.003	0.793	0.003	0.057	0.001	0.046	0.004	0.039	0.007	0.914	0.006
0.1247	0.4517	0.4235	0.172	0.003	0.759	0.003	0.069	0.001	0.064	0.004	0.048	0.007	0.888	0.006
0.1502	0.4501	0.3997	0.195	0.003	0.721	0.003	0.084	0.001	0.089	0.004	0.061	0.007	0.850	0.005

* Standard uncertainties u(T) = 0.05 K, u(p) = 0.5 kPa, and u(w_i) = 0.0001 for the initial mixture¹⁶.

Table S-10. Phase compositions calculated through indirect method for the system propanone (4) + GVL (2) + n-tetradecane (3) at 298.15 K and p = 94.2 kPa^{16*}.

Initial mixture				GVL rich phase (extract)				n-tetradecane rich phase (raffinate)						
w ₄	w ₂	w ₃	w ₄	u(w ₄)	w ₂	u(w ₂)	w ₃	u(w ₃)	w ₄	u(w ₄)	w ₂	u(w ₂)	w ₃	u(w ₃)
0.0633	0.4498	0.4869	0.116	0.007	0.859	0.007	0.025	0.0002	0.019	0.002	0.020	0.003	0.962	0.002
0.0999	0.4501	0.4500	0.166	0.007	0.805	0.007	0.029	0.0002	0.031	0.010	0.020	0.014	0.949	0.010
0.1503	0.4489	0.4009	0.228	0.006	0.736	0.006	0.036	0.0002	0.048	0.005	0.021	0.007	0.931	0.005
0.0198	0.4506	0.5296	0.047	0.008	0.933	0.008	0.020	0.0001	0.004	0.005	0.019	0.007	0.977	0.005
0.2499	0.4500	0.3001	0.323	0.005	0.627	0.005	0.050	0.0003	0.091	0.002	0.022	0.003	0.887	0.002
0.3000	0.4509	0.2492	0.356	0.005	0.588	0.005	0.056	0.0004	0.128	0.003	0.023	0.004	0.848	0.003

* Standard uncertainties u(T) = 0.05 K, u(p) = 0.5 kPa, and u(w_i) = 0.0001 for the initial mixture¹⁶.

Table S-11. Phase compositions calculated through indirect method for the system 2-butanone (5) + GVL (2) + n-tetradecane (3) at 298.15 K and p = 94.2 kPa^{16*}.

Initial mixture				GVL rich phase (extract)				n-tetradecane rich phase (raffinate)						
w ₅	w ₂	w ₃	w ₅	u(w ₅)	w ₂	u(w ₂)	w ₃	u(w ₃)	w ₅	u(w ₅)	w ₂	u(w ₂)	w ₃	u(w ₃)
0.0996	0.4505	0.4499	0.152	0.005	0.810	0.005	0.038	0.001	0.046	0.004	0.026	0.007	0.927	0.006
0.0501	0.4500	0.4998	0.073	0.004	0.899	0.004	0.027	0.001	0.033	0.005	0.022	0.007	0.945	0.006
0.1487	0.4493	0.4020	0.224	0.005	0.725	0.005	0.051	0.001	0.052	0.004	0.028	0.007	0.919	0.005
0.2001	0.4500	0.3499	0.282	0.005	0.651	0.005	0.067	0.002	0.058	0.004	0.030	0.007	0.912	0.005
0.2498	0.4499	0.3004	0.325	0.005	0.590	0.005	0.085	0.002	0.065	0.005	0.033	0.008	0.902	0.007
0.2998	0.4495	0.2507	0.355	0.005	0.539	0.005	0.106	0.002	0.093	0.004	0.044	0.006	0.863	0.005
0.1250	0.4492	0.4257	0.192	0.005	0.764	0.005	0.045	0.001	0.048	0.004	0.027	0.007	0.925	0.006

* Standard uncertainties u(T) = 0.05 K, u(p) = 0.5 kPa, and u(w_i) = 0.0001 for the initial mixture¹⁶.

Table S-12. Phase compositions calculated through indirect method for the system 2-heptanone (6) + GVL (2) + n-tetradecane (3) at 298.15 K and p = 94.2 kPa^{16*}.

Initial mixture				GVL rich phase (extract)				n-tetradecane rich phase (raffinate)						
w ₆	w ₂	w ₃	w ₆	u(w ₆)	w ₂	u(w ₂)	w ₃	u(w ₃)	w ₆	u(w ₆)	w ₂	u(w ₂)	w ₃	u(w ₃)
0.0499	0.4496	0.5005	0.075	0.002	0.897	0.002	0.028	0.0003	0.036	0.005	0.028	0.007	0.935	0.005
0.1000	0.4499	0.4501	0.133	0.002	0.824	0.002	0.042	0.0004	0.062	0.005	0.039	0.007	0.900	0.005
0.1500	0.4505	0.3995	0.185	0.002	0.753	0.002	0.063	0.0005	0.093	0.005	0.053	0.006	0.854	0.004
0.0250	0.4498	0.5252	0.037	0.003	0.941	0.003	0.022	0.0002	0.024	0.005	0.023	0.007	0.953	0.005
0.0750	0.4497	0.4753	0.104	0.002	0.861	0.002	0.034	0.0003	0.056	0.005	0.036	0.007	0.908	0.005
0.1249	0.4501	0.4250	0.161	0.002	0.787	0.002	0.052	0.0004	0.073	0.005	0.044	0.006	0.884	0.004
0.1749	0.4502	0.3749	0.208	0.001	0.715	0.002	0.076	0.001	0.113	0.004	0.064	0.006	0.823	0.004

* Standard uncertainties u(T) = 0.05 K, u(p) = 0.5 kPa, and u(w_i) = 0.0001 for the initial mixture¹⁶.