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Supplementary material

SUPPLEMENTARY MATERIAL TO

Excess molar volumes of 1,3-propanediol + (C_1–C_5) alkan-1-ols: application of a cubic equation of state

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TABLE I-S. Densities, ρ, of the pure components at various temperatures and the corresponding literature values

Compound	T / K	ρ / g cm^{-3}	
		This work	Lit.
1,3-Propanediol	293.15	1.05265	–
	298.15	1.04955	1.049717 9
	303.15	1.04665	1.046718 9
	313.15	1.03970	1.040207 9
Methanol	293.15	0.79155	0.79115 10
	298.15	0.78630	0.78637 11
	303.15	0.78165	0.78170 11
	313.15	0.77215	0.77226 10
Ethanol	293.15	0.78945	0.78933 10
	298.15	0.78498	0.78493 11
	303.15	0.78071	0.78064 11
	313.15	0.77212	0.77254 10
1-Propanol	293.15	0.80352	0.80323 10
	298.15	0.79960	0.79960 11
	303.15	0.79554	0.79560 11
	313.15	0.78747	0.78759 10
1-Butanol	293.15	0.80950	0.80943 12
	298.15	0.80570	0.80584 11
	303.15	0.80212	0.80220 11
	313.15	0.79415	–
1-Pentanol	293.15	0.81480	0.81492 11
	298.15	0.81082	0.81080 11
	303.15	0.80707	0.8072 11
	313.15	0.79940	–

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TABLE II-S. Densities, ρ, and excess molar volumes, V_m^E, for 1,3 propanediol (1) + alkanols (2) mixtures at various temperatures

x_1	ρ / g cm^{-3}	V_m^E / cm^3 mol^{-1}
1,3-propanediol (1) + methanol (2), T = 293.15 K		
0.0000	0.79155	–
0.0776	0.82915	–0.181
0.1581	0.86417	–0.371
0.2356	0.89422	–0.535
0.3482	0.93132	–0.680
0.4529	0.96009	–0.731
0.5399	0.98021	–0.700
0.6482	1.00150	–0.592
0.7394	1.01690	–0.459
0.8369	1.03104	–0.265
0.9280	1.04358	–0.121
1.0000	1.05265	–
1,3-propanediol (1) + methanol (2), T = 298.15 K		
0.0000	0.78630	–
0.0776	0.82379	–0.169
0.1581	0.85886	–0.353
0.2356	0.88872	–0.498
0.3482	0.92601	–0.639
0.4529	0.95503	–0.689
0.5399	0.97538	–0.658
0.6482	0.99704	–0.555
0.7394	1.01250	–0.411
0.8369	1.02730	–0.245
0.9280	1.03997	–0.096
1.0000	1.04955	–
1,3-propanediol (1) + methanol (2), T = 303.15 K		
0.0000	0.78165	–
0.0776	0.81918	–0.166
0.1581	0.85411	–0.337
0.2356	0.88386	–0.469
0.3482	0.92088	–0.582
0.4529	0.94999	–0.624
0.5399	0.97084	–0.610
0.6482	0.99305	–0.526
0.7394	1.00909	–0.407
0.8369	1.02412	–0.244
0.9280	1.03693	–0.094
1.0000	1.04665	–

TABLE II-S. Continued

x_1	ρ / g cm^{-3}	V_m^E / cm^3 mol^{-1}
1,3-propanediol (1) + methanol (2), T = 313.15 K		
0.0000	0.77215	–
0.0776	0.80968	–0.161
0.1581	0.84437	–0.311
0.2356	0.87411	–0.433
0.3482	0.91144	–0.547
0.4529	0.94083	–0.587
0.5399	0.96188	–0.569
0.6482	0.98455	–0.492
0.7394	1.00100	–0.380
0.8369	1.01658	–0.234
0.9280	1.02965	–0.084
1.0000	1.03970	–
1,3-propanediol (1) + ethanol (2), T = 293.15 K		
0.0000	0.78945	
0.0786	0.81642	–0.132
0.1840	0.85128	–0.312
0.2408	0.86931	–0.399
0.3310	0.89660	–0.501
0.4449	0.92878	–0.570
0.5545	0.95729	–0.565
0.6345	0.97657	–0.513
0.7331	0.99893	–0.416
0.8551	1.02443	–0.237
0.9361	1.04059	–0.116
1.0000	1.05265	
1,3-propanediol (1) + ethanol (2), T = 298.15 K		
0.0000	0.78498	–
0.0786	0.81184	–0.120
0.1840	0.84670	–0.295
0.2408	0.86465	–0.372
0.3310	0.89213	–0.481
0.4449	0.92449	–0.552
0.5545	0.95321	–0.551
0.6345	0.97262	–0.499
0.7331	0.99505	–0.396
0.8551	1.02085	–0.222
0.9361	1.03705	–0.093
1.0000	1.04955	–

TABLE II-S. Continued

x_1	ρ / g cm^{-3}	V_m^E / cm^3 mol^{-1}
1,3-propanediol (1) + ethanol (2), T = 303.15 K		
0.0000	0.78071	–
0.0786	0.80744	–0.107
0.1840	0.84198	–0.252
0.2408	0.86012	–0.339
0.3310	0.88745	–0.431
0.4449	0.92005	–0.510
0.5545	0.94901	–0.514
0.6345	0.96861	–0.467
0.7331	0.99137	–0.374
0.8551	1.01740	–0.202
0.9361	1.03400	–0.091
1.0000	1.04665	–
1,3-propanediol (1) + ethanol (2),T = 313.15 K		
0.0000	0.77212	–
0.0786	0.79872	–0.095
0.1840	0.83311	–0.225
0.2408	0.85122	–0.307
0.3310	0.87865	–0.399
0.4449	0.91121	–0.464
0.5545	0.94024	–0.460
0.6345	0.96019	–0.426
0.7331	0.98317	–0.333
0.8551	1.00990	–0.189
0.9361	1.02680	–0.085
1.0000	1.03970	–
1,3-propanediol (1) + 1-propanol (2), T = 293.15 K		
0.0000	0.80352	–
0.0794	0.82401	–0.119
0.1737	0.84823	–0.231
0.2385	0.86498	–0.306
0.3480	0.89298	–0.387
0.4425	0.91691	–0.421
0.5594	0.94622	–0.421
0.6433	0.96697	–0.389
0.7345	0.98915	–0.318
0.8453	1.01579	–0.200
0.9309	1.03637	–0.104
1.0000	1.05265	–

TABLE II-S. Continued

x_1	ρ / g cm^{-3}	V_m^E / cm^3 mol^{-1}
1,3-propanediol (1) + 1-propanol (2), T =298.15 K		
0.0000	0.79960	
0.0794	0.81998	–0.108
0.1737	0.84415	–0.213
0.2385	0.86085	–0.282
0.3480	0.88895	–0.367
0.4425	0.91295	–0.402
0.5594	0.94235	–0.403
0.6433	0.96319	–0.371
0.7345	0.98533	–0.291
0.8453	1.01230	–0.188
0.9309	1.03290	–0.085
1.0000	1.04955	
1,3-propanediol (1) + 1-propanol (2), T =303.15 K		
0.0000	0.79554	
0.0794	0.81571	–0.085
0.1737	0.83982	–0.181
0.2385	0.85651	–0.246
0.3480	0.88470	–0.332
0.4425	0.90881	–0.370
0.5594	0.93830	–0.368
0.6433	0.95916	–0.331
0.7345	0.98160	–0.263
0.8453	1.00870	–0.157
0.9309	1.02960	–0.066
1.0000	1.04665	
1,3-propanediol (1) + 1-propanol (2), T = 313.15 K		
0.0000	0.78747	
0.0794	0.80756	–0.077
0.1737	0.83153	–0.159
0.2385	0.84820	–0.220
0.3480	0.87638	–0.301
0.4425	0.90055	–0.338
0.5594	0.93018	–0.338
0.6433	0.95124	–0.308
0.7345	0.97388	–0.245
0.8453	1.00130	–0.149
0.9309	1.02250	–0.066
1.0000	1.03970	

TABLE II-S. Continued

x_1	ρ / g cm^{-3}	V_m^E / cm^3 mol^{-1}
1,3-propanediol (1) + 1-butanol (2), T = 293.15 K		
0.0000	0.80950	–
0.0964	0.82945	–0.115
0.1636	0.84349	–0.154
0.2400	0.85980	–0.180
0.3523	0.88456	–0.193
0.4471	0.90637	–0.195
0.5605	0.93369	–0.191
0.6669	0.96070	–0.186
0.7576	0.98474	–0.173
0.8510	1.01032	–0.134
0.9062	1.02595	–0.107
1.0000	1.05265	–
1,3-propanediol (1) + 1-butanol (2), T = 298.15 K		
0.0000	0.80570	–
0.0964	0.82555	–0.102
0.1636	0.83957	–0.138
0.2400	0.85592	–0.166
0.3523	0.88077	–0.184
0.4471	0.90263	–0.186
0.5605	0.93003	–0.183
0.6669	0.95706	–0.174
0.7576	0.98113	–0.157
0.8510	1.00675	–0.114
0.9062	1.02260	–0.099
1.0000	1.04955	–
1,3-propanediol (1) + 1-butanol (2), T = 303.15 K		
0.0000	0.80212	–
0.0964	0.82190	–0.093
0.1636	0.83590	–0.125
0.2400	0.85227	–0.153
0.3523	0.87719	–0.174
0.4471	0.89913	–0.180
0.5605	0.92660	–0.177
0.6669	0.95370	–0.167
0.7576	0.97780	–0.146
0.8510	1.00355	–0.106
0.9062	1.01931	–0.080
1.0000	1.04665	–

TABLE II-S. Continued

x_1	ρ / g cm^{-3}	V_m^E / cm^3 mol^{-1}
	1,3-propanediol (1) + 1-butanol (2), T = 313.15 K	
0.0000	0.79415	–
0.0964	0.81373	–0.070
0.1636	0.82785	–0.114
0.2400	0.84425	–0.143
0.3523	0.86925	–0.167
0.4471	0.89125	–0.172
0.5605	0.91885	–0.172
0.6669	0.94601	–0.157
0.7576	0.97022	–0.135
0.8510	0.99615	–0.097
0.9062	1.01200	–0.069
1.0000	1.03970	–
	1,3-propanediol (1) + 1-pentanol (2), T = 293.15 K	
0.0000	0.81480	–
0.0847	0.82833	0.041
0.1739	0.84329	0.103
0.2451	0.85591	0.152
0.3546	0.87675	0.212
0.4381	0.89402	0.236
0.5138	0.91079	0.244
0.6511	0.94442	0.216
0.7384	0.96814	0.179
0.8521	1.00228	0.104
0.9391	1.03112	0.036
1.0000	1.05265	–
	1,3-propanediol (1) + 1-pentanol (2), T = 298.15 K	
0.0000	0.81082	–
0.0847	0.82422	0.062
0.1739	0.83914	0.132
0.2451	0.85179	0.180
0.3546	0.87275	0.232
0.4381	0.89008	0.254
0.5138	0.90692	0.261
0.6511	0.94066	0.232
0.7384	0.96450	0.192
0.8521	0.99881	0.114
0.9391	1.02770	0.051
1.0000	1.04955	–

TABLE II-S. Continued

x_1	ρ / g cm^{-3}	V_m^E / cm^3 mol^{-1}
1,3-propanediol (1) + 1-pentanol (2), T = 303.15 K		
0.0000	0.80707	
0.0847	0.82028	0.090
0.1739	0.83513	0.172
0.2451	0.84781	0.219
0.3546	0.86887	0.264
0.4381	0.88627	0.282
0.5138	0.90320	0.284
0.6511	0.93698	0.260
0.7384	0.96089	0.220
0.8521	0.99533	0.140
0.9391	1.02445	0.069
1.0000	1.04665	
1,3-propanediol (1) + 1-pentanol (2), T = 313.15 K		
0.0000	0.79940	
0.0847	0.81239	0.121
0.1739	0.82717	0.214
0.2451	0.83988	0.258
0.3546	0.86101	0.296
0.4381	0.87852	0.305
0.5138	0.89549	0.306
0.6511	0.92931	0.285
0.7384	0.95321	0.251
0.8521	0.98765	0.180
0.9391	1.01715	0.087
1.0000	1.03970	