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SUPPLEMENTARY MATERIAL TO

Prediction of excess molar volumes of binary mixtures by Prigogine–Flory–Patterson (PFP) and extended real association solution (ERAS) models

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TABLE S-I. Parameters of the pure components used in PFP and ERAS models calculations at 298.15 K

Substance	K	$\alpha\times10^4$ / K^{-1}	$\kappa\times10^{10}$ / Pa^{-1}	P^* / J cm^{-3}	V^* / cm^{3}mol^{-1}	Δh^* / kJ mol^{-1}	Δv^* / cm^3 mol^{-1}	S / nm^{-1}
Methanol[1]	986	11.89	11.92	443.6	32.13	–25.1	–5.6	16.49
Ethanol[2]	317	11.20	11.53	411.8	46.90	–25.1	–5.6	15.43
Propan-1-ol[2]	197	10.20	10.06	414.1	61.10	–25.1	–5.6	14.90
Butan-1-ol[2]	175	9.32	9.42	422.7	75.70	–25.1	–5.6	14.56
Butan-2-ol[2]	68	10.30	10.40	388.7	75.40	–25.1	–5.6	14.07
Pentan-1-ol[3]	153	9.05	8.84	411.0	89.76	–25.1	–5.6	14.58
Acetonitrile[4]	0	11.10	11.70	408.0	42.20	–13.2	–2.8	15.19
Hexan-1-amine[5]	0.874	10.68	9.30	495.0	106.87	–13.2	–2.8	0
Benzene[6]	0.6	12.18	9.66	626.3	69.26	–15.0	0	12.43
Chlorobenzene[7]	0.8	9.91	7.65	611.0	82.26	–3.5	–3.0	12.34

TABLE S-II. Interactional parameters, χ_{12}, and contributions of the PFP theory, interactional, free volume and pressure contribution P^* for binary mixtures at T = 298.15 K

Mixture	χ_{12} / J cm^{-3}	Interactional	Free volume	P^* effect
Methanol+benzene	–1.51	–0.01208	–0.00025	0.01210
Ethanol+benzene	–7.77	–0.08232	–0.01058	0.10101
Propan-1-ol+benzene	–6.87	–0.08524	–0.04066	0.21342
Butan-1-ol+benzene	–1.74	–0.02428	–0.07624	0.29901
Butan-2-ol+benzene	25.36	0.35358	–0.03830	0.17076
Methanol+chlorobenzene	–213.72	–1.55626	–0.02805	–0.09270
Ethanol+chlorobenzene	–18.62	–0.18219	–0.01087	–0.07843
Propan-1-ol+chlorobenzene	–15.05	–0.17473	–0.00051	–0.01834

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TABLE S-II. Continued

Mixture	χ_{12} / J cm^{-3}	Interactional	Free volume	P^* effect
Butan-1-ol+chlorobenzene	–12.12	–0.15616	–0.00125	0.03448
Butan-2-ol+chlorobenzene	11.49	0.15262	–0.00212	–0.02818
Pentan-1-ol+chlorobenzene	–9.98	–0.14546	–0.00825	0.07790
Butan-1-ol+n-heptane	–19.79	0.40173	–0.11869	–0.07583
Butan-2-ol+n-heptane	35.46	0.72049	–0.06458	–0.11480
Butan-1-ol+hexylamine	–7.30	–1.15015	–0.01841	0.07602
Methanol+acetonitrile	–18.84	–0.15338	–0.00375	0.00546
Ethanol+acetonitrile	–3.13	–0.03198	–0.00013	0.00007
Hexan-1-amine+*n*-heptane	24.08	0.59286	–0.05009	–0.19555

TABLE S-III. ERAS parameters for binary mixtures at atmospheric pressure and 298.15 K

Mixture	Δv_{AB}^* / cm^3 mol^{-1}	X_{AB} / J cm^{-3}	K_{AB}
Methanol+benzene	–6.68	–12.63	2.64
Ethanol+benzene	–5.74	10.12	179.13
Propan-1-ol+benzene	–6.00	17.92	121.92
Butan-1-ol+benzene	–2.14	–53.42	59.12
Butan-2-ol+benzene	–4.75	6.53	22.16
Methanol+chlorobenzene	–9.27	–25.41	3.44
Ethanol+chlorobenzene	–4.19	–54.56	33.48
Propan-1-ol+chlorobenzene	–3.68	–61.65	28.61
Butan-1-ol+chlorobenzene	–3.38	–67.85	43.87
butan-2-ol+chlorobenzene	–3.55	–36.18	16.79
Pentan-1-ol+chlorobenzene	–3.82	–52.24	23.80
Butan-1-ol+*n*-heptane	–3.28	7.08	22.72
Butan-2-ol+*n*-heptane	–2.73	7.21	22.87
Butan-1-ol+hexan-1-amine	–12.06	56.44	498.5
Methanol+acetonitrile	–5.22	–14.86	27.07
Ethanol+acetonitrile	–5.29	13.25	13.25
Hexan-1-amine+*n*-heptane	–0.50	16.64	–0.51

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