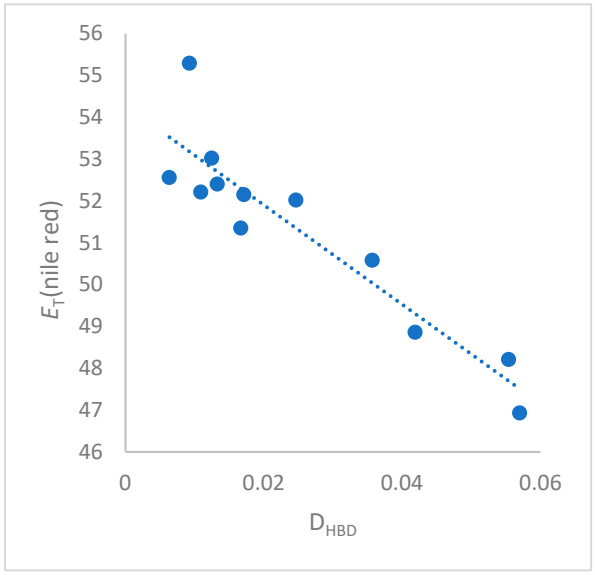
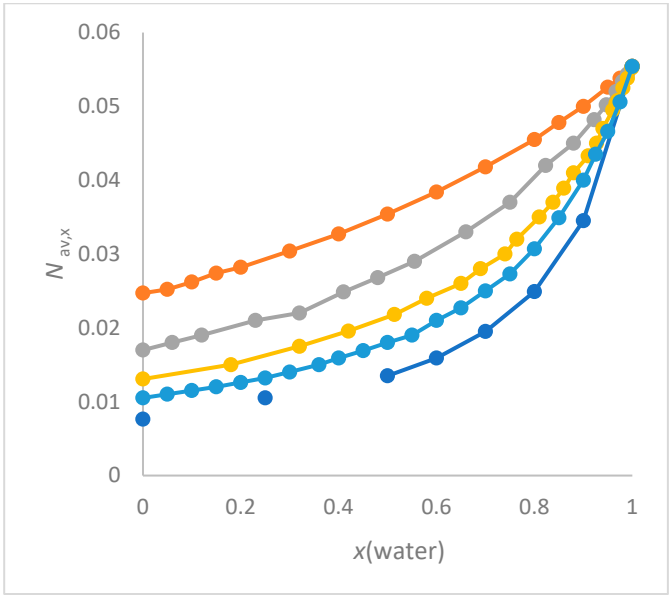
Supplementary material





(**a**) (**b**)

Figure S1a (left panel) Correlation of E_T(nile red) (kcal/mol) as a function of D_{HBD} (mol/cm^3) for protic solvents including water, methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-methyl-2-propanol, ethanolamine, 1,2-ethandiols, 2,2,2-trifluoroethanol and 1,1,1,3,3,3-hexafluoro-2-propanol. The UV/vis-spectroscopic data are taken from ref. [72] and the D_{HBD} parameter from [62]. E_T(nile red) = -118.8 D_{HBD} + 54.3, n = 12, r = 0.924. The correlation supports the D_{HBD} parameter for 2,2,2-trifluoroethanol and 1,1,1,3,3,3-hexafluoro-2-propanol from ref. [62].
FigS1b. (right panel) Plots of $N_{av,x}$ (sum of total OH dipoles) (in mol/cm^3) as a function of x(water) for methanol/water (red dots), ethanol/water (grey dots) 2-propanol/water (yellow dots), 2-methyl-2-propanol/water (light blue dots); 2-n-butoxyethanol/water (deep blue) mixtures, physical data from references [191, 198-202].

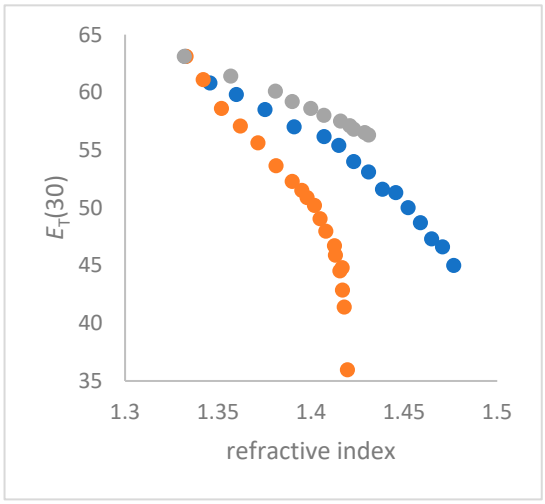


Figure. S2 Plots of E_T(30) (kcal/mol) as a function of n_D^{20} for 1,2-ethanediol/water (grey), DMSO/water (blue) and 1,4-dioxane/water (red) mixtures.

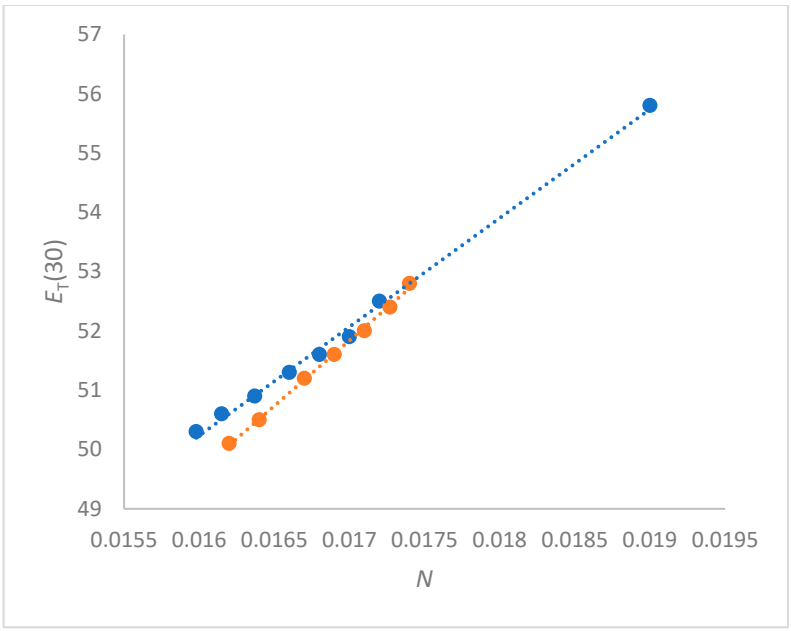
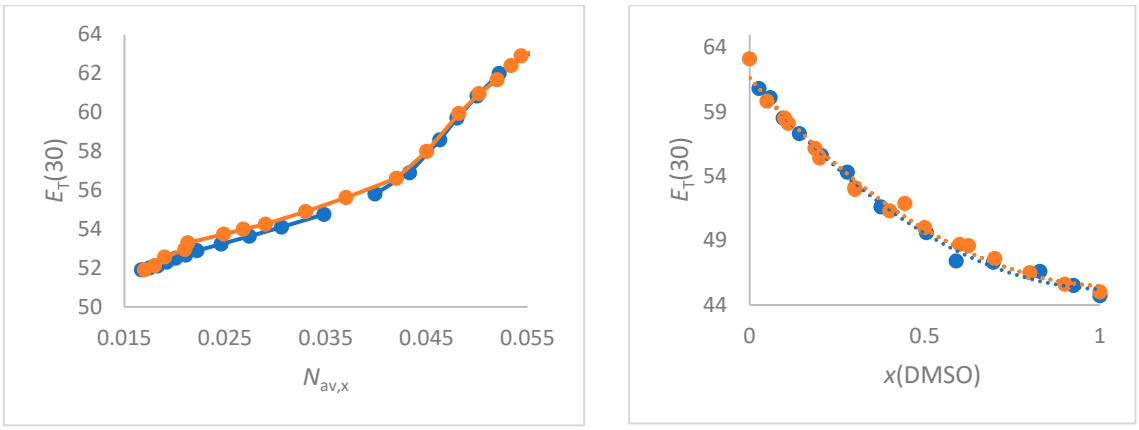


Figure S3. Correlation of E_T30) (in kcal/mol) as a function of N (in mol/cm^3) in the temperature range from -75 to + 75 °C, Reichardt [1] (blue dots) and Linert [116] (red dots). Densities see ref. [218].



(**a**) (**b**)

Figure S4a (left panel). Comparison of $E_T(30)$ (kcal/mol) as a function of $N_{av,x}$ (mol/cm^3) for ethanol/water mixtures. Data from Dimroth/Reichardt [2] (red dots) and data from Rosés [18] (blue dots), (25°C); Figure S4b (right panel). Comparison of $E_T(30)$ (kcal/mol) as a function of x(DMSO) for DMSO/water mixtures data from [12,14, 121, 122] (red dots) (25°C) and data from Connors [15] (blue dots).

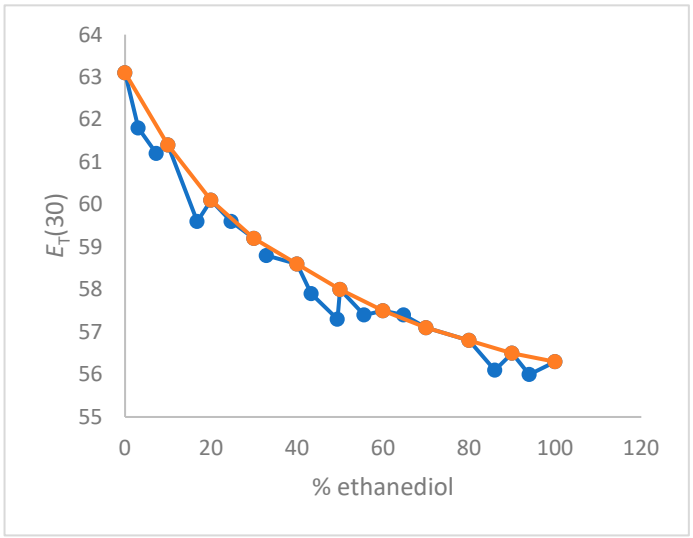


Figure S5. Comparison of $E_T(30)$ (kcal/mol) as a function of x(1,2-ethanediol) (in mol %) for 1,2-ethanediol/water mixtures, data from Kosower/Marcus [12] (red dots) (25 °C) ; data from Connors [15] (blue dots).

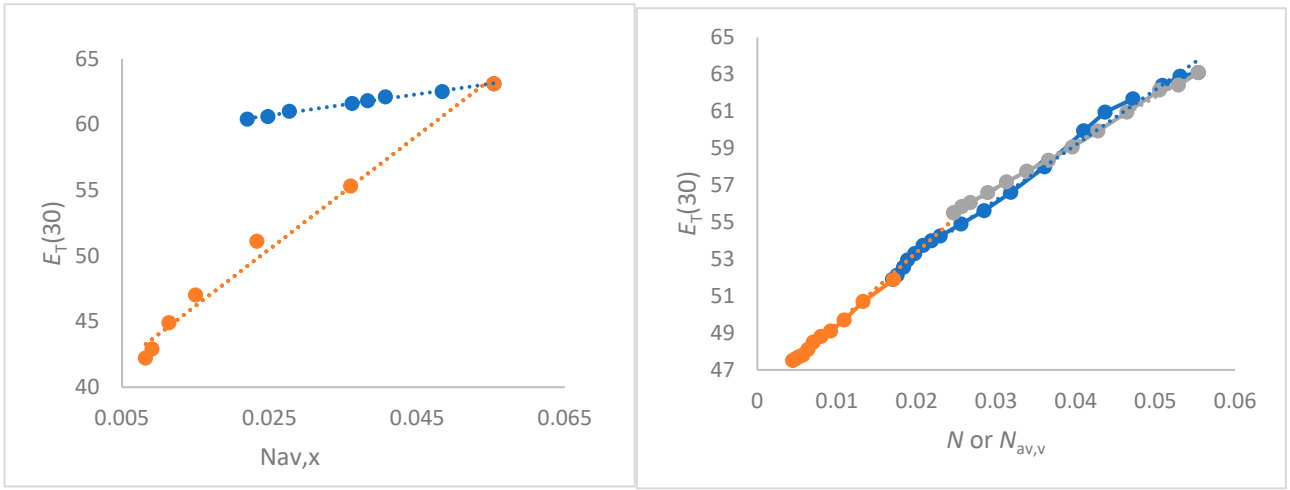


Figure S6a.(left panel) $E_T(30)$ (kcal/mol) as a function of $N_{av,x}$ (mol/cm³) for urea/water (blue) and *N,N`*-dimethylpropyleneurea/water (red) mixtures; data from [143, 144]. $E_T(30)$ (urea/water) = 80.3 + 58.7; n = 8, r = 0.996; $E_T(30)$ *N,N`*-dimethylpropyleneurea /water) = 432 + 39.7; n = 7, r = 0.994; Figure S6b (right panel). Overall correlation of $E_T(30)$ (kcal/mol) as a function of *N* for the homologous series of primary alcohols (red dots) as well as $E_T(30)$ as function of $N_{av,v}$ (mol/cm³) for ethanol/water mixtures (blue dots) and methanol/water mixtures (grey dots). All $E_T(30)$ data are taken from [2,18] and [34].

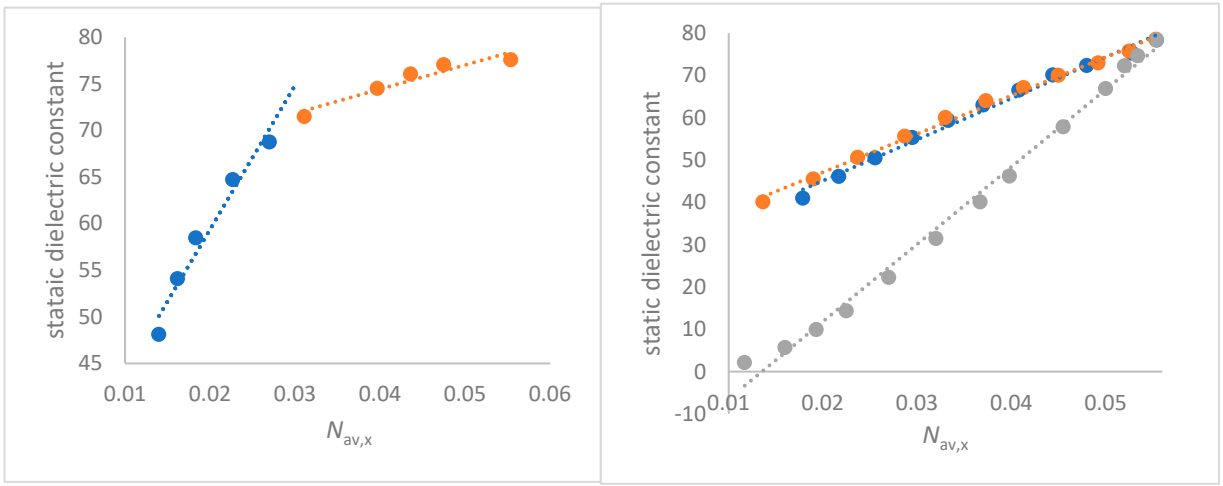


Figure S7a.(left pamel) Correlation of the static dielectric constant of DMSO /water mixtures [151] as a function of $N_{av,x}$ (mol/cm³); Figure S7b (right panel). Correlation of the static dielectric constant ε_r as function of $N_{av,x}$ (mol/cm³) for several co-solvent/water mixtures including the pure co-solvents, 1,4-dioxane/water mixtures [162]: ε_r = 1827 $N_{av,x}$ - 25; n = 11; r = 0.996 (grey dots). The 1,2-ethanediol/water mixtures, ε_r = 975 $N_{av,x}$ + 25; n = 11; r = 0.994 (blue dots) and the glycerol/water mixtures, εr = 908 $N_{av,x}$ - 29; n = 11; r = 0.999 (red dots), are used as independent reference.

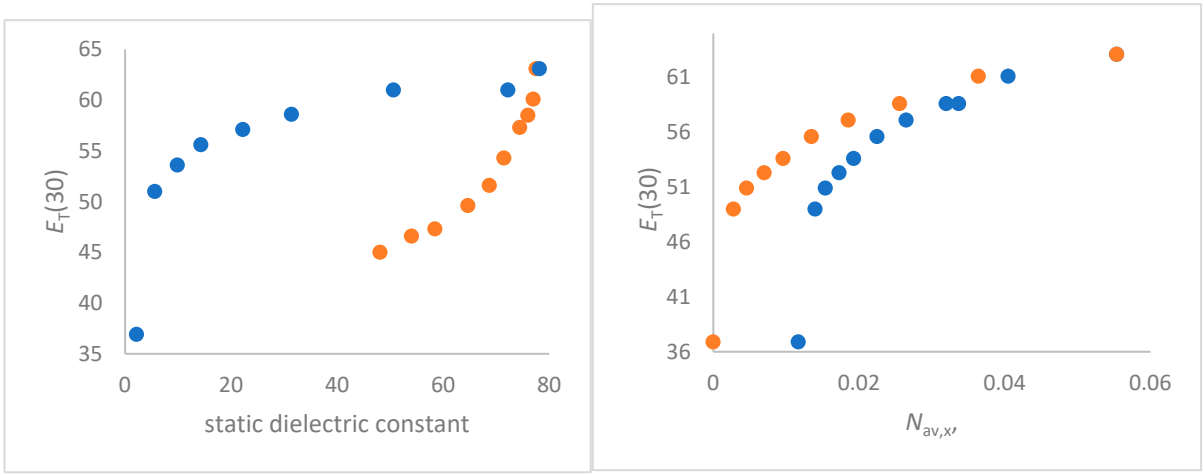


Figure S8a. (left panel) Correlation of $E_T(30)$ (kcal/mol) as a function of the static dielectric constant ε_r for DMSO/water (red) [151] and 1,4-dioxane/water mixtures [162] (blue). Fig. S8b. (right panel) Correlation of $E_T(30)$ (kcal/mol) as a function of $N_{av,x}$ (blue) and $N_{av,x}$(water) (red) for 1,4.dioxane/water mixtures.

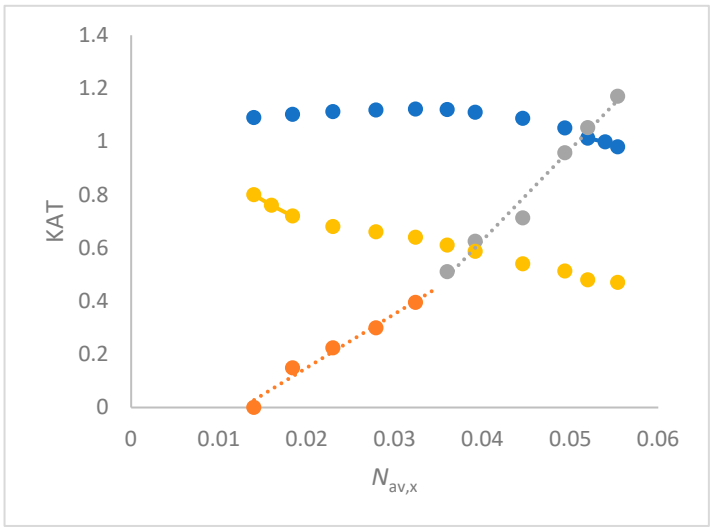


Figure S9 Plots of Kamlet-Taft (KAT) α HBD parameter (red and grey dots), β (HBA) parameter) (yellow dots) and π^* dipolarity/polarizability parameter (blue dots) as a function of $N_{av,x}$ (mol/cm^3) for DMSO/water mixtures [157]. Note the maximum KAT value for π^* corresponds exactly to the kink in the curve for KAT α as a function of $N_{av,x}$ and the inflection point of β versus $N_{av,x}$ at the same composition.

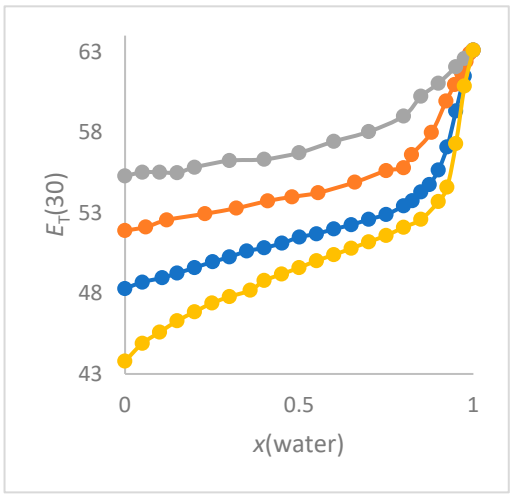


Figure S10. Correlations of $E_T(30)$ as function of x(water) for methanol/water (grey), ethanol/water (red), 2-propanol/water (blue), and 2-methyl-2-propanol/water (yellow) mixtures. Data from [2, 17-19].

Table S1 $E_T(30)$ values for ethanol measured at various temperatures; data from Reichardt and Linert [1, 116] and densities at various temperatures of the ethanol/water mixture [218].

T / °C	Density g/cm³	N mol/cm³	$E_T(30)$ kcal/mol
-75	0.87	0.019	55.8
15	0.7936	0.0172	52.5
25	0.785	0.017	51.9
35	0.7767	0.0168	51.6
45	0.768	0.0166	51.3
55	0.759	0.01637	50.9
65	0.7512	0.01615	50.6
75	0.7428	0.01598	50.3
3.9	0.80309	0.0174	52.8
11.5	0.7956	0.01727	52.4
20.2	0.789	0.0171	52
29.5	0.78138	0.0169	51.6
41.8	0.7709	0.0167	51.2
58	0.7572	0.7572	50.5
67.5	0.749	0.0162	50.1

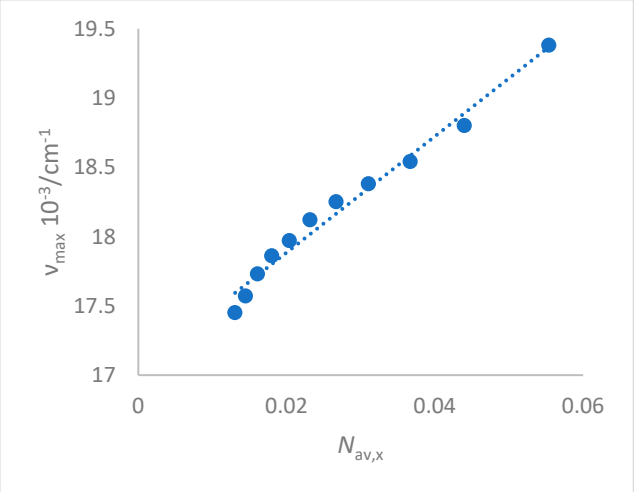


Figure S11. Plot of ν_{max}(**Fe**) [10^3 cm^{-1}] as function of $N_{av,x}$ (mol/cm³) for the 2-propanol/water mixtures [126]. Linear fit: ν_{max}(**Fe**) [10^3 cm^{-1}] = 41.95 $N_{av,x}$ + 17.05; r = 0.99, n = 11.

Table S2. Physical properties of the 1,2-ethanediol/water mixture in terms of mole fractions as well as refractive index and $E_T(30)$ values [12, 130]. $D_{av,x,HBD}$ values are the total concentration of OH dipoles when the partial OH concentration of the 1,2-ethanediol component is taken into account according to Equation (9).

X(water)	Density g/cm³	n_D^{20}	$M_{av,x}$	$N_{av,x}$ mol/cm³	$N_{av,xCH)}$ mol/cm³	$Dav,x,_{HBD}$ mol/cm³	$E_T(30)$ Kcal/mol
1	0.998	1.332	18.015	0.0554	0	0.0554	63.1
0.9	1.03293	1.357	22.42	0.046	0.0184	0.0506	61.4
0.8	1.05685	1.381	26.82	0.0394	0.0315	0.0473	60.1

0.7	1.0734	1.39	31.23	0.0344	0.0413	0.0447	59.2
0.6	1.0844	1.4	35.64	0.0304	0.0486	0.0425	58.6
0.5	1.0921	1.407	40.05	0.0273	0.0546	0.041	58
0.4	1.09744	1.416	44.45	0.0247	0.0593	0.039	57.5
0.3	1.102	1.421	48.84	0.0225	0.063	0.038	57.1
0.2	1.10518	1.423	53.26	0.02075	0.0664	0.037	56.8
0.1	1.1078	1.429	57.66	0.0192	0.069	0.0365	56.5
0	1.10986	1.431	62.07	0.01788	0.0715	0.0357	56.3

Table S3. Physical data of methanol/water mixtures with respect to mole, volume and mass fraction, and $E_T(30)$ values [18]. Physical data from [215-217].

X(water)	$M_{av,v}$ / $M_{av,x}$	Density g/cm³	$M_{av.x}$ g/mol	$M_{av.v}$ g/mol	$N_{av,x}$ mol/cm³	$N_{av,v}$ mol/cm³	$N_{av,w}$ mol/cm³	$E_T(30)$ kcal/mol
1	1	0.998	18.015	18.015	0.0554	0.0554	0.0554	63.1
0.977	1.018	0.988	18.34	18.67	0.0538	0.0529	0.0532	62.42
0.958	1.052	0.98475	18.56	19.54	0.053	0.05054	0.0516	62.15
0.845	1.055	0.971	19.83	20.92	0.049	0.04643	0.0476	60.96
0.84	1.108	0.960	20.24	22.43	0.047	0.0428	0.0449	59.93
0.77	1.122	0.945	21.27	23.88	0.044	0.03957	0.04148	59.07
0.69	1.13	0.927	22.3	25.34	0.0415	0.03658	0.038	58.35
0.6	1.138	0.91	23.62	26.88	0.0385	0.03385	0.036	57.76
0.49	1.123	0.885	25.16	28.256	0.035	0.03132	0.0328	57.18
0.36	1.096	0.85688	26.97	29.57	0.0318	0.02897	0.03	56.6
0.198	1.054	0.8259	29.27	30.85	0.0282	0.02677	0.0272	56.06
0.106	1.031	0.81	30.54	31.49	0.0265	0.02572	0.026	55.84
0	1	0.791	32.04	32.04	0.0247	0.02471	0.02471	55.5

Table S4. $E_T(30)$ and $E_T(1)$ values, density, average molar masses, average molar concentrations in ethanol/water mixtures. Data from Reichardt [1,2]. Physical solvent mixture are data from [215-217].

X(water)	density	$M_{av.x}$ g/mol	$N_{av,x}$ mol/cm³	M_{avw} g/mol	$M_{av.w}$ / $M_{av.x}$	$N_{av,w}$ mol/cm³	$M_{av.w}$ g/mol	$E_T(30)$ Kcal/mol	$E_T(1)$ Kcal/mol
1	0.9982	18.015	0.0554	18.015	1	0.0554	18.015	63.1	69.1
0.99	0.9945	18.29	0.0544	18.57	1.015	0.0535	18.71	62.9	
0.98	0.99106	18.57	0.0533	19.13	1.03	0.0518	19.414	62.4	
0.967	0.98476	18.94	0.052	20.26	1.07	0.0486	20.8	61.68	68.6
0.947	0.97897	19.5	0.0519	21.38	1.096	0.0458	22.2	60.96	
0.922	0.9736	20.2	0.0464	22.5	1.114	0.0433	23.6	59.94	67.4
0.88	0.9622	21.4	0.045	24.89	1.163	0.0386	26.43	57.99	66.2
0.823	0.9485	22.5	0.042	27.27	1.212	0.0348	29.34	56.61	64.8
0.8	0.9415	23.6	0.0399	28.96	1.227			55.8	
0.75	0.93017	25.03	0.0372	29.9	1.194	0.0311	32.035	55.62	64.0
0.66	0.90916	27.55	0.033	32.59	1.183	0.0279	34.84	54.9	63.5
0.555	0.8856	30.5	0.029	35.185	1.15	0.0252	37.65	54.25	63
0.48	0.8728	32.6	0.0267	37.035	1.136	0.0236	39.05	53.99	
0.41	0.8593	34.56	0.0247	38.55	1.115	0.0223	40.46	53.74	62.6
0.32	0.8449	37.08	0.0228	40.41	1.09	0.0209	41.86	53.29	
0.23	0.8293	39.61	0.0209	42.086	1.0625	0.0197	43.28	52.95	61.9
0.12	0.81145	42.7	0.019	43.96	1.03	0.0185	44.66	52.56	
0.06	0.80165	44.38		44.95	1.013	0.0178	45.33	52.12	
0	0.7893	46.07	0.017	46.07	1	0.017	46.07	51.9	61.2

Table S5. Physical properties and $E_T(30)$ values of the formamide/water mixtures [21, 120, 137, 138].

X(water)	Density g/ml	$M_{av.x}$ g/mol	$N_{av.x}$ mol/cm^3	$E_T(30)$ kcal/mol
0	1.1273	45.04	0.025	55.8
0.02	1.1261	44.49	0.0253	55.9
0.04	1.1235	43.96	0.0255	56
0.1	1.1152	42.33	0.026	56.3
0.102	1.115	42.28	0.02637	56.3
0.1083	1.1049	49.62	0.02756	56.6
0.3	1.0923	37.48	0.029	57
0.35	1.0832	35.58	0.0304	57.3
0.36	1.0819	35.3	0.0306	57.3
0.4	1.076	34.23	0.0314	57.4
0.422	1.074	33.63	0.0319	57.6
0.488	1.065	31.85	0.033	57.9
0.516	1.0612	31.15	0.0341	58.0
0.528	1.06	30.76	0.0345	58.2
0.56	1.0559	29.9	0.0353	58.2
0.6	1.0509	28.82	0.036	58.5
0.613	1.049	28.47	0.0368	58.4
0.638	1.0457	27.77	0.0376	58.6
0.7	1.0379	26.12	0.0397	59.3
0.8	1.025	23.42	0.0437	60.2
0.9	1.012	20.24	0.05	61.4
1	0.998	18.015	0.0554	63.1

Table S6. The *N*-methylformamide (NMF) /water mixtures. X(water), M_{avx}, $N_{av,x}$. Data from [139, 219]. $E_T(30)$data from [21].

X(water)	M_{avx}	Density g/cm^3	$N_{av,x}$ mol/cm^3	$E_T(30)$ kcal/mol
1	18.015	0.997	0.0554	63.1
0.91	21.7	1.009	0.0465	60.1
0.89	22.53	1.0103	0.0448	59,6
0.83	24.99	1.013	0.0405	58,8
0.78	27.05	1.015	0.0375	58,2
0.71	29.92	1.01657	0.034	57,4
0.66	31.99	1.01625	0.0317	57,2
0.62	33.6	1.015	0.0302	56,9
0.55	36.51	1.014	0.0278	56,45
0.32	45.9	1.007	0.022	55,4
0.3	46.75	1.006	0.0215	55,2
0.16	52.5	1.002	0.0191	54,6
0.13	53.72	1.002	0.0186	54,5
0.07	56.19	1.00072	0.0178	54,3
0	59.067	0.99929	0.017	54,1

Table S7. The dimethylformamide (DMF)/water mixtures, physical data and $E_T(30)$ values [21, 141, 142, 220].

X(water)	Density g/cm3	$M_{av.x}$ g/mol	$N_{av.x}$ mol/cm^3	$E_T(30)$ kcal/mol
1	0.998	18.015	0.0554	63.1

0.96				60.2
0.945	0.9955	21.13	0.0469	59.9
0.93	0.996	21.32	0.0467	59.2
0.92	0.997	22.421	0.0448	58.5
0.91	0.997	22.97	0.0434	58.2
0.85	0.9968	26.27	0.0379	56.2
0.75	0.9937	31.78	0.03126	54
0.65	0.964	37.3	0.0258	51.9
0.55	0.9799	42.78	0.0229	50.05
0.45	0.971	48.29	0.02	49.3
0.355	0.964	53.5	0.018	48
0.25	0.9578	59.3	0.0162	46.8
0.214	0.956	61.34	0.0156	46.4
0.17	0.9533	63.8	0.0149	45.8
0.12	0.95	66.48	0.0143	45.2
0.06	0.947	69.6	0.0136	44.4
0.055	0.9462	70.07	0.0135	44.0
0	0.943	73.09	0.0129	43.7

Table S8. The *N*-formylmorpholine /water mixtures, $N_{av.x}$, refractive index and $E_T(30)$ values [32, 221, 222].

X(water)	Density g/cm³	M_{avx} g/mol	$N_{av.x}$ mol/cm³	$N_{av,xCH)}$ mol/cm³	n_D^{20}	$E_T(30)$ Kcal/mol
0	1.146	115.13	0.0099	0.0891	1.4898	44.63
0.05	1.145	110.3	0.0104			45.12
0.15	1.144	100.56	0.01137	0.087	1.4878	46.14
0.2	1.143	95.7	0.012	0.0864	1.485	46.66
0.25	1.142	90.85	0.0125			47.2
0.3	1.14	86	0.01325	0.08347	1.481	47.47
0.35	1.139	81.13	0.014			48.3
0.4	1.138	76.3	0.0157	0.08478	1.475	48.82
0.45	1.1365	71.4	0.0159			49.36
0.5	1.135	66.57	0.017	0.0765	1.470	49.93
0.55	1.1325	61.7	0.01835			50.61
0.6	1.13	56.85	0.02			51.29
0.65	1.125	51.99	0.02164	0.068	1.458	51.93
0.7	1.122	47.14	0.0238	0.06426	1.448	52.82
0.75	1.115	42.28	0.0264			53.58
0.8	1.1	37.43	0.0294	0.053	1.433	54.71
0.85	1.088	32.57	0.0334			55.82
0.9	1.06	27.7	0.0382	0.03438	1.396	57.25
0.95	1.043	22.86	0.0456			59.9
1	0.997	18.015	0.05541	0	1.335	63.1

Table S9. Physical properties and $E_T(30)$ values of DMSO/water mixtures from different literature sources [12,15], Density from [146, 148].

X(water)	Density g/cm³	$M_{av.x}$ g/mol	$N_{av.x}$ mol/cm³	$E_T(30)$ kcal/mol
1	0,997	18,015	0,0554	63,1
0,973	1,0116	19,64	0,0515	60,8
0,9451	1,02145	21,3	0,0479	59,8
0,941	1,0242	21,56	0,0475	60,1

0,904	1,0387	23,79	0,0436	58,5
0,9	1,04209	24,03	0,043	58,5
0,8895	1,045	24,66	0,0423	58,1
0,858	1,055	26,55	0,0397	57,3
0,8129	1,06865	29,26	0,0365	56,16
0,8	1,07163	30,04	0,0357	55,4
0,721	1,0837	34,8	0,0311	54,3
0,6984	1,088	36,14	0,03	52,96
0,7	1,085	36,05	0,03	53,1
0,625	1,094	40,56	0,027	51,6
0,6	1,09515	42,06	0,026	51,3
0,5569	1,097	44,65	0,0245	51,9
0,5	1,09794	48,07	0,0228	50
0,495	1,098	48,38	0,0227	49,6
0,41	1,0989	53,48	0,0205	47,4
0,4	1,0989	54,1	0,0203	48,7
0,375	1,0989	55,58	0,0197	48,6
0,305	1,0986	59,86	0,01835	47,3
0,3	1,09844	60,1	0,0183	47,6
0,2	1,0967	66,1	0,0166	46,5
0,171	1.0966	67,85	0,0162	46,6
0,1	1,0965	72	0,0152	45,6
0,075	1,096	73,63	0,0149	45,5
0	1,09528	78,13	0,014	45

Table S10. Physical properties of the 1,4-dioxane/water mixtures in terms of mole and volume fractions as well as refractive index and $E_T(30)$ values, data from [2, 159-162, 165].

X(water)	Density g/cm^3	n_D^{20}	$M_{av,x}$ g/mol	$N_{av,x}$ mol/cm^3	$M_{av,v}$ g/mol	$N_{av,v}$ mol/cm^3	$E_T(30)$ kcal/mol
1	0.9971	1.333	18.015	0.0554	18.015	0.0554	63.1
0.985	1.004		19.06	0.0527			61.9
0.977	1.0068	1.3422	19.63	0.0513	25.02	0.0402	61.09
0.971	1.0095		20.04	0.0504			60.5
0.95	1.0158	1.352	21.52	0.0472	32.03	0.0317	58.6
0.943	1.018		22.01	0.0463			58.4
0.917	1.023	1.3621	23.83	0.0429	39.03	0.0262	57.07
0.913	1.0235		24.11	0.0424			57
0.877	1.0285	1.3716	26.63	0.0386	46.05	0.0223	55.62
0.857	1.031		28.04	0.0367			54.8
0.826	1.034	1.3813	30.21	0.034	53.06	0.0189	53.64
0.759	1.0365	1.39	34.9	0.0297	60.08	0.0173	52.27
0.74	1.0367		36.24	0.0286			52.1
0.718	1.037	1.3952	37.78	0.0274	63.57	0.0163	51.5
0.67	1.0372	1.398	41.14	0.0252	67.08	0.0155	50.87
0.612	1.0366	1.402	44.58	0.0232	70.58	0.0147	50.2
0.542	1.035	1.405	49.98	0.0207	74.09	0.014	49.04
0.515	1.0340		52.01	0.0199			48.8

0.455	1.0344	1.4081	56.2	0.0184	77.59	0.0133	47.97
0.345	1.0328	1.4127	63.9	0.0162	81.1	0.0127	46.7
0.34	1.0328		64.28	0.01606			46.5
0.3	1.0322	1.4132	67.08	0.0154	82.5	0.0125	45.89
0.25	1.0315	1.4156	70.58	0.0146	83.9	0.0123	44.53
0.199	1.0307	1.4168	74.16	0.0139	84.6	0.0122	44.8
0.17	1.03	1.417	76.2	0.0135	85.3	0.0121	42.86
0.1	1.0294	1.418	81.1	0.0127	86.7	0.0118	41.4
0	1.028	1.4197	88.11	0.01166	88.11	0.01166	35.96

Table S11. Physical properties of 2-propanol/water mixtures [215-217] and $E_T(30)$ values [2,18,19].

X(water)	density	$M_{av.x}$	$N_{av.x}$ Mol/cm^3	$M_{av.w}$	$M_{av.w}$ / $M_{av.x}$	$E_T(30)$ Kcal/mol
0	0.7835	60.095	0.01304	60.095	1	48.3
0.05	0.788	58	0.0136	59.17	1.02	48.7
0.107	0.793	55.6	0.01426	58.04	1.044	48.97
0.15	0.795	53.78	0.01478	57.98	1.078	49.26
0.2	0.801	51.68	0.0155			49.6
0.252	0.804	49.57	0.0162			49.97
0.3	0.812	47.44	0.017	55.31	1.166	50.26
0.35	0.819	45.36	0.018			50.63
0.4	0.827	43.27	0.019	53.09	1.227	50.83
0.451	0.835	41.16	0.02			51.12
0.501	0.84	39.05	0.0215	50.4	1.29	51.5
0.55	0.85	36.95	0.023		1.3188	51.7
0.6	0.858	34.85	0.0246	47.04	1.349	52.00
0.65	0.866	32.74	0.02645		1.377	52.26
0.7	0.877	30.64	0.0286	44.55	1.3967	52.6
0.75	0.894	28.53	0.0313		1.407	52.9
0.8	0.9117	26.42	0.0345	37.15	1.406	53.43
0.825	0.9203	25.36	0.0363			53.75
0.85	0.9288	24.3	0.0382	33.6	1.383	54.3
0.874	0.937	23.27	0.0403			54.75
0.9	0.945	22.3	0.0424	29.5	1.323	55.66
0.925	0.953	21.17	0.045			57.09
0.95	0.968	20.11	0.0481	24.3	1.208	59.32
0.975	0.982	19.06	0.051			61.49
1	0.997	18.015	0.0053	18.015	1	63.1

Table 12a. $E_T(30)$, density, various average molar masses and corresponding molar concentrations of 2-methyl-2-propanol/water mixtures, data from [173, 174]. $E_T(30)$values, data from [19]..

X (water)	Density g/cm^3	$M_{av.x}$ g/mol	$N_{av,x}$ mol/cm^3	$M_{av.w}$ g/mol	$M_{av.w}$ / $M_{av.x}$	$N_{av,w}$ mol/cm^3	$E_T(30)$ kcal/mol
0	0.78	74.12	0.0105	74.12	1	0.0105	43.8
0.05	0.783	71.3	0.011	73.38	1.03	0.0107	44.9
0.10	0.787	68.5	0.0115	72.9	1.064	0.0108	45.6
0.15	0.79	65.7	0.012	71.8	1.093	0.011	46.3
0.20	0.794	62.9	0.0126	70.91	1.127	0.0112	46.86
0.25	0.795	60.1	0.0132	69.9	1.163	0.01137	47.4
0.30	0.802	57.3	0.014	68.83	1.2	0.01165	47.8
0.36	0.812	53.9	0.015	67.38	1.25	0.012	48.2
0.40	0.825	51.67	0.0159	66.3	1.283	0.0124	48.8
0.45	0.826	48.87	0.0169	64.52	1.32	0.0128	49.2

Table 12a. $E_T(30)$, density, various average molar masses and corresponding molar concentrations of 2-methyl-2-propanol/water mixtures, data from [173, 174]. $E_T(30)$values, data from [19]..

X (water)	Density g/cm³	$M_{av.x}$ g/mol	$N_{av,x}$ mol/cm³	$M_{av.w}$ g/mol	$M_{av.w}$ / $M_{av.x}$	$N_{av,w}$ mol/cm³	$E_T(30)$ kcal/mol
0.50	0.833	46.07	0.018	63.11	1.37	0.0132	49.6
0.55	0.848	43.3	0.02194	60.76	1.403	0.014	50.03
0.60	0.85	40.46	0.021	59.14	1.462	0.0143	50.4
0.65	0.857	37.65	0.0227	56.67	1.505	0.0151	50.8
0.70	0.872	34.8	0.025	53.8	1.546	0.0162	51.2
0.75	0.8734	32.04	0.0273	50.44	1.574	0.0173	51.6
0.80	0.898	29.23	0.0307	46.46	1.59	0.019	52.1
0.85	0.922	26.43	0.0349	41.63	1.575	0.022	52.6
0.90	0.947	23.62	0.04	35.63	1.508	0.0266	53.7
0.925	0.958	22.03	0.0435	31.7	1.439	0.0302	54.6
0.95	0.97	20.8	0.0466	27.93	1.32	0.0347	57.3
0.975	0.983	19.413	0.0506	23.36	1.2	0.042	60.87
1	0.997	18.015	0.0554	18.015	1	0.0554	63.1

Table S12b. Refractive index, density, average molar masses, average molar concentrations of 2-methyl-2-propanol/water mixtures, data from [173,174]. $E_T(30)$values, data from [19].].

$M_{av.v}$ g/mol	$N_{av,v}$ mol/cm³	n_D^{20}	$N_{av,x,CH}$ mol/cm³	$N_{av,x}$ mol/cm³	$E_T(30)$ kcal/mol
18.015	0.0554	1.332	0	0.0554	63.1
28.8	0.0345	1.3483	0.0114	0.0506	57.3
37.3	0.025	1.3588	0.021	0.0466	53.7
43.4	0.0213	1.3655	0.0294	0.0435	52.6
48.44	0.0187	1.3698	0.036	0.04	52.1
52.1	0.0169	1.3725	0.0471	0.0349	51.6
55.18	0.0158	1.3744	0.0553	0.0307	51.6
58	0.0149	1.3759	0.0614	0.0273	51.2
60.1	0.014	1.3771	0.0675	0.025	50.8
61.98	0.0135	1.3782	0.0715	0.0227	50.4
63.68	0.013	1.3792	0.0756	0.021	50
65.12	0.0127	1.38	0.0794	0.0196	49.6
66.4	0.0124	1.3805	0.081	0.018	49.2
67.6	0.012	1.3809	0.0856	0.0169	48.8
68.56	0.0119	1.3813	0.0858	0.0159	48.2
69.5	0.0116	1.3816	0.0864	0.015	
70.42	0.0114	1.3818	0.0882	0.014	47.8
71.15	0.0112	1.3819	0.0891	0.0132	47.4
71.9	0.011	1.382	0.0907	0.0126	46.8
73.3	0.0107	1.3821	0.0918	0.012	46.3
73.1	0.0107	1.3821	0.09315	0.0115	45.6
73.63	0.01063	1.382	0.094	0.011	44.9
74.12	0.0105	1.3822	0.0945	0.0105	43.8

Table S13. Physical data and $E_T(30)$values, data from [8], for the 2-Butoxyethanol (BE)/water mixtures at 25°C, physical data from [191].

X(water)	Density g/cm³ (293K)	n_D^{20}	$M_{av,x}$ g/mol	$N_{av,x}$ mol/cm³	$N_{av,x,CH}$ Mol/cm³	$E_T(30)$ kcal/mol
1	0.998	1.333	18.015	0.0554	0	63.1
0.989	0.99643		19.12	0.052	0.00744	59.9
0.98	0.9949		20.018	0.0497	0.013	55.04
0.97	0.9893		21.02	0.0468	0.018	53.58
0.96	0.9872		22.021	0.0448	0.0233	53.24
0.95	0.984		23.022	0.04274	0.0278	53.04
0.914	0.976		25.52	0.0382	0.0372	53.16
0.9	0.969	1.3766	28.03	0.0346	0.045	53.11
0.8	0.95015	1.394	38.04	0.0249	0.0647	
0.7	0.9375	1.4036	48.06	0.0195	0.076	
0.6	0.92776	1.4091	58.07	0.0159	0.0827	
0.5	0.92	1.4128	68.1	0.0135	0.08775	
0.4	0.915	1.4153	78.1	0.0117	0.09126	
0.3	0.9105	1.417	88.1	0.01033	0.094	
0.2	0.9068	1.4182	98.12	0.0092	0.0955	
0.1	0.9038	1.4191	108.15	0.0083	0.09711	
0	0.90118	1.4196	118.17	0.00762	0.099	50.1