Supplementary matrial

for "1-Propanol Probing Methodology: Two-dimensional Characterization of the Effect of Solute on H2O"

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Table S1
Hydrophobicity/hydrophilicity Indices

# in map	solute	abbrev.	Class	ref.	hydrophobicity *a*	hydrophilicity *b* (kJ/mol)	*nH*	error +/- for *nH*
{0}	H2O	H2O	origin	1	0.00	0		
{1}	methanol	ME	hydrophobe	2	-0.21	-905	3	1
{2}	Ethanol	ET	hydrophobe	3	-0.47	-788	9	1
{3}	2-propanol	2P	hydrophobe	4	-0.80	-167	16	1
{4}	1-propanol	1P	hydrophobe	1	-1.00	0	20	0.5
{5}	t-butanol	TBA	hydrophobe	6	-1.44	943	29	1
{6}	2-butoxyethanol	BE	hydrophobe	7	-2.83	0	58	1
{7}	Glycerol	Gly	hydrophile	8	-0.15	-1180	2	1
{8}	urea	UR	hydrophile	7	0.00	-1210		
{8A}		UR(agg)	hydrophile	7	0.00	-390		
{9}	DMSO	DMSO	amphiphile	3	-0.17	-1388	3	1
{10}	Na+	Na+	hydration center	9, 10	-0.30	0	5.2	
{11}	F-	F-	hydration center	9	-0.72	0	14	2
{12}	Cl-	Cl-	hydration center	9, 10	-0.16	0	2.3	0.6
{13}	SO4-(2-)	SO4(2-)	hydrophobe-like hydration center	11	-0.72	3890	14	2
{14}	Br-	Br-	hydrophile	9	0.00	-920		
{15}	I-	I-	hydrophile	9	0.00	-2050		
{16}	Ethylene glycol	EG	hydrophile	2	-0.15	-1100	2	1
{17}	1,2-propanediol	12P	amphiphile	12	-0.52	-790	10	2
{18}	1,3-propendiol	13P	amphiphile	12	-0.43	-1020	8	2
{19}	acetone	AC	amphiphile	13	-0.58	-1448	11	2
{20}	PEG-200	PEG-2	amphiphile	6	-0.57	-3834	11	2

{21}	PEG-600	PEG-6	amphiphile	6	-2.19	-8870	44	5
{22}	Glucose	GL	amphiphile	1	-0.20	-1262	3	1
{23}	fructose	FR	amphiphile	14	-0.37	-1262	7	2
{24}	sucrose	SUC	amphiphile	1	-0.70	-2100	14	2
{24A}		SUC(agg)	amphiphile	1	-0.14	-2100	2	1
{25}	trehalose	TRE	amphiphile	1	-0.71	-2100	14	2
{25A}		TRE(agg)	amphiphile	1	-0.20	-2100	3	1
{26}	trimethyl ammonium oxide	TMAO	amphiphile	7	-0.35	-328	6	2
{27}	tetramethyl urea	TMU	amphiphile	13	-0.63	-3406	12	3
{28}	tetra-methyl-ammonium	TMA+	hydrophile	15	0.00	-1182		
{29}	NH4+	(NH4)+	hydration center	15	-0.10	0	1	1
{33}	Ca(2+)		hydration center	15	-0.34	0	6	2
{34}	ClO4-		hydrophile	16	-0.02	-2798	0	1
{35}	SCN-		hydrophile	16	-0.02	-2798	0	1
{36}	Tartrate-	TRT(2-)	hydrophobe-like hydration center	11	-0.72	2270	14	2
{37}	formate-	Ofm-	hydration center	17	-0.11	0	1.2	0.5
{38}	acetate-	Oac-	hydrophobe	16,17	-0.22	0	3.7	0.7
{39}	propionate-	Opr-	hydrophobe	17	-0.48	0	9	2
{40}	1-ethyl-3-methylimidazolium	C2mim]+	amphiphile	18	-0.39	-1970	7	2
{41}	1-butyl-3-methylimidazolium	[C4mim]+	amphiphile	19	-1.31	-3227	26	4
{41A}		(agg)	amphiphile	19	-0.49	-1390	9	2
{42}	1-butyl-2,3-dimethyl IM	[C4C1mir	amphiphile	18	-1.85	-6760	37	5
{42A}		(agg)	amphiphile	18	-0.24	-2300	4	1
{43}	PF6-	PF6-	amphiphile	20	-0.67	-3835.0409	13	3
{44}	trifluoromethylsufonate	Otf-	amphiphile	20	-0.67	-2370.00903	13	3
{45}	bis(trifluoromethylsulfonyl)imid	NTf2-	amphiphile	20	-4.08	-8150.04487	84	7
{46}	tetraethylammonium ion	TEA+	hydrophile	5	-0.09	-2270	0.9	0.5

#	solute	Abbre	class	ref	*a*	*b*	*nH*	error +/-

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D	state change
0.00	
-0.21	
-0.39	
-0.64	
0.80	
1.16	
2.26	
-0.21	
-0.17	xUR<0.08
-0.06	0.08<xUR<0.2
-0.24	
0.24	
0.58	
0.13	
0.80	
-0.13	
-0.29	
-0.20	
-0.43	
-0.37	
-0.51	
-0.71	

-2.16	
-0.24	
-0.35	
-0.64	0<xS0<0.007
-0.32	0.007<xS0< 0.03
-0.64	0<xS0<0.009
-0.34	0.009<xS0< 0.03
-0.29	
-0.70	
-0.17	
0.08	
0.27	
-0.40	
-0.40	
0.66	
0.08	
0.18	
0.38	
-0.42	
-1.14	xS0<0.013
-0.44	xS0 > 0.013
-1.77	xS0<0.006
-0.38	xS0 > 0.006
-0.77	
-0.63	
-3.47	
-0.33	

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