Comparison of Implicit and Explicit Solvent Models for the Calculation of Solvation Free Energy in Organic Solvents

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1 List of molecules name

Table S1: Molecule name and CAS number for each molecule

Molecule name	Formula	CAS number
1,2-dichloroethane	$C_2H_4Cl_2$	107-06-2
1-butanol	$C_4H_{10}O$	71-36-3
1-chlorobutane	C_4H_9Cl	109-69-3
1-octanol	$C_8H_{18}O$	111-87-5
1-pentanol	$C_5H_{12}O$	71-41-0
2-hexanone	$C_6H_{12}O$	591-78-6
2-methyl-2-butanol	$C_5H_{12}O$	75-85-4
2-methyl-2-propanol	$C_4H_{10}O$	75-65-0
2-methylpyridine	C_6H_7N	109-06-8
3-methylpyridine	C_6H_7N	108-99-6
acetone	C_3H_6O	67-64-1
acetonitrile	C_2H_3N	75-05-8
acetophenone	C_8H_8O	98-86-2
anisole	C_7H_8O	100-66-3
benzaldehyde	C_7H_6O	100-52-7
benzonitrile	C_7H_5N	100-47-0
chloroform	$CHCl_3$	67-66-3
cyclohexanone	$C_6H_{10}O$	108-94-1
dibromomethane	CH_2Br_2	74-95-3
dibutyl ether	$C_8H_{18}O$	142-96-1
dichloromethane	CH_2Cl_2	75-09-2
diethylamine	$C_4H_{11}N$	109-89-7
diethyl sulfide	$C_4H_{10}S$	352-93-2

Table S1: Molecule name and CAS number for each molecule

Molecule name	Formula	CAS number
diisopropyl ether	$C_6H_{14}O$	108-20-3
dimethyl ether	C_2H_6O	115-10-6
dimethyl sulfoxide	C_2H_6SO	67-68-5
ethanol	C_2H_6O	64-17-5
ethyl acetate	$C_4H_8O_2$	141-78-6
ethylbenzene	$C_8H_{10}O$	100-41-4
formaldehyde	CH_2O	50-00-0
isopropylbenzene	C_9H_{12}	98-82-8
methanol	CH_4O	67-56-1
methyl acetate	$C_3H_6O_2$	79-20-9
morpholine	C_4H_9NO	110-91-8
n-butylamine	$C_4H_{11}N$	109-73-9
nitrobenzene	$C_6H_5NO_2$	98-95-3
nitromethane	CH_3NO_2	75-52-5
N-methylformamide	C_2H_5NO	123-39-7
N,N-dimethylacetamide	C_4H_9NO	127-19-5
N,N-dimethylformamide	C_3H_7NO	68-12-2
o-xylene	C_8H_{10}	95-47-6
phenol	C_6H_6O	108-95-2
pyridine	C_5H_5N	110-86-1
tetrahydrofuran	C_4H_8O	109-99-9
thiophene	C_4H_4S	110-02-1
toluene	C_7H_8	108-88-3
triethylamine	$C_6H_{15}N$	121-44-8

Table S1: Molecule name and CAS number for each molecule

Molecule name	Formula	CAS number
triethyl phosphate	$C_6H_{15}PO_4$	78-40-0

2 Solvent properties

Table S2: Experimental dielectric constants (ε), density (ρ), molar mass (M), surface tension (γ) and isothermal compressibility (κ_T) of solvents at room temperature and number of heavy atoms per solvent molecule (N_{heavy}). Data from Web server at `http://virtualchemistry.org`[1–4]

IUPAC name	ε	ρ (kg/m^3)	M (g/mol)	γ (mN/m)	κ_T (GPa^{-1})	N_{heavy}
1-octanol	9.86	821.80	130.23	27.10	0.76	9
acetone	20.49	784.40	58.08	22.72	1.32	4
acetonitrile	35.69	776.00	41.05	28.66	1.07	3
acetophenone	17.22	1023.40	120.15	39.04	0.56	9
benzonitrile	25.59	1001.00	103.12	38.79	0.68[a]	8
chloroform	4.71	1479.10	119.38	26.67	1.03	4
cyclohexanone	15.62	941.90	98.14	34.57	0.66	7
dibutyl ether	3.05	764.00	130.23	22.40	0.96[b]	9
dimethyl sulfoxide	46.40	1095.00	78.13	42.92	0.52	4
ethyl acetate	5.99	894.00	88.10	23.39	1.20	6
methanol	31.49	786.60	32.04	22.07	1.25	2
methyl acetate	6.68	927.00	74.08	24.73	1.14	5
N-methylformamide	181.56	999.00	59.07	38.50	0.56	4
nitromethane	36.56	1129.00	61.04	36.53	0.72	4

[a] calculated at 288K[1]
[b] calculated at 298.15K[1]

Table S2: Experimental dielectric constants (ε), density (ρ), molar mass (M), surface tension (γ) and isothermal compressibility (κ_T) of solvents at room temperature and number of heavy atoms per solvent molecule (N_{heavy}). Data from Web server at `http://virtualchemistry.org`[1–4]

IUPAC name	ε	ρ (kg/m^3)	M (g/mol)	γ (mN/m)	κ_T (GPa^{-1})	N_{heavy}
N,N-dimethylacetamide	37.78	936.80	87.12	33.10	0.63	6
N,N-dimethylformamide	37.22	943.30	73.09	35.74	0.64	5
o-xylene	2.55	875.80	106.17	29.76	0.81	8
pyridine	12.98	981.90	79.10	36.56	0.72	6
toluene	2.37	861.90	92.14	27.73	0.92	7
ethanol	25.00	784.80	46.07	21.97	1.15	3

3 Root mean square deviation (RMSD) and mean signed error (MSE)

Table S3: Root mean square deviation (RMSD) and mean signed error (MSE) of PB calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent[a]

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-octanol	29	10.8 ± 1.1	-9.6 ± 0.9	8.8 ± 0.8	-7.8 ± 0.7	6.2 ± 0.7	-5.4 ± 0.6	3.1 ± 0.3	-2.4 ± 0.4
N-methylformamide	9	7.7 ± 1.2	-6.8 ± 1.2	8.4 ± 1.3	-7.7 ± 1.2	3.0 ± 1.2	-1.7 ± 0.8	6.3 ± 0.6	-5.9 ± 0.7
N,N-dimethylacetamide	9	9.5 ± 1.6	-8.3 ± 1.6	8.5 ± 1.0	-8.0 ± 1.0	4.0 ± 0.9	-2.8 ± 1.0	5.4 ± 0.4	-5.2 ± 0.4
N,N-dimethylformamide	9	11.7 ± 1.8	-10.6 ± 1.7	9.6 ± 0.8	-9.2 ± 0.9	3.2 ± 0.6	-2.5 ± 0.7	6.8 ± 0.4	-6.7 ± 0.4
acetone	12	19.5 ± 1.4	-19.0 ± 1.3	18.1 ± 1.1	-17.8 ± 1.0	6.0 ± 1.1	-4.9 ± 1.0	13.0 ± 0.4	-12.9 ± 0.4
acetonitrile	6	15.9 ± 1.0	-15.7 ± 1.0	16.3 ± 0.6	-16.2 ± 0.6	4.5 ± 1.0	-3.7 ± 1.1	12.5 ± 0.5	-12.5 ± 0.5
acetophenone	8	15.6 ± 2.2	-14.6 ± 1.9	14.0 ± 0.7	-13.8 ± 0.8	5.0 ± 0.7	-4.4 ± 0.8	9.5 ± 0.4	-9.4 ± 0.4
benzonitrile	6	23.5 ± 2.4	-22.9 ± 2.2	21.9 ± 0.8	-21.8 ± 0.8	6.5 ± 1.0	-5.9 ± 1.1	16.0 ± 0.7	-15.9 ± 0.8
chloroform	28	7.4 ± 0.9	-5.6 ± 0.9	5.2 ± 0.6	-3.7 ± 0.7	3.6 ± 0.4	-2.8 ± 0.4	2.3 ± 0.3	-0.9 ± 0.4
cyclohexanone	9	14.2 ± 2.0	-13.0 ± 1.9	12.4 ± 0.9	-12.1 ± 0.9	5.6 ± 0.8	-4.8 ± 1.0	7.4 ± 0.4	-7.3 ± 0.4
dibutyl ether	5	8.4 ± 1.3	-7.8 ± 1.4	9.5 ± 1.2	-9.1 ± 1.2	4.5 ± 0.8	-4.0 ± 0.9	5.2 ± 0.4	-5.1 ± 0.4
dimethyl sulfoxide	9	7.7 ± 1.8	4.1 ± 2.2	5.8 ± 1.6	3.8 ± 1.5	3.1 ± 0.4	0.2 ± 1.0	5.4 ± 1.3	3.5 ± 1.4
ethanol	13	15.3 ± 1.6	-14.5 ± 1.3	13.4 ± 0.6	-13.2 ± 0.5	4.8 ± 0.8	-4.2 ± 0.6	9.1 ± 0.2	-9.1 ± 0.2

[a]N is the number of solutes tested. $\Delta G_{Exper.}$: experimental solvation free energy. $\Delta G_{Expl.}$: Solvation free energy calculated with explicit solvent model. ΔG_{polar}: Polar contribulation. ΔG_{apolar}: Non-polar contribulation.

Table S3: Root mean square deviation (RMSD) and mean signed error (MSE) of PB calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent[a]

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
ethyl acetate	13	20.7 ± 1.3	-20.1 ± 1.3	18.6 ± 1.0	-18.2 ± 1.0	3.2 ± 0.6	-1.6 ± 0.8	16.7 ± 0.5	-16.6 ± 0.5
methanol	20	15.6 ± 1.0	-14.9 ± 1.0	13.1 ± 0.4	-13.0 ± 0.4	2.9 ± 0.5	-1.8 ± 0.5	11.3 ± 0.3	-11.2 ± 0.3
methyl acetate	7	18.9 ± 1.6	-18.5 ± 1.5	16.4 ± 0.9	-16.3 ± 0.9	1.8 ± 0.3	-0.3 ± 0.7	16.0 ± 0.6	-16.0 ± 0.6
nitromethane	10	21.9 ± 1.6	-21.4 ± 1.5	21.9 ± 0.7	-21.9 ± 0.6	2.2 ± 0.5	-1.4 ± 0.5	20.6 ± 0.8	-20.4 ± 0.8
o-xylene	5	12.6 ± 0.8	-12.5 ± 0.8	12.2 ± 0.6	-12.1 ± 0.6	1.9 ± 0.5	-1.4 ± 0.6	10.7 ± 0.2	-10.7 ± 0.2
pyridine	8	19.3 ± 2.0	-18.6 ± 1.7	19.0 ± 0.6	-18.9 ± 0.6	4.7 ± 0.6	-4.2 ± 0.8	14.8 ± 0.5	-14.7 ± 0.5
toluene	11	16.9 ± 0.8	-16.7 ± 0.8	15.3 ± 0.4	-15.2 ± 0.4	1.6 ± 0.1	-1.5 ± 0.1	13.8 ± 0.4	-13.7 ± 0.4
total	226	14.8 ± 0.5	-12.6 ± 0.5	13.4 ± 0.4	-11.5 ± 0.4	4.3 ± 0.2	-3.1 ± 0.2	10.6 ± 0.4	-8.5 ± 0.4

Table S4: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-octanol	29	13.7 ± 1.4	6.6 ± 2.2	13.9 ± 1.3	8.4 ± 2.1	15.8 ± 1.5	-14.0 ± 1.4	23.4 ± 1.3	22.4 ± 1.3

Table S4: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
N-methylformamide	9	13.8 ± 2.2	9.1 ± 3.5	12.8 ± 2.0	8.3 ± 3.2	9.7 ± 2.6	-7.0 ± 2.2	15.9 ± 1.3	15.3 ± 1.4
N,N-dimethylacetamide	9	11.3 ± 2.6	4.8 ± 3.4	10.8 ± 2.2	5.2 ± 3.1	12.3 ± 2.0	-10.5 ± 2.2	16.7 ± 1.8	15.7 ± 1.9
N,N-dimethylformamide	9	12.1 ± 2.7	0.9 ± 4.0	10.4 ± 2.7	2.2 ± 3.4	14.0 ± 2.4	-12.0 ± 2.5	15.5 ± 2.0	14.2 ± 2.0
acetone	12	12.7 ± 1.7	1.5 ± 3.7	11.2 ± 1.6	2.7 ± 3.1	17.6 ± 2.8	-14.8 ± 2.7	18.2 ± 1.2	17.6 ± 1.4
acetonitrile	6	12.1 ± 2.8	5.1 ± 4.5	11.1 ± 2.7	4.7 ± 4.1	11.8 ± 2.2	-10.1 ± 2.5	15.4 ± 1.8	14.7 ± 1.9
acetophenone	8	13.7 ± 2.1	2.7 ± 4.7	11.6 ± 1.8	3.5 ± 4.0	15.4 ± 2.8	-13.3 ± 2.8	18.5 ± 2.9	16.8 ± 2.8
benzonitrile	6	13.7 ± 2.7	0.8 ± 5.6	10.9 ± 2.3	1.9 ± 4.4	17.0 ± 3.3	-14.9 ± 3.2	18.0 ± 2.5	16.8 ± 2.6
chloroform	28	16.7 ± 1.3	13.2 ± 1.9	17.9 ± 1.4	15.0 ± 1.9	13.0 ± 0.9	-11.9 ± 1.0	28.3 ± 1.7	26.9 ± 1.7
cyclohexanone	9	12.7 ± 2.4	3.1 ± 4.1	10.8 ± 1.9	3.9 ± 3.4	16.8 ± 2.5	-14.7 ± 2.8	19.6 ± 2.0	18.6 ± 2.1
dibutyl ether	5	13.9 ± 4.4	8.0 ± 5.1	13.1 ± 3.8	6.7 ± 5.0	12.4 ± 2.3	-11.1 ± 2.5	18.8 ± 2.7	17.8 ± 2.7
dimethyl sulfoxide	9	13.3 ± 2.3	4.7 ± 4.1	11.0 ± 2.0	4.3 ± 3.3	12.2 ± 3.4	-8.0 ± 3.1	13.2 ± 1.4	12.3 ± 1.5
ethanol	13	14.5 ± 2.2	5.3 ± 3.8	12.9 ± 1.9	6.6 ± 3.1	14.3 ± 2.4	-12.3 ± 2.0	19.8 ± 1.5	18.9 ± 1.6
ethyl acetate	13	11.5 ± 2.0	3.7 ± 3.0	10.6 ± 1.9	5.6 ± 2.5	14.4 ± 2.3	-12.1 ± 2.2	18.4 ± 1.3	17.7 ± 1.4
methanol	20	15.2 ± 1.8	7.2 ± 3.0	14.1 ± 1.6	9.2 ± 2.4	12.2 ± 1.7	-10.0 ± 1.5	20.1 ± 1.3	19.2 ± 1.3

Table S4: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
methyl acetate	7	10.0 ± 2.5	1.0 ± 3.8	8.1 ± 2.5	3.2 ± 2.8	12.4 ± 2.5	-10.6 ± 2.4	14.4 ± 1.6	13.8 ± 1.6
nitromethane	10	11.8 ± 1.9	1.1 ± 3.7	8.7 ± 1.4	0.6 ± 2.7	12.4 ± 2.1	-10.4 ± 2.1	12.0 ± 1.4	11.0 ± 1.5
o-xylene	5	15.1 ± 3.8	12.9 ± 3.5	15.4 ± 3.8	13.2 ± 3.5	9.3 ± 1.8	-8.3 ± 1.8	22.1 ± 2.3	21.5 ± 2.2
pyridine	8	12.9 ± 2.5	4.2 ± 4.2	10.8 ± 2.3	3.9 ± 3.6	15.1 ± 2.7	-13.0 ± 2.7	17.6 ± 1.6	17.0 ± 1.7
toluene	11	12.7 ± 1.7	10.6 ± 2.1	13.9 ± 1.6	12.0 ± 2.1	10.1 ± 0.7	-9.7 ± 0.9	22.6 ± 1.6	21.8 ± 1.8
total	226	13.7 ± 0.5	6.1 ± 0.8	13.0 ± 0.5	7.1 ± 0.7	13.8 ± 0.5	-11.7 ± 0.5	20.3 ± 0.5	18.8 ± 0.5

Table S5: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-octanol	29	14.0 ± 1.4	8.5 ± 2.1	14.6 ± 1.5	10.3 ± 1.9	14.4 ± 1.4	-12.5 ± 1.3	23.7 ± 1.2	22.8 ± 1.2
N-methylformamide	9	13.5 ± 2.0	10.3 ± 2.9	12.7 ± 1.9	9.5 ± 2.8	8.9 ± 2.4	-6.5 ± 2.0	16.6 ± 1.4	16.0 ± 1.4
N,N-dimethylacetamide	9	11.6 ± 2.5	6.8 ± 3.1	11.3 ± 2.0	7.1 ± 2.9	11.3 ± 2.2	-9.3 ± 2.1	17.4 ± 1.8	16.5 ± 1.9

Table S5: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
N,N-dimethylformamide	9	11.7 ± 2.8	3.2 ± 3.7	10.6 ± 3.0	4.5 ± 3.2	13.0 ± 2.3	-10.6 ± 2.5	16.3 ± 1.9	15.2 ± 1.9
acetone	12	11.9 ± 1.7	3.7 ± 3.3	10.8 ± 1.7	4.9 ± 2.8	15.6 ± 2.3	-13.3 ± 2.4	18.7 ± 1.2	18.1 ± 1.3
acetonitrile	6	11.4 ± 2.9	6.8 ± 3.8	10.5 ± 2.6	6.3 ± 3.4	10.2 ± 1.8	-9.2 ± 1.9	16.2 ± 2.0	15.5 ± 1.9
acetophenone	8	12.8 ± 1.9	4.4 ± 4.3	11.2 ± 1.9	5.2 ± 3.5	14.3 ± 2.5	-12.6 ± 2.4	19.5 ± 2.9	17.8 ± 2.8
benzonitrile	6	11.8 ± 2.4	2.5 ± 4.8	9.3 ± 2.3	3.6 ± 3.5	15.8 ± 2.8	-14.3 ± 2.8	19.2 ± 2.8	17.9 ± 2.9
chloroform	28	18.2 ± 1.3	15.1 ± 1.9	19.6 ± 1.5	16.9 ± 1.9	11.8 ± 0.8	-10.7 ± 0.9	29.0 ± 1.7	27.6 ± 1.7
cyclohexanone	9	12.0 ± 2.3	4.6 ± 3.7	10.5 ± 1.9	5.5 ± 3.0	15.8 ± 2.2	-13.9 ± 2.5	20.2 ± 1.9	19.4 ± 1.9
dibutyl ether	5	13.8 ± 4.2	9.4 ± 4.5	12.9 ± 3.8	8.1 ± 4.4	11.4 ± 1.9	-10.4 ± 2.0	19.6 ± 2.7	18.6 ± 2.8
dimethyl sulfoxide	9	12.2 ± 2.4	6.8 ± 3.4	10.2 ± 1.9	6.4 ± 2.7	9.5 ± 2.4	-6.4 ± 2.3	13.7 ± 1.5	12.9 ± 1.6
ethanol	13	14.7 ± 2.2	7.2 ± 3.5	13.5 ± 2.0	8.6 ± 2.9	13.2 ± 2.2	-11.1 ± 2.0	20.4 ± 1.4	19.6 ± 1.5
ethyl acetate	13	11.1 ± 2.1	5.6 ± 2.7	10.8 ± 1.8	7.5 ± 2.1	12.7 ± 1.8	-10.9 ± 1.9	19.1 ± 1.3	18.4 ± 1.4
methanol	20	15.6 ± 1.9	9.3 ± 2.8	15.1 ± 1.7	11.3 ± 2.2	10.5 ± 1.6	-8.3 ± 1.4	20.4 ± 1.2	19.6 ± 1.3
methyl acetate	7	9.6 ± 2.7	3.2 ± 3.4	8.7 ± 2.6	5.4 ± 2.6	11.2 ± 2.3	-9.4 ± 2.3	15.3 ± 1.5	14.8 ± 1.5
nitromethane	10	10.6 ± 1.8	2.8 ± 3.2	7.8 ± 1.4	2.4 ± 2.3	11.1 ± 1.8	-9.5 ± 1.8	12.7 ± 1.4	11.9 ± 1.4

Table S5: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
o-xylene	5	15.6 ± 3.2	14.0 ± 3.0	15.9 ± 3.3	14.4 ± 3.0	8.4 ± 1.4	-7.8 ± 1.4	22.8 ± 2.4	22.2 ± 2.3
pyridine	8	12.5 ± 2.3	6.4 ± 3.8	10.4 ± 2.3	6.1 ± 3.0	13.1 ± 2.4	-11.5 ± 2.2	18.3 ± 1.6	17.6 ± 1.7
toluene	11	13.9 ± 1.6	12.3 ± 1.9	15.2 ± 1.6	13.7 ± 2.0	9.0 ± 0.7	-8.6 ± 0.8	23.0 ± 1.5	22.3 ± 1.7
total	226	13.8 ± 0.5	8.0 ± 0.7	13.5 ± 0.5	9.0 ± 0.7	12.4 ± 0.5	-10.5 ± 0.4	20.9 ± 0.5	19.5 ± 0.5

Table S6: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-I calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-octanol	29	14.5 ± 1.5	8.4 ± 2.2	15.1 ± 1.6	10.1 ± 2.1	16.3 ± 1.5	-14.3 ± 1.5	25.3 ± 1.2	24.4 ± 1.3
N-methylformamide	9	14.2 ± 2.0	10.4 ± 3.2	13.5 ± 2.0	9.6 ± 3.2	10.8 ± 2.7	-8.2 ± 2.4	18.3 ± 1.5	17.7 ± 1.5
N,N-dimethylacetamide	9	12.0 ± 2.5	6.4 ± 3.4	11.7 ± 2.2	6.8 ± 3.2	13.2 ± 2.3	-11.3 ± 2.3	18.9 ± 1.8	18.0 ± 1.9
N,N-dimethylformamide	9	12.8 ± 3.0	2.6 ± 4.2	11.4 ± 3.3	3.9 ± 3.6	15.3 ± 2.5	-12.8 ± 2.8	17.7 ± 2.0	16.7 ± 2.0
acetone	12	12.8 ± 1.7	3.1 ± 3.6	11.6 ± 1.7	4.3 ± 3.1	17.9 ± 2.5	-15.4 ± 2.6	20.2 ± 1.2	19.6 ± 1.3

Table S6: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-I calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
acetonitrile	6	11.9 ± 2.8	6.3 ± 4.1	10.9 ± 2.7	5.8 ± 3.8	12.4 ± 2.1	-11.2 ± 2.1	17.8 ± 2.1	17.0 ± 2.0
acetophenone	8	13.6 ± 2.0	3.8 ± 4.6	11.7 ± 1.8	4.6 ± 3.8	16.7 ± 2.8	-14.8 ± 2.7	21.1 ± 3.1	19.4 ± 2.9
benzonitrile	6	12.8 ± 2.4	1.7 ± 5.2	10.1 ± 2.1	2.7 ± 4.0	18.5 ± 3.2	-16.8 ± 3.1	21.0 ± 3.1	19.6 ± 3.1
chloroform	28	18.6 ± 1.3	15.2 ± 2.0	20.0 ± 1.6	17.0 ± 2.0	13.8 ± 1.0	-12.5 ± 1.1	30.8 ± 1.7	29.5 ± 1.7
cyclohexanone	9	12.6 ± 2.3	4.0 ± 4.0	10.8 ± 1.9	4.9 ± 3.2	18.1 ± 2.5	-16.1 ± 2.8	21.8 ± 1.9	21.0 ± 1.9
dibutyl ether	5	14.4 ± 4.6	9.5 ± 4.7	13.5 ± 4.1	8.2 ± 4.7	13.0 ± 2.0	-12.0 ± 2.3	21.2 ± 2.8	20.2 ± 2.9
dimethyl sulfoxide	9	12.7 ± 2.4	6.2 ± 3.7	10.6 ± 2.0	5.8 ± 2.9	11.5 ± 2.7	-8.7 ± 2.5	15.3 ± 1.6	14.5 ± 1.7
ethanol	13	15.5 ± 2.4	6.9 ± 3.9	14.1 ± 2.1	8.2 ± 3.2	15.4 ± 2.5	-13.0 ± 2.3	22.0 ± 1.4	21.2 ± 1.5
ethyl acetate	13	11.7 ± 2.1	5.3 ± 2.9	11.1 ± 2.0	7.2 ± 2.3	14.8 ± 1.9	-12.8 ± 2.0	20.6 ± 1.3	20.0 ± 1.4
methanol	20	16.5 ± 2.1	9.1 ± 3.1	15.7 ± 1.8	11.0 ± 2.5	12.6 ± 1.8	-10.1 ± 1.7	21.9 ± 1.3	21.1 ± 1.3
methyl acetate	7	10.3 ± 2.8	2.5 ± 3.7	8.9 ± 2.8	4.7 ± 2.9	13.3 ± 2.5	-11.4 ± 2.6	16.7 ± 1.5	16.2 ± 1.5
nitromethane	10	11.5 ± 1.9	2.2 ± 3.5	8.5 ± 1.3	1.7 ± 2.6	13.5 ± 2.1	-11.7 ± 2.1	14.3 ± 1.4	13.4 ± 1.5
o-xylene	5	16.1 ± 3.2	14.5 ± 3.1	16.4 ± 3.3	14.9 ± 3.2	9.7 ± 1.6	-9.0 ± 1.5	24.5 ± 2.5	23.9 ± 2.4
pyridine	8	13.0 ± 2.4	5.6 ± 4.1	10.8 ± 2.3	5.3 ± 3.3	15.5 ± 2.7	-13.8 ± 2.5	19.8 ± 1.7	19.2 ± 1.8

Table S6: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-I calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
toluene	11	14.3 ± 1.7	12.5 ± 2.1	15.5 ± 1.6	13.9 ± 2.0	10.5 ± 0.7	-10.1 ± 0.9	24.7 ± 1.5	24.0 ± 1.8
total	226	14.4 ± 0.5	7.7 ± 0.8	14.0 ± 0.5	8.7 ± 0.7	14.5 ± 0.5	-12.4 ± 0.5	22.5 ± 0.5	21.1 ± 0.5

Table S7: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-II calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-octanol	29	13.9 ± 1.4	8.3 ± 2.1	14.5 ± 1.5	10.1 ± 1.9	14.7 ± 1.5	-12.5 ± 1.4	23.5 ± 1.2	22.6 ± 1.2
N-methylformamide	9	13.5 ± 1.9	10.2 ± 2.9	12.7 ± 1.9	9.3 ± 2.9	9.4 ± 2.4	-6.6 ± 2.2	16.5 ± 1.3	16.0 ± 1.3
N,N-dimethylacetamide	9	11.7 ± 2.4	6.6 ± 3.2	11.4 ± 2.0	7.0 ± 3.1	11.7 ± 2.2	-9.6 ± 2.2	17.5 ± 1.7	16.7 ± 1.8
N,N-dimethylformamide	9	11.8 ± 2.8	2.9 ± 3.8	10.6 ± 3.1	4.2 ± 3.3	13.5 ± 2.3	-11.0 ± 2.6	16.2 ± 1.8	15.2 ± 1.9
acetone	12	12.0 ± 1.6	3.5 ± 3.3	10.9 ± 1.7	4.7 ± 2.9	16.1 ± 2.3	-13.6 ± 2.4	18.8 ± 1.2	18.3 ± 1.2
acetonitrile	6	11.4 ± 2.7	6.5 ± 3.8	10.4 ± 2.5	6.0 ± 3.5	10.8 ± 1.9	-9.7 ± 1.9	16.4 ± 1.9	15.8 ± 1.9
acetophenone	8	12.9 ± 1.8	4.2 ± 4.2	11.2 ± 1.8	5.0 ± 3.6	14.8 ± 2.5	-13.1 ± 2.4	19.6 ± 2.9	18.1 ± 2.8

Table S7: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-II calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solvent	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
benzonitrile	6	11.8 ± 2.3	2.1 ± 4.7	9.2 ± 2.0	3.2 ± 3.5	16.5 ± 2.9	-15.0 ± 2.8	19.5 ± 2.8	18.2 ± 2.8
chloroform	28	18.3 ± 1.3	15.0 ± 1.9	19.7 ± 1.5	16.8 ± 1.9	12.1 ± 0.9	-10.7 ± 1.0	28.9 ± 1.6	27.6 ± 1.6
cyclohexanone	9	11.9 ± 2.2	4.3 ± 3.7	10.4 ± 1.9	5.2 ± 3.0	16.2 ± 2.3	-14.4 ± 2.5	20.3 ± 1.8	19.6 ± 1.8
dibutyl ether	5	13.7 ± 4.3	9.2 ± 4.5	12.8 ± 3.9	7.9 ± 4.5	11.8 ± 1.9	-10.9 ± 2.1	19.8 ± 2.7	18.8 ± 2.8
dimethyl sulfoxide	9	12.1 ± 2.4	6.4 ± 3.3	10.0 ± 1.9	6.1 ± 2.6	9.8 ± 2.4	-6.9 ± 2.3	13.8 ± 1.4	13.0 ± 1.5
ethanol	13	14.8 ± 2.2	7.0 ± 3.6	13.5 ± 2.0	8.3 ± 2.9	13.6 ± 2.3	-11.3 ± 2.1	20.3 ± 1.3	19.7 ± 1.5
ethyl acetate	13	11.1 ± 2.0	5.4 ± 2.7	10.7 ± 1.8	7.3 ± 2.2	13.1 ± 1.8	-11.3 ± 1.9	19.2 ± 1.2	18.6 ± 1.3
methanol	20	15.6 ± 2.0	9.1 ± 2.9	15.0 ± 1.7	11.1 ± 2.3	10.9 ± 1.7	-8.3 ± 1.6	20.1 ± 1.1	19.4 ± 1.2
methyl acetate	7	9.8 ± 2.8	3.0 ± 3.6	8.8 ± 2.7	5.2 ± 2.7	11.7 ± 2.3	-9.9 ± 2.4	15.6 ± 1.5	15.1 ± 1.5
nitromethane	10	10.6 ± 1.8	2.5 ± 3.3	7.8 ± 1.3	2.1 ± 2.4	11.6 ± 1.9	-10.0 ± 1.8	12.9 ± 1.4	12.1 ± 1.4
o-xylene	5	15.2 ± 3.0	13.8 ± 2.9	15.6 ± 3.0	14.2 ± 2.9	8.6 ± 1.4	-8.1 ± 1.3	22.8 ± 2.3	22.3 ± 2.1
pyridine	8	12.4 ± 2.3	6.0 ± 3.9	10.3 ± 2.2	5.7 ± 3.0	13.7 ± 2.4	-12.1 ± 2.2	18.5 ± 1.6	17.8 ± 1.7
toluene	11	13.6 ± 1.6	12.0 ± 1.9	14.9 ± 1.5	13.5 ± 1.9	9.2 ± 0.7	-8.8 ± 0.9	22.9 ± 1.5	22.2 ± 1.6
total	226	13.8 ± 0.5	7.7 ± 0.8	13.5 ± 0.5	8.8 ± 0.7	12.8 ± 0.5	-10.8 ± 0.5	20.8 ± 0.5	19.6 ± 0.5

Table S8: Root mean square deviation (RMSD) and mean signed error (MSE) of SMD calculations at B3LYP/6-31+G(d,p) level of theory from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solvent	N	RMSD	MSE	RMSD	MSE
1-octanol	29	6.96 ± 0.82	-4.94 ± 0.92	5.75 ± 0.63	-3.17 ± 0.88
N-methylformamide	9	6.68 ± 1.03	-3.21 ± 1.95	6.22 ± 0.63	-4.03 ± 1.58
N,N-dimethylacetamide	9	5.60 ± 0.86	-2.41 ± 1.72	5.52 ± 1.04	-2.04 ± 1.68
N,N-dimethylformamide	9	5.36 ± 0.90	-2.32 ± 1.63	6.01 ± 0.94	-0.96 ± 1.99
acetone	12	6.89 ± 1.12	-5.49 ± 1.22	6.43 ± 0.97	-4.28 ± 1.39
acetonitrile	6	4.70 ± 1.03	-3.48 ± 1.27	5.09 ± 1.10	-3.94 ± 1.32
acetophenone	8	5.38 ± 0.97	-3.94 ± 1.30	6.00 ± 1.19	-3.15 ± 1.81
benzonitrile	6	4.99 ± 0.90	-4.06 ± 1.16	5.11 ± 1.22	-2.99 ± 1.69
chloroform	28	4.10 ± 0.46	-1.23 ± 0.74	5.32 ± 1.20	0.59 ± 1.02
cyclohexanone	9	5.67 ± 0.93	-3.55 ± 1.46	5.95 ± 1.09	-2.70 ± 1.75
dibutyl ether	5	3.92 ± 1.27	0.53 ± 1.74	3.31 ± 0.83	-0.75 ± 1.43
dimethyl sulfoxide	9	5.38 ± 0.67	0.31 ± 1.79	5.64 ± 0.83	-0.02 ± 1.87
ethanol	13	6.48 ± 0.81	-5.12 ± 1.10	5.80 ± 0.63	-3.81 ± 1.21
ethyl acetate	13	4.49 ± 0.60	-2.94 ± 0.92	5.40 ± 0.66	-1.04 ± 1.47
methanol	20	7.53 ± 1.02	-5.66 ± 1.12	6.32 ± 0.63	-3.72 ± 1.14
methyl acetate	7	3.55 ± 0.80	-2.29 ± 1.02	5.84 ± 0.81	-0.08 ± 2.24
nitromethane	10	4.86 ± 0.82	-3.67 ± 1.01	7.60 ± 1.11	-4.13 ± 2.02
o-xylene	5	1.94 ± 0.30	-1.83 ± 0.29	1.69 ± 0.33	-1.46 ± 0.39
pyridine	8	4.27 ± 0.97	-1.45 ± 1.41	4.55 ± 0.96	-1.73 ± 1.52
toluene	11	1.77 ± 0.34	0.24 ± 0.53	3.24 ± 0.91	1.68 ± 0.84
total	226	5.56 ± 0.25	-3.13 ± 0.31	5.64 ± 0.23	-2.07 ± 0.35

Table S9: Root mean square deviation (RMSD) and mean signed error (MSE) of SMD calculations at HF/6-31+G(d,p) level of theory from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solvent	N	RMSD	MSE	RMSD	MSE
1-octanol	29	9.52 ± 1.25	-7.90 ± 0.98	7.63 ± 0.97	-6.13 ± 0.86
N-methylformamide	9	8.59 ± 1.45	-6.99 ± 1.68	8.89 ± 1.34	-7.81 ± 1.42
N,N-dimethylacetamide	9	6.83 ± 1.19	-4.74 ± 1.64	6.83 ± 1.27	-4.37 ± 1.71
N,N-dimethylformamide	9	6.16 ± 1.19	-4.22 ± 1.48	6.17 ± 1.41	-2.86 ± 1.80
acetone	12	9.53 ± 1.42	-8.31 ± 1.34	8.74 ± 1.30	-7.10 ± 1.47
acetonitrile	6	6.78 ± 1.10	-6.04 ± 1.26	7.33 ± 1.12	-6.49 ± 1.41
acetophenone	8	8.31 ± 1.33	-7.25 ± 1.46	8.35 ± 1.56	-6.45 ± 1.87
benzonitrile	6	8.48 ± 1.22	-7.70 ± 1.47	8.02 ± 1.57	-6.63 ± 1.85
chloroform	28	4.96 ± 0.56	-3.60 ± 0.64	4.73 ± 0.64	-1.78 ± 0.83
cyclohexanone	9	7.40 ± 1.06	-6.51 ± 1.17	7.31 ± 1.32	-5.65 ± 1.56
dibutyl ether	5	2.48 ± 1.14	-1.30 ± 0.95	3.04 ± 0.83	-2.59 ± 0.71
dimethyl sulfoxide	9	6.31 ± 1.34	-2.79 ± 1.90	6.87 ± 0.95	-3.13 ± 2.00
ethanol	13	9.52 ± 1.02	-8.62 ± 1.12	7.85 ± 0.75	-7.31 ± 0.79
ethyl acetate	13	6.33 ± 0.79	-5.41 ± 0.92	6.25 ± 0.69	-3.50 ± 1.43
methanol	20	11.89 ± 1.62	-10.12 ± 1.40	9.30 ± 1.13	-8.18 ± 0.98
methyl acetate	7	5.01 ± 0.88	-3.95 ± 1.15	5.85 ± 0.75	-1.74 ± 2.10
nitromethane	10	7.11 ± 0.74	-6.62 ± 0.81	9.08 ± 1.27	-7.08 ± 1.80
o-xylene	5	2.74 ± 0.37	-2.62 ± 0.36	2.49 ± 0.43	-2.25 ± 0.48
pyridine	8	5.77 ± 1.06	-3.85 ± 1.51	5.69 ± 1.11	-4.13 ± 1.38
toluene	11	1.71 ± 0.39	-1.12 ± 0.39	1.93 ± 0.33	0.32 ± 0.56
total	226	7.73 ± 0.39	-5.92 ± 0.34	7.09 ± 0.29	-4.86 ± 0.34

Table S10: Root mean square deviation (RMSD) and mean signed error (MSE) of SMD calculations at M06-2X/6-31+G(d,p) level of theory from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solvent	N	RMSD	MSE	RMSD	MSE
1-octanol	29	7.31 ± 0.93	-6.10 ± 0.74	5.53 ± 0.70	-4.33 ± 0.65
N-methylformamide	9	6.67 ± 1.25	-5.11 ± 1.45	6.61 ± 0.82	-5.93 ± 0.96
N,N-dimethylacetamide	9	6.20 ± 1.28	-3.82 ± 1.59	5.93 ± 1.05	-3.45 ± 1.59
N,N-dimethylformamide	9	5.71 ± 1.19	-3.70 ± 1.45	5.30 ± 1.17	-2.34 ± 1.56
acetone	12	8.16 ± 1.21	-7.01 ± 1.20	6.90 ± 0.90	-5.80 ± 1.08
acetonitrile	6	6.06 ± 1.15	-5.21 ± 1.27	6.53 ± 1.05	-5.66 ± 1.34
acetophenone	8	6.93 ± 1.15	-5.98 ± 1.23	6.39 ± 1.06	-5.19 ± 1.33
benzonitrile	6	7.70 ± 1.53	-6.73 ± 1.53	6.49 ± 1.22	-5.65 ± 1.31
chloroform	28	3.97 ± 0.43	-2.17 ± 0.63	5.03 ± 1.10	-0.35 ± 0.93
cyclohexanone	9	6.79 ± 1.02	-5.75 ± 1.18	6.10 ± 1.10	-4.89 ± 1.23
dibutyl ether	5	3.25 ± 1.60	-1.29 ± 1.33	3.57 ± 1.38	-2.58 ± 1.11
dimethyl sulfoxide	9	5.52 ± 0.95	-1.72 ± 1.72	6.02 ± 0.89	-2.06 ± 1.87
ethanol	13	7.50 ± 0.78	-6.95 ± 0.77	6.22 ± 0.54	-5.64 ± 0.72
ethyl acetate	13	5.48 ± 0.69	-4.50 ± 0.86	5.06 ± 0.62	-2.60 ± 1.19
methanol	20	8.72 ± 1.11	-7.58 ± 0.97	6.84 ± 0.65	-5.64 ± 0.86
methyl acetate	7	5.06 ± 1.07	-3.65 ± 1.33	4.96 ± 0.70	-1.44 ± 1.77
nitromethane	10	6.36 ± 0.69	-5.84 ± 0.79	7.79 ± 1.06	-6.30 ± 1.44
o-xylene	5	2.80 ± 0.58	-2.51 ± 0.55	2.46 ± 0.48	-2.14 ± 0.54
pyridine	8	6.12 ± 1.35	-3.67 ± 1.71	5.33 ± 1.12	-3.96 ± 1.27
toluene	11	1.79 ± 0.40	-0.96 ± 0.45	2.16 ± 0.36	0.48 ± 0.64
total	226	6.36 ± 0.28	-4.71 ± 0.29	5.78 ± 0.23	-3.65 ± 0.30

Table S11: Root mean square deviation (RMSD) and mean signed error (MSE) with SMD calculations at M06-2X/cc-pVTZ level of theory from the calculations with explicit solvent model or from experimental data (kJ/mol) per solvent

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solvent	N	RMSD	MSE	RMSD	MSE
1-octanol	29	5.05 ± 0.67	-3.20 ± 0.73	4.09 ± 0.62	-1.43 ± 0.71
N-methylformamide	9	4.55 ± 1.14	-2.72 ± 1.20	4.17 ± 0.68	-3.54 ± 0.72
N,N-dimethylacetamide	9	5.80 ± 1.06	-2.28 ± 1.78	5.67 ± 1.03	-1.91 ± 1.77
N,N-dimethylformamide	9	5.02 ± 1.01	-1.92 ± 1.50	5.54 ± 0.96	-0.56 ± 1.81
acetone	12	5.94 ± 1.03	-4.51 ± 1.11	5.20 ± 0.85	-3.30 ± 1.18
acetonitrile	6	4.31 ± 0.83	-2.83 ± 1.31	4.84 ± 0.75	-3.28 ± 1.44
acetophenone	8	5.41 ± 0.97	-4.08 ± 1.27	5.46 ± 1.09	-3.28 ± 1.54
benzonitrile	6	5.84 ± 1.15	-4.62 ± 1.44	5.13 ± 1.16	-3.55 ± 1.52
chloroform	28	3.29 ± 0.35	-0.66 ± 0.61	4.69 ± 0.95	1.17 ± 0.86
cyclohexanone	9	5.62 ± 0.91	-4.16 ± 1.26	5.45 ± 1.10	-3.31 ± 1.44
dibutyl ether	5	3.43 ± 1.38	-0.44 ± 1.52	3.39 ± 1.61	-1.73 ± 1.30
dimethyl sulfoxide	9	5.13 ± 0.91	0.45 ± 1.68	5.80 ± 1.40	0.11 ± 1.90
ethanol	13	5.27 ± 0.86	-4.42 ± 0.80	4.51 ± 0.63	-3.11 ± 0.89
ethyl acetate	13	4.23 ± 0.58	-2.87 ± 0.87	4.80 ± 0.68	-0.96 ± 1.32
methanol	20	5.75 ± 0.83	-4.60 ± 0.76	4.66 ± 0.44	-2.67 ± 0.85
methyl acetate	7	4.27 ± 0.88	-2.10 ± 1.41	5.39 ± 0.69	0.12 ± 2.03
nitromethane	10	4.87 ± 0.61	-3.95 ± 0.90	7.00 ± 0.94	-4.41 ± 1.73
o-xylene	5	2.44 ± 0.83	-1.69 ± 0.78	2.15 ± 0.63	-1.33 ± 0.77
pyridine	8	5.32 ± 1.01	-1.71 ± 1.76	4.54 ± 0.98	-1.99 ± 1.45
toluene	11	1.85 ± 0.35	-0.02 ± 0.57	2.79 ± 0.40	1.43 ± 0.72
total	226	4.81 ± 0.21	-2.67 ± 0.27	4.83 ± 0.22	-1.61 ± 0.30

Table S12: Root mean square deviation (RMSD) and mean signed error (MSE) of PB calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute[a]

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-butanol	6	15.6 ± 1.8	-14.9 ± 1.8	14.2 ± 2.1	-13.2 ± 2.0	4.2 ± 0.7	-3.8 ± 0.7	10.8 ± 1.9	-9.4 ± 2.2
1-chlorobutane	4	16.4 ± 2.3	-15.4 ± 2.8	18.1 ± 2.7	-17.0 ± 3.1	2.3 ± 0.9	-1.5 ± 0.8	17.3 ± 3.1	-15.5 ± 3.9
1-octanol	1	-6.0	-6.0	-2.5	-2.5	-3.8	-3.8	1.3	1.3
1-pentanol	4	14.4 ± 2.4	-13.5 ± 2.4	11.4 ± 2.4	-10.4 ± 2.3	3.8 ± 1.1	-3.2 ± 1.1	9.7 ± 3.0	-7.2 ± 3.3
1,2-dichloroethane	3	14.6 ± 2.2	-14.1 ± 2.1	14.1 ± 1.9	-13.7 ± 1.9	3.8 ± 1.9	-2.5 ± 1.6	12.3 ± 3.0	-11.2 ± 3.0
2-hexanone	3	16.4 ± 2.3	-15.9 ± 2.4	13.0 ± 2.5	-12.1 ± 2.7	3.0 ± 1.1	-2.4 ± 1.0	11.5 ± 3.0	-9.7 ± 3.6
2-methyl-2-butanol	1	-17.4	-17.4	-8.9	-8.9	3.2	3.2	-12.1	-12.1
2-methyl-2-propanol	2	9.2 ± 0.0	-9.2 ± 0.0	4.3 ± 0.7	-4.2 ± 0.7	2.8 ± 1.4	-2.1 ± 1.3	2.3 ± 0.7	-2.1 ± 0.7
2-methylpyridine	1	0.4	0.4	-1.7	-1.7	-1.2	-1.2	-0.5	-0.5
3-methylpyridine	1	1.1	1.1	-1.3	-1.3	-1.2	-1.2	-0.1	-0.1
N-methylformamide	2	18.0 ± 3.5	-17.3 ± 3.4	20.3 ± 3.1	-19.8 ± 3.2	10.1 ± 1.4	-9.9 ± 1.4	10.2 ± 1.8	-9.9 ± 1.8
N,N-dimethylacetamide	1	-7.7	-7.7	-6.9	-6.9	-5.5	-5.5	-1.5	-1.5
N,N-dimethylformamide	6	19.2 ± 1.7	-18.8 ± 1.7	16.1 ± 2.0	-15.5 ± 1.8	6.0 ± 1.0	-5.4 ± 1.1	11.1 ± 1.8	-10.1 ± 1.9

[a]N is the number of solvents tested.

Table S12: Root mean square deviation (RMSD) and mean signed error (MSE) of PB calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute[a]

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
acetone	17	15.5 ± 1.1	-14.5 ± 1.3	14.7 ± 1.2	-13.6 ± 1.4	4.4 ± 0.4	-4.0 ± 0.4	11.2 ± 1.3	-9.5 ± 1.4
acetonitrile	12	13.8 ± 1.0	-13.3 ± 1.0	15.1 ± 0.9	-14.7 ± 1.0	5.4 ± 0.8	-4.7 ± 0.7	10.8 ± 1.2	-10.0 ± 1.2
acetophenone	2	11.1 ± 3.6	-9.9 ± 3.5	10.0 ± 4.8	-7.5 ± 4.7	4.8 ± 1.6	-4.3 ± 1.5	5.5 ± 2.3	-3.2 ± 3.2
anisole	2	5.4 ± 1.0	-5.2 ± 1.0	5.2 ± 2.3	-4.1 ± 2.3	5.1 ± 2.1	-4.2 ± 2.1	0.3 ± 0.1	0.1 ± 0.2
benzaldehyde	1	-5.2	-5.2	-3.3	-3.3	-3.1	-3.1	-0.2	-0.2
benzonitrile	3	16.3 ± 4.7	-14.3 ± 4.5	15.7 ± 5.0	-13.3 ± 4.8	7.8 ± 2.0	-7.0 ± 1.9	10.6 ± 5.8	-6.3 ± 4.9
chloroform	15	11.2 ± 1.1	-9.1 ± 1.7	12.9 ± 1.3	-11.2 ± 1.6	1.4 ± 0.2	-0.3 ± 0.4	12.5 ± 1.4	-10.8 ± 1.6
cyclohexanone	1	-12.8	-12.8	-11.1	-11.1	-6.9	-6.9	-4.2	-4.2
dibromomethane	1	-5.8	-5.8	-6.7	-6.7	-4.6	-4.6	-2.0	-2.0
dibutyl ether	2	12.2 ± 5.0	-10.0 ± 5.0	11.1 ± 5.0	-8.7 ± 4.9	1.8 ± 0.6	-1.6 ± 0.6	10.5 ± 5.2	-7.1 ± 5.5
dichloromethane	14	12.0 ± 1.0	-10.6 ± 1.5	13.3 ± 1.1	-12.1 ± 1.4	1.4 ± 0.2	-0.5 ± 0.3	12.7 ± 1.1	-11.7 ± 1.3
diethyl sulfide	1	4.8	4.8	-2.0	-2.0	-0.5	-0.5	-1.5	-1.5
diethylamine	3	10.7 ± 3.3	-8.8 ± 3.5	11.5 ± 2.8	-10.0 ± 3.4	0.7 ± 0.1	-0.6 ± 0.1	11.0 ± 2.8	-9.4 ± 3.3
diisopropyl ether	3	7.9 ± 0.4	-7.8 ± 0.4	3.0 ± 0.5	-0.8 ± 1.6	1.4 ± 0.4	0.3 ± 0.8	2.4 ± 1.0	-1.2 ± 1.2

Table S12: Root mean square deviation (RMSD) and mean signed error (MSE) of PB calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute[a]

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
dimethyl ether	2	8.5 ± 0.1	-8.5 ± 0.1	9.8 ± 0.2	-9.8 ± 0.2	3.7 ± 1.2	-3.2 ± 1.2	6.7 ± 1.0	-6.5 ± 1.0
dimethyl sulfoxide	5	19.1 ± 3.1	-17.3 ± 3.7	16.0 ± 3.8	-13.3 ± 4.1	6.5 ± 1.4	-5.0 ± 1.9	10.9 ± 2.2	-8.3 ± 3.2
ethanol	19	14.7 ± 1.1	-13.5 ± 1.3	13.8 ± 1.1	-12.4 ± 1.3	3.9 ± 0.5	-2.6 ± 0.7	10.9 ± 1.0	-9.8 ± 1.1
ethyl acetate	8	20.3 ± 2.6	-18.3 ± 3.0	16.0 ± 2.7	-13.2 ± 3.2	5.5 ± 0.9	-4.9 ± 0.9	12.5 ± 2.8	-8.2 ± 3.3
ethylbenzene	6	9.9 ± 2.2	-2.5 ± 3.9	9.7 ± 1.9	-3.8 ± 3.7	2.5 ± 0.6	-1.5 ± 0.8	7.9 ± 1.7	-2.3 ± 3.1
formaldehyde	1	-19.1	-19.1	-8.2	-8.2	-3.6	-3.6	-4.6	-4.6
isopropylbenzene	1	-13.9	-13.9	-14.4	-14.4	-2.2	-2.2	-12.2	-12.2
methanol	17	14.7 ± 1.0	-13.9 ± 1.2	14.0 ± 1.1	-13.0 ± 1.2	4.9 ± 0.6	-3.7 ± 0.8	9.9 ± 0.8	-9.3 ± 0.8
methyl acetate	4	18.1 ± 2.1	-17.4 ± 2.3	13.5 ± 1.8	-12.8 ± 2.2	6.2 ± 2.1	-5.0 ± 1.8	9.0 ± 2.2	-7.7 ± 2.4
morpholine	1	-5.2	-5.2	-2.6	-2.6	-3.4	-3.4	0.8	0.8
n-butylamine	3	11.0 ± 2.7	-10.0 ± 2.6	10.2 ± 3.0	-9.1 ± 2.7	2.7 ± 0.6	-2.6 ± 0.5	8.5 ± 3.5	-6.5 ± 3.2
nitrobenzene	1	-11.9	-11.9	-3.3	-3.3	-5.1	-5.1	1.8	1.8
nitromethane	12	27.3 ± 0.9	-27.1 ± 0.9	17.8 ± 0.9	-17.5 ± 0.9	7.3 ± 0.9	-6.5 ± 0.9	11.7 ± 1.1	-11.0 ± 1.2
o-xylene	3	7.5 ± 2.5	-6.2 ± 2.4	7.3 ± 2.1	-6.5 ± 1.9	2.5 ± 0.9	-2.1 ± 0.8	6.2 ± 2.4	-4.5 ± 2.5

Table S12: Root mean square deviation (RMSD) and mean signed error (MSE) of PB calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute[a]

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
phenol	1	-4.4	-4.4	-7.3	-7.3	-6.6	-6.6	-0.7	-0.7
pyridine	3	9.8 ± 2.6	-8.1 ± 3.2	11.2 ± 2.4	-10.0 ± 2.9	3.2 ± 1.1	-2.6 ± 1.0	8.8 ± 2.5	-7.4 ± 2.7
tetrahydrofuran	5	12.0 ± 1.7	-11.4 ± 1.6	11.0 ± 1.6	-10.5 ± 1.6	3.1 ± 0.4	-3.0 ± 0.4	8.4 ± 1.6	-7.4 ± 1.7
thiophene	1	2.3	2.3	-3.6	-3.6	-1.5	-1.5	-2.1	-2.1
toluene	17	11.5 ± 1.3	-8.3 ± 2.0	13.0 ± 1.4	-10.2 ± 1.9	2.2 ± 0.3	-1.6 ± 0.4	11.7 ± 1.6	-8.6 ± 1.9
triethyl phosphate	1	-6.7	-6.7	4.7	4.7	-0.4	-0.4	5.2	5.2
triethylamine	3	6.4 ± 0.8	-6.2 ± 0.8	9.9 ± 1.9	-9.1 ± 2.2	0.4 ± 0.1	-0.3 ± 0.2	9.6 ± 1.9	-8.9 ± 2.0

Table S13: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-butanol	6	7.9 ± 0.6	7.8 ± 0.5	9.7 ± 0.7	9.5 ± 0.7	13.1 ± 0.9	-12.9 ± 0.8	22.5 ± 0.6	22.4 ± 0.6
1-chlorobutane	4	14.4 ± 0.7	14.4 ± 0.7	13.1 ± 1.3	12.8 ± 1.3	6.8 ± 0.8	-6.7 ± 0.8	19.8 ± 1.6	19.5 ± 1.7

Table S13: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-octanol	1	21.4	21.4	24.9	24.9	-13.0	-13.0	38.0	38.0
1-pentanol	4	11.7 ± 1.1	11.5 ± 1.1	14.7 ± 0.8	14.6 ± 0.8	12.5 ± 1.4	-12.1 ± 1.4	26.8 ± 1.3	26.7 ± 1.3
1,2-dichloroethane	3	8.9 ± 2.0	8.2 ± 2.1	9.4 ± 2.1	8.6 ± 2.2	11.6 ± 1.8	-11.2 ± 1.7	19.8 ± 0.6	19.8 ± 0.6
2-hexanone	3	11.6 ± 3.5	10.2 ± 3.2	14.4 ± 2.2	14.0 ± 2.0	13.2 ± 1.2	-13.1 ± 1.2	27.1 ± 1.3	27.0 ± 1.3
2-methyl-2-butanol	1	9.3	9.3	17.7	17.7	-2.2	-2.2	19.9	19.9
2-methyl-2-propanol	2	7.0 ± 0.1	7.0 ± 0.1	12.0 ± 0.6	12.0 ± 0.5	9.5 ± 2.1	-9.0 ± 2.1	21.1 ± 1.6	21.0 ± 1.6
2-methylpyridine	1	22.9	22.9	20.8	20.8	-8.4	-8.4	29.2	29.2
3-methylpyridine	1	23.1	23.1	20.7	20.7	-8.9	-8.9	29.5	29.5
N-methylformamide	2	4.5 ± 0.7	-4.4 ± 0.7	6.9 ± 0.4	-6.8 ± 0.4	22.6 ± 1.6	-22.5 ± 1.6	15.8 ± 1.2	15.7 ± 1.2
N,N-dimethylacetamide	1	7.1	7.1	7.9	7.9	-18.1	-18.1	26.0	26.0
N,N-dimethylformamide	6	1.3 ± 0.1	-0.5 ± 0.5	3.5 ± 0.8	2.9 ± 0.9	17.7 ± 1.1	-17.5 ± 1.1	20.4 ± 0.4	20.4 ± 0.4
acetone	17	4.8 ± 0.4	-3.4 ± 0.8	4.3 ± 0.4	-2.4 ± 0.8	16.7 ± 0.5	-16.6 ± 0.5	14.4 ± 0.6	14.2 ± 0.6
acetonitrile	12	6.6 ± 0.7	-6.0 ± 0.8	7.9 ± 0.7	-7.4 ± 0.8	16.2 ± 0.8	-16.0 ± 0.8	8.8 ± 0.5	8.6 ± 0.5
acetophenone	2	15.6 ± 1.8	15.4 ± 1.8	18.3 ± 3.0	17.8 ± 3.0	16.3 ± 1.4	-16.2 ± 1.4	34.1 ± 1.6	34.0 ± 1.6

Table S13: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
anisole	2	19.0 ± 1.7	18.9 ± 1.7	20.3 ± 2.9	19.9 ± 2.9	11.6 ± 1.8	-11.3 ± 1.8	31.2 ± 1.1	31.2 ± 1.1
benzaldehyde	1	16.1	16.1	18.0	18.0	-13.3	-13.3	31.3	31.3
benzonitrile	3	10.1 ± 1.9	9.6 ± 1.8	11.3 ± 2.4	10.6 ± 2.2	17.6 ± 1.9	-17.3 ± 1.8	27.9 ± 1.0	27.9 ± 1.0
chloroform	15	17.8 ± 0.4	17.8 ± 0.4	15.9 ± 0.5	15.7 ± 0.6	3.7 ± 0.3	-3.5 ± 0.4	19.4 ± 0.6	19.2 ± 0.6
cyclohexanone	1	9.6	9.6	11.2	11.2	-18.2	-18.2	29.4	29.4
dibromomethane	1	8.8	8.8	7.9	7.9	-13.0	-13.0	20.8	20.8
dibutyl ether	2	24.4 ± 0.8	24.4 ± 0.8	25.6 ± 0.8	25.6 ± 0.8	8.7 ± 0.7	-8.7 ± 0.7	34.3 ± 1.4	34.3 ± 1.4
dichloromethane	14	9.3 ± 0.4	9.1 ± 0.4	8.0 ± 0.6	7.6 ± 0.6	6.2 ± 0.3	-6.1 ± 0.4	13.9 ± 0.5	13.7 ± 0.6
diethyl sulfide	1	27.0	27.0	20.3	20.3	-7.0	-7.0	27.3	27.3
diethylamine	3	21.3 ± 1.0	21.3 ± 1.0	20.2 ± 1.3	20.1 ± 1.4	3.3 ± 0.3	-3.3 ± 0.3	23.5 ± 1.6	23.3 ± 1.6
diisopropyl ether	3	12.5 ± 1.3	12.2 ± 1.4	20.0 ± 3.2	19.2 ± 3.2	6.0 ± 0.4	-6.0 ± 0.4	25.8 ± 3.2	25.2 ± 3.3
dimethyl ether	2	2.1 ± 0.1	2.1 ± 0.1	0.8 ± 0.1	0.8 ± 0.1	10.2 ± 1.1	-10.1 ± 1.1	11.0 ± 1.0	10.9 ± 0.9
dimethyl sulfoxide	5	12.7 ± 0.9	-12.5 ± 0.9	9.4 ± 1.6	-8.6 ± 1.8	27.6 ± 1.8	-27.3 ± 1.8	18.9 ± 1.0	18.8 ± 1.0
ethanol	19	2.2 ± 0.3	0.1 ± 0.5	2.9 ± 0.4	1.2 ± 0.6	11.0 ± 0.7	-10.6 ± 0.7	11.9 ± 0.4	11.8 ± 0.5

Table S13: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
ethyl acetate	8	5.2 ± 1.1	0.5 ± 1.8	7.7 ± 1.8	5.6 ± 1.9	17.7 ± 1.0	-17.5 ± 1.0	23.4 ± 1.2	23.1 ± 1.3
ethylbenzene	6	23.3 ± 0.9	23.2 ± 0.9	22.3 ± 1.6	22.0 ± 1.5	3.7 ± 0.7	-3.1 ± 0.8	25.5 ± 1.8	25.1 ± 1.8
formaldehyde	1	-14.9	-14.9	-4.1	-4.1	-11.4	-11.4	7.3	7.3
isopropylbenzene	1	25.8	25.8	25.3	25.3	-1.4	-1.4	26.7	26.7
methanol	17	6.7 ± 0.6	-6.3 ± 0.5	6.2 ± 0.6	-5.5 ± 0.7	13.2 ± 0.7	-12.7 ± 0.8	7.4 ± 0.3	7.3 ± 0.4
methyl acetate	4	6.0 ± 1.0	-1.7 ± 2.9	6.4 ± 1.2	3.0 ± 2.8	18.4 ± 2.4	-17.9 ± 2.2	21.0 ± 1.0	20.9 ± 1.0
morpholine	1	16.0	16.0	18.7	18.7	-13.4	-13.4	32.1	32.1
n-butylamine	3	17.9 ± 0.9	17.8 ± 0.9	18.8 ± 0.2	18.8 ± 0.2	4.7 ± 0.8	-4.4 ± 0.8	23.3 ± 1.1	23.2 ± 1.0
nitrobenzene	1	8.7	8.7	17.3	17.3	-21.6	-21.6	38.9	38.9
nitromethane	12	18.4 ± 0.8	-18.2 ± 0.8	9.1 ± 0.8	-8.6 ± 0.9	27.6 ± 0.9	-27.4 ± 0.9	18.8 ± 0.3	18.8 ± 0.3
o-xylene	3	24.6 ± 1.6	24.4 ± 1.7	24.3 ± 1.6	24.1 ± 1.6	2.7 ± 0.8	-2.3 ± 0.9	26.7 ± 2.3	26.4 ± 2.3
phenol	1	15.3	15.3	12.4	12.4	-15.9	-15.9	28.3	28.3
pyridine	3	14.5 ± 1.7	14.1 ± 1.8	12.7 ± 1.8	12.2 ± 1.9	11.3 ± 1.3	-11.1 ± 1.3	23.4 ± 0.7	23.3 ± 0.8
tetrahydrofuran	5	10.3 ± 0.3	10.3 ± 0.3	11.3 ± 0.1	11.3 ± 0.1	10.5 ± 0.3	-10.5 ± 0.3	21.7 ± 0.3	21.7 ± 0.3

Table S13: Root mean square deviation (RMSD) and mean signed error (MSE) of Still calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
thiophene	1	21.6	21.6	15.6	15.6	-7.0	-7.0	22.7	22.7
toluene	17	21.7 ± 0.4	21.6 ± 0.4	19.8 ± 0.5	19.7 ± 0.5	3.1 ± 0.3	-2.6 ± 0.4	22.5 ± 0.7	22.3 ± 0.7
triethyl phosphate	1	20.3	20.3	31.7	31.7	-21.7	-21.7	53.4	53.4
triethylamine	3	24.8 ± 1.7	24.6 ± 1.7	21.7 ± 0.6	21.7 ± 0.6	3.6 ± 0.2	-3.6 ± 0.2	25.3 ± 0.7	25.3 ± 0.7

Table S14: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-butanol	6	10.7 ± 0.4	10.7 ± 0.4	12.4 ± 0.6	12.4 ± 0.6	10.2 ± 0.9	-9.9 ± 0.8	22.4 ± 0.7	22.3 ± 0.7
1-chlorobutane	4	15.0 ± 0.8	14.9 ± 0.8	13.6 ± 1.3	13.3 ± 1.4	6.3 ± 0.8	-6.1 ± 0.7	19.7 ± 1.6	19.4 ± 1.7
1-octanol	1	23.5	23.5	27.0	27.0	-9.9	-9.9	36.9	36.9
1-pentanol	4	14.1 ± 0.8	14.0 ± 0.7	17.2 ± 0.5	17.1 ± 0.5	9.7 ± 1.5	-9.3 ± 1.5	26.6 ± 1.4	26.4 ± 1.3
1,2-dichloroethane	3	10.4 ± 2.0	9.7 ± 2.0	10.8 ± 2.0	10.1 ± 2.1	10.4 ± 1.7	-10.0 ± 1.6	20.2 ± 0.6	20.1 ± 0.6

Table S14: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
2-hexanone	3	12.6 ± 3.3	11.4 ± 3.0	15.6 ± 2.0	15.2 ± 2.0	12.1 ± 1.1	-11.9 ± 1.1	27.2 ± 1.3	27.1 ± 1.3
2-methyl-2-butanol	1	11.8	11.8	20.3	20.3	0.9	0.9	19.4	19.4
2-methyl-2-propanol	2	9.5 ± 0.0	9.5 ± 0.0	14.6 ± 0.7	14.5 ± 0.7	6.9 ± 2.2	-6.1 ± 2.2	20.8 ± 1.6	20.6 ± 1.6
2-methylpyridine	1	24.1	24.1	22.1	22.1	-8.3	-8.3	30.4	30.4
3-methylpyridine	1	24.9	24.9	22.5	22.5	-8.3	-8.3	30.8	30.8
N-methylformamide	2	2.4 ± 0.7	-2.1 ± 0.7	4.6 ± 0.5	-4.6 ± 0.5	21.8 ± 1.7	-21.7 ± 1.7	17.2 ± 1.2	17.1 ± 1.2
N,N-dimethylacetamide	1	9.0	9.0	9.8	9.8	-16.7	-16.7	26.6	26.6
N,N-dimethylformamide	6	1.2 ± 0.2	-0.0 ± 0.5	3.9 ± 0.8	3.3 ± 0.9	18.4 ± 1.1	-18.2 ± 1.1	21.5 ± 0.4	21.5 ± 0.4
acetone	17	3.3 ± 0.4	-0.7 ± 0.8	3.3 ± 0.6	0.3 ± 0.8	15.1 ± 0.5	-14.9 ± 0.5	15.4 ± 0.6	15.2 ± 0.6
acetonitrile	12	6.1 ± 0.7	-5.4 ± 0.8	7.4 ± 0.7	-6.8 ± 0.8	18.4 ± 0.8	-18.2 ± 0.8	11.5 ± 0.5	11.4 ± 0.5
acetophenone	2	17.5 ± 1.8	17.4 ± 1.8	20.2 ± 3.0	19.8 ± 3.0	15.8 ± 1.3	-15.7 ± 1.3	35.5 ± 1.6	35.4 ± 1.6
anisole	2	21.4 ± 1.7	21.3 ± 1.7	22.7 ± 2.9	22.3 ± 2.9	10.5 ± 1.8	-10.2 ± 1.8	32.6 ± 1.2	32.5 ± 1.1
benzaldehyde	1	16.9	16.9	18.8	18.8	-14.5	-14.5	33.3	33.3
benzonitrile	3	10.0 ± 2.0	9.4 ± 2.0	11.2 ± 2.6	10.3 ± 2.4	20.6 ± 1.9	-20.4 ± 1.9	30.8 ± 1.0	30.7 ± 1.0

Table S14: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
chloroform	15	18.5 ± 0.4	18.4 ± 0.4	16.5 ± 0.5	16.4 ± 0.6	3.5 ± 0.3	-3.2 ± 0.4	19.7 ± 0.6	19.6 ± 0.6
cyclohexanone	1	10.2	10.2	11.8	11.8	-17.2	-17.2	29.0	29.0
dibromomethane	1	9.1	9.1	8.2	8.2	-12.8	-12.8	21.0	21.0
dibutyl ether	2	28.2 ± 0.7	28.1 ± 0.7	29.4 ± 0.7	29.4 ± 0.7	4.6 ± 0.8	-4.5 ± 0.8	33.9 ± 1.5	33.9 ± 1.5
dichloromethane	14	10.5 ± 0.4	10.4 ± 0.4	9.1 ± 0.6	8.9 ± 0.6	5.5 ± 0.3	-5.3 ± 0.3	14.4 ± 0.5	14.2 ± 0.6
diethyl sulfide	1	28.5	28.5	21.8	21.8	-4.5	-4.5	26.3	26.3
diethylamine	3	23.6 ± 1.1	23.6 ± 1.1	22.5 ± 1.2	22.4 ± 1.2	1.4 ± 0.4	-1.0 ± 0.6	23.6 ± 1.6	23.4 ± 1.6
diisopropyl ether	3	17.0 ± 1.1	16.9 ± 1.2	24.4 ± 2.9	23.9 ± 2.9	1.3 ± 0.4	-0.9 ± 0.5	25.5 ± 3.1	24.8 ± 3.3
dimethyl ether	2	6.7 ± 0.0	6.7 ± 0.0	5.5 ± 0.2	5.4 ± 0.2	6.6 ± 1.2	-6.4 ± 1.2	11.9 ± 0.9	11.9 ± 0.9
dimethyl sulfoxide	5	6.3 ± 0.8	-6.0 ± 0.9	4.5 ± 0.8	-2.1 ± 1.8	19.8 ± 1.8	-19.3 ± 1.8	17.4 ± 1.0	17.2 ± 1.0
ethanol	19	3.9 ± 0.4	3.3 ± 0.5	5.0 ± 0.5	4.3 ± 0.6	8.4 ± 0.6	-7.7 ± 0.7	12.3 ± 0.4	12.1 ± 0.5
ethyl acetate	8	5.7 ± 1.7	2.9 ± 1.8	9.5 ± 1.9	8.0 ± 1.8	16.1 ± 1.0	-15.9 ± 1.0	24.2 ± 1.2	23.9 ± 1.3
ethylbenzene	6	22.6 ± 1.0	22.5 ± 0.9	21.6 ± 1.7	21.3 ± 1.6	5.2 ± 0.8	-4.8 ± 0.8	26.5 ± 1.8	26.1 ± 1.8
formaldehyde	1	-15.3	-15.3	-4.4	-4.4	-13.6	-13.6	9.2	9.2

Table S14: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
isopropylbenzene	1	22.9	22.9	22.4	22.4	-5.1	-5.1	27.5	27.5
methanol	17	3.6 ± 0.6	-3.0 ± 0.5	3.5 ± 0.5	-2.1 ± 0.7	10.9 ± 0.7	-10.4 ± 0.8	8.4 ± 0.3	8.2 ± 0.4
methyl acetate	4	5.7 ± 0.8	1.2 ± 2.8	8.0 ± 1.7	5.9 ± 2.7	16.8 ± 2.3	-16.2 ± 2.2	22.3 ± 1.0	22.2 ± 1.0
morpholine	1	22.3	22.3	25.0	25.0	-5.5	-5.5	30.5	30.5
n-butylamine	3	16.6 ± 1.0	16.5 ± 1.1	17.5 ± 0.4	17.5 ± 0.4	5.7 ± 0.8	-5.5 ± 0.8	23.1 ± 1.1	23.0 ± 1.1
nitrobenzene	1	10.9	10.9	19.5	19.5	-20.8	-20.8	40.3	40.3
nitromethane	12	14.4 ± 0.7	-14.2 ± 0.8	5.4 ± 0.8	-4.5 ± 0.9	24.2 ± 0.9	-24.0 ± 0.9	19.5 ± 0.3	19.5 ± 0.3
o-xylene	3	22.8 ± 2.0	22.5 ± 2.0	22.5 ± 2.0	22.2 ± 1.9	5.4 ± 0.8	-5.2 ± 0.8	27.7 ± 2.3	27.4 ± 2.3
phenol	1	17.0	17.0	14.1	14.1	-15.4	-15.4	29.5	29.5
pyridine	3	16.7 ± 1.7	16.4 ± 1.7	14.9 ± 1.7	14.5 ± 1.8	10.5 ± 1.2	-10.3 ± 1.2	24.9 ± 0.7	24.9 ± 0.7
tetrahydrofuran	5	14.6 ± 0.3	14.6 ± 0.3	15.6 ± 0.2	15.6 ± 0.2	5.0 ± 0.4	-4.9 ± 0.4	20.5 ± 0.3	20.5 ± 0.3
thiophene	1	21.7	21.7	15.8	15.8	-7.1	-7.1	22.9	22.9
toluene	17	20.1 ± 0.5	20.0 ± 0.5	18.2 ± 0.6	18.1 ± 0.5	5.8 ± 0.3	-5.6 ± 0.4	23.8 ± 0.7	23.6 ± 0.8
triethyl phosphate	1	25.5	25.5	36.9	36.9	-15.4	-15.4	52.3	52.3

Table S14: Root mean square deviation (RMSD) and mean signed error (MSE) of HCT calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
triethylamine	3	27.6 ± 1.7	27.5 ± 1.7	24.6 ± 0.6	24.5 ± 0.6	0.6 ± 0.2	-0.5 ± 0.2	25.1 ± 0.7	25.1 ± 0.7

Table S15: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-I calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-butanol	6	10.0 ± 0.6	9.9 ± 0.6	11.7 ± 0.7	11.6 ± 0.7	12.5 ± 0.9	-12.4 ± 0.8	24.0 ± 0.7	24.0 ± 0.7
1-chlorobutane	4	15.9 ± 0.8	15.9 ± 0.8	14.6 ± 1.3	14.3 ± 1.4	7.0 ± 0.8	-6.8 ± 0.7	21.4 ± 1.6	21.1 ± 1.8
1-octanol	1	22.3	22.3	25.8	25.8	-12.7	-12.7	38.6	38.6
1-pentanol	4	13.4 ± 1.0	13.2 ± 1.0	16.4 ± 0.7	16.3 ± 0.6	12.1 ± 1.5	-11.8 ± 1.5	28.2 ± 1.3	28.1 ± 1.4
1,2-dichloroethane	3	11.1 ± 2.1	10.4 ± 2.1	11.5 ± 2.2	10.8 ± 2.3	11.4 ± 1.8	-11.0 ± 1.7	21.9 ± 0.7	21.8 ± 0.6
2-hexanone	3	12.7 ± 3.6	11.4 ± 3.3	15.6 ± 2.3	15.1 ± 2.1	13.9 ± 1.2	-13.7 ± 1.2	28.9 ± 1.4	28.8 ± 1.4
2-methyl-2-butanol	1	10.8	10.8	19.3	19.3	-1.2	-1.2	20.5	20.5
2-methyl-2-propanol	2	9.1 ± 0.1	9.1 ± 0.1	14.1 ± 0.6	14.1 ± 0.6	8.3 ± 2.2	-7.8 ± 2.1	22.0 ± 1.6	21.9 ± 1.6

Table S15: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-I calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
2-methylpyridine	1	24.6	24.6	22.6	22.6	-9.9	-9.9	32.5	32.5
3-methylpyridine	1	25.3	25.3	22.9	22.9	-10.0	-10.0	32.9	32.9
N-methylformamide	2	4.0 ± 0.6	-3.9 ± 0.6	6.4 ± 0.4	-6.4 ± 0.4	25.2 ± 1.6	-25.1 ± 1.6	18.8 ± 1.2	18.8 ± 1.2
N,N-dimethylacetamide	1	8.3	8.3	9.1	9.1	-19.0	-19.0	28.1	28.1
N,N-dimethylformamide	6	1.8 ± 0.3	-1.2 ± 0.5	3.0 ± 0.7	2.2 ± 0.9	21.1 ± 1.1	-21.0 ± 1.1	23.2 ± 0.4	23.2 ± 0.4
acetone	17	3.8 ± 0.4	-1.3 ± 0.9	3.6 ± 0.5	-0.3 ± 0.9	17.4 ± 0.5	-17.2 ± 0.6	17.1 ± 0.6	16.9 ± 0.6
acetonitrile	12	6.5 ± 0.7	-5.8 ± 0.8	7.8 ± 0.7	-7.2 ± 0.8	20.1 ± 0.8	-19.9 ± 0.8	12.8 ± 0.5	12.7 ± 0.5
acetophenone	2	17.5 ± 1.9	17.2 ± 1.9	20.2 ± 3.1	19.7 ± 3.1	18.1 ± 1.5	-18.0 ± 1.5	37.8 ± 1.6	37.7 ± 1.6
anisole	2	22.2 ± 1.7	22.1 ± 1.7	23.5 ± 2.9	23.1 ± 3.0	11.9 ± 1.8	-11.6 ± 1.8	34.8 ± 1.2	34.7 ± 1.2
benzaldehyde	1	17.1	17.1	18.9	18.9	-16.7	-16.7	35.7	35.7
benzonitrile	3	10.4 ± 2.2	9.7 ± 2.1	11.6 ± 2.7	10.7 ± 2.5	22.7 ± 2.0	-22.5 ± 1.9	33.2 ± 1.0	33.2 ± 1.0
chloroform	15	19.2 ± 0.4	19.1 ± 0.4	17.2 ± 0.6	17.1 ± 0.6	4.2 ± 0.3	-4.0 ± 0.4	21.2 ± 0.6	21.1 ± 0.6
cyclohexanone	1	9.6	9.6	11.2	11.2	-19.1	-19.1	30.2	30.2
dibromomethane	1	8.8	8.8	7.9	7.9	-14.4	-14.4	22.3	22.3

Table S15: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-I calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
dibutyl ether	2	30.9 ± 0.7	30.9 ± 0.7	32.1 ± 0.7	32.1 ± 0.7	3.8 ± 0.8	-3.6 ± 0.8	35.8 ± 1.5	35.7 ± 1.5
dichloromethane	14	10.8 ± 0.5	10.6 ± 0.4	9.4 ± 0.6	9.1 ± 0.6	6.5 ± 0.4	-6.4 ± 0.4	15.6 ± 0.5	15.5 ± 0.6
diethyl sulfide	1	29.7	29.7	23.0	23.0	-5.2	-5.2	28.1	28.1
diethylamine	3	25.1 ± 1.1	25.0 ± 1.1	23.9 ± 1.3	23.8 ± 1.2	1.5 ± 0.4	-1.2 ± 0.5	25.2 ± 1.6	25.0 ± 1.6
diisopropyl ether	3	20.1 ± 1.0	20.0 ± 1.1	27.4 ± 2.8	27.0 ± 2.8	1.2 ± 0.5	0.7 ± 0.5	26.9 ± 3.2	26.3 ± 3.2
dimethyl ether	2	7.4 ± 0.0	7.4 ± 0.0	6.1 ± 0.2	6.1 ± 0.2	7.3 ± 1.2	-7.1 ± 1.2	13.3 ± 0.9	13.3 ± 0.9
dimethyl sulfoxide	5	8.0 ± 0.8	-7.7 ± 0.9	5.5 ± 1.1	-3.8 ± 1.8	22.8 ± 1.8	-22.4 ± 1.8	18.8 ± 1.0	18.6 ± 1.0
ethanol	19	3.1 ± 0.4	2.1 ± 0.5	4.1 ± 0.5	3.2 ± 0.6	10.8 ± 0.7	-10.4 ± 0.7	13.7 ± 0.4	13.5 ± 0.5
ethyl acetate	8	5.7 ± 1.6	2.0 ± 1.9	9.0 ± 2.0	7.2 ± 1.9	18.9 ± 1.1	-18.6 ± 1.1	26.1 ± 1.3	25.8 ± 1.3
ethylbenzene	6	23.4 ± 1.0	23.3 ± 1.0	22.4 ± 1.8	22.1 ± 1.6	6.5 ± 0.8	-6.1 ± 0.8	28.6 ± 1.8	28.2 ± 1.8
formaldehyde	1	-15.5	-15.5	-4.6	-4.6	-15.2	-15.2	10.6	10.6
isopropylbenzene	1	22.9	22.9	22.4	22.4	-7.0	-7.0	29.4	29.4
methanol	17	5.1 ± 0.6	-4.6 ± 0.5	4.7 ± 0.6	-3.8 ± 0.7	13.6 ± 0.7	-13.2 ± 0.8	9.5 ± 0.3	9.4 ± 0.4
methyl acetate	4	6.0 ± 0.6	0.5 ± 3.0	7.7 ± 1.8	5.2 ± 2.9	19.3 ± 2.5	-18.8 ± 2.4	24.0 ± 1.0	23.9 ± 1.0

Table S15: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-I calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
morpholine	1	23.5	23.5	26.2	26.2	-5.3	-5.3	31.5	31.5
n-butylamine	3	16.1 ± 1.2	16.0 ± 1.3	17.0 ± 0.6	16.9 ± 0.6	7.7 ± 0.7	-7.6 ± 0.8	24.6 ± 1.2	24.5 ± 1.2
nitrobenzene	1	10.0	10.0	18.6	18.6	-24.0	-24.0	42.6	42.6
nitromethane	12	17.1 ± 0.8	-16.8 ± 0.8	7.9 ± 0.8	-7.2 ± 0.9	28.3 ± 0.9	-28.2 ± 0.9	21.0 ± 0.3	21.0 ± 0.3
o-xylene	3	23.1 ± 2.1	22.8 ± 2.1	22.8 ± 2.1	22.5 ± 2.2	7.0 ± 0.8	-6.9 ± 0.8	29.6 ± 2.3	29.3 ± 2.3
phenol	1	16.6	16.6	13.7	13.7	-18.0	-18.0	31.7	31.7
pyridine	3	17.0 ± 1.8	16.7 ± 1.9	15.2 ± 1.9	14.8 ± 2.0	12.5 ± 1.4	-12.3 ± 1.4	27.1 ± 0.7	27.0 ± 0.8
tetrahydrofuran	5	15.8 ± 0.3	15.8 ± 0.3	16.8 ± 0.2	16.8 ± 0.2	5.1 ± 0.4	-5.0 ± 0.4	21.8 ± 0.3	21.8 ± 0.3
thiophene	1	22.2	22.2	16.3	16.3	-8.6	-8.6	24.9	24.9
toluene	17	20.6 ± 0.5	20.5 ± 0.5	18.7 ± 0.6	18.5 ± 0.6	7.4 ± 0.3	-7.3 ± 0.4	26.0 ± 0.7	25.8 ± 0.7
triethyl phosphate	1	24.4	24.4	35.8	35.8	-18.7	-18.7	54.5	54.5
triethylamine	3	29.9 ± 1.7	29.8 ± 1.7	26.9 ± 0.6	26.9 ± 0.6	0.6 ± 0.2	0.6 ± 0.2	26.4 ± 0.7	26.3 ± 0.7

Table S16: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-II calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
1-butanol	6	10.0 ± 0.4	10.0 ± 0.4	11.8 ± 0.6	11.7 ± 0.6	10.6 ± 0.9	-10.4 ± 0.8	22.1 ± 0.7	22.0 ± 0.7
1-chlorobutane	4	14.7 ± 0.8	14.6 ± 0.8	13.4 ± 1.3	13.1 ± 1.4	6.4 ± 0.8	-6.2 ± 0.7	19.6 ± 1.6	19.3 ± 1.7
1-octanol	1	21.7	21.7	25.2	25.2	-10.4	-10.4	35.6	35.6
1-pentanol	4	13.2 ± 0.8	13.1 ± 0.8	16.2 ± 0.5	16.2 ± 0.5	10.1 ± 1.5	-9.7 ± 1.5	26.1 ± 1.4	25.9 ± 1.4
1,2-dichloroethane	3	10.7 ± 2.0	10.1 ± 2.1	11.1 ± 2.1	10.5 ± 2.2	10.4 ± 1.7	-10.1 ± 1.6	20.6 ± 0.7	20.5 ± 0.6
2-hexanone	3	12.1 ± 3.3	10.9 ± 3.1	15.0 ± 2.0	14.7 ± 1.9	12.0 ± 1.1	-11.8 ± 1.1	26.6 ± 1.4	26.5 ± 1.4
2-methyl-2-butanol	1	11.5	11.5	20.0	20.0	1.5	1.5	18.5	18.5
2-methyl-2-propanol	2	9.4 ± 0.0	9.4 ± 0.0	14.4 ± 0.7	14.4 ± 0.6	6.5 ± 2.3	-5.6 ± 2.2	20.2 ± 1.6	20.0 ± 1.6
2-methylpyridine	1	24.3	24.3	22.3	22.3	-8.1	-8.1	30.4	30.4
3-methylpyridine	1	24.9	24.9	22.6	22.6	-8.3	-8.3	30.8	30.8
N-methylformamide	2	2.7 ± 0.7	-2.6 ± 0.7	5.0 ± 0.4	-5.0 ± 0.4	22.5 ± 1.7	-22.4 ± 1.6	17.5 ± 1.2	17.4 ± 1.2
N,N-dimethylacetamide	1	8.7	8.7	9.5	9.5	-16.7	-16.7	26.2	26.2
N,N-dimethylformamide	6	1.4 ± 0.2	-0.7 ± 0.5	3.3 ± 0.8	2.6 ± 0.9	19.1 ± 1.1	-18.9 ± 1.1	21.5 ± 0.4	21.5 ± 0.4
acetone	17	3.4 ± 0.4	-0.9 ± 0.8	3.4 ± 0.6	0.1 ± 0.8	15.5 ± 0.5	-15.3 ± 0.5	15.6 ± 0.6	15.4 ± 0.6

Table S16: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-II calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
acetonitrile	12	6.2 ± 0.7	-5.6 ± 0.8	7.5 ± 0.7	-6.9 ± 0.8	18.9 ± 0.8	-18.7 ± 0.8	11.9 ± 0.5	11.8 ± 0.5
acetophenone	2	17.4 ± 1.8	17.2 ± 1.8	20.1 ± 2.9	19.6 ± 2.9	15.7 ± 1.3	-15.6 ± 1.3	35.3 ± 1.6	35.2 ± 1.6
anisole	2	21.6 ± 1.7	21.5 ± 1.7	22.9 ± 2.9	22.5 ± 2.9	10.2 ± 1.7	-9.9 ± 1.7	32.5 ± 1.2	32.4 ± 1.1
benzaldehyde	1	16.6	16.6	18.5	18.5	-15.0	-15.0	33.5	33.5
benzonitrile	3	9.9 ± 2.1	9.2 ± 2.0	11.1 ± 2.6	10.2 ± 2.4	21.1 ± 1.9	-20.8 ± 1.9	31.1 ± 1.0	31.1 ± 1.0
chloroform	15	18.9 ± 0.4	18.8 ± 0.4	16.9 ± 0.6	16.8 ± 0.6	3.7 ± 0.3	-3.4 ± 0.4	20.3 ± 0.6	20.1 ± 0.6
cyclohexanone	1	9.3	9.3	10.9	10.9	-17.3	-17.3	28.2	28.2
dibromomethane	1	9.0	9.0	8.1	8.1	-13.3	-13.3	21.5	21.5
dibutyl ether	2	29.2 ± 0.7	29.2 ± 0.7	30.5 ± 0.7	30.5 ± 0.7	2.5 ± 0.9	-2.2 ± 0.9	32.7 ± 1.5	32.7 ± 1.5
dichloromethane	14	10.7 ± 0.4	10.5 ± 0.4	9.3 ± 0.6	9.0 ± 0.6	5.8 ± 0.3	-5.6 ± 0.4	14.8 ± 0.5	14.6 ± 0.6
diethyl sulfide	1	28.4	28.4	21.7	21.7	-4.5	-4.5	26.2	26.2
diethylamine	3	24.2 ± 1.2	24.1 ± 1.2	23.0 ± 1.2	22.9 ± 1.2	1.2 ± 0.2	-0.1 ± 0.7	23.2 ± 1.6	23.0 ± 1.7
diisopropyl ether	3	19.3 ± 1.0	19.2 ± 1.0	26.6 ± 2.7	26.2 ± 2.8	2.5 ± 0.6	2.3 ± 0.6	24.6 ± 3.2	23.9 ± 3.3
dimethyl ether	2	7.2 ± 0.0	7.2 ± 0.0	6.0 ± 0.3	5.9 ± 0.3	6.3 ± 1.2	-6.1 ± 1.2	12.1 ± 0.9	12.0 ± 0.9

Table S16: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-II calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
dimethyl sulfoxide	5	6.6 ± 0.8	-6.3 ± 0.9	4.6 ± 0.8	-2.4 ± 1.8	20.0 ± 1.8	-19.6 ± 1.9	17.4 ± 1.0	17.2 ± 1.0
ethanol	19	3.5 ± 0.4	2.8 ± 0.5	4.6 ± 0.5	3.9 ± 0.6	8.9 ± 0.7	-8.4 ± 0.7	12.4 ± 0.4	12.3 ± 0.5
ethyl acetate	8	5.6 ± 1.6	2.5 ± 1.8	9.2 ± 1.8	7.7 ± 1.8	16.4 ± 1.0	-16.2 ± 1.0	24.2 ± 1.3	23.9 ± 1.3
ethylbenzene	6	22.1 ± 1.0	22.0 ± 0.9	21.1 ± 1.7	20.8 ± 1.6	5.4 ± 0.8	-5.0 ± 0.8	26.1 ± 1.8	25.7 ± 1.8
formaldehyde	1	-15.4	-15.4	-4.5	-4.5	-14.5	-14.5	10.0	10.0
isopropylbenzene	1	21.2	21.2	20.7	20.7	-6.0	-6.0	26.7	26.7
methanol	17	4.1 ± 0.6	-3.6 ± 0.5	3.9 ± 0.5	-2.7 ± 0.7	11.8 ± 0.7	-11.3 ± 0.8	8.7 ± 0.3	8.6 ± 0.4
methyl acetate	4	5.7 ± 0.8	1.2 ± 2.8	8.0 ± 1.8	5.9 ± 2.7	17.0 ± 2.4	-16.4 ± 2.2	22.4 ± 1.0	22.3 ± 1.0
morpholine	1	24.5	24.5	27.2	27.2	-2.6	-2.6	29.8	29.8
n-butylamine	3	15.3 ± 1.1	15.1 ± 1.2	16.1 ± 0.5	16.1 ± 0.5	6.6 ± 0.8	-6.4 ± 0.7	22.6 ± 1.1	22.6 ± 1.1
nitrobenzene	1	10.6	10.6	19.2	19.2	-21.2	-21.2	40.4	40.4
nitromethane	12	15.0 ± 0.7	-14.8 ± 0.8	6.0 ± 0.8	-5.1 ± 0.9	25.2 ± 0.9	-25.0 ± 0.9	19.9 ± 0.3	19.8 ± 0.3
o-xylene	3	21.4 ± 2.0	21.1 ± 2.1	21.1 ± 2.1	20.8 ± 2.1	6.3 ± 0.8	-6.1 ± 0.8	27.2 ± 2.3	26.9 ± 2.3
phenol	1	16.9	16.9	13.9	13.9	-15.7	-15.7	29.7	29.7

Table S16: Root mean square deviation (RMSD) and mean signed error (MSE) of OBC-II calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$		ΔG_{polar}		ΔG_{apolar}	
Solute	N	RMSD	MSE	RMSD	MSE	RMSD	MSE	RMSD	MSE
pyridine	3	17.0 ± 1.7	16.8 ± 1.8	15.2 ± 1.7	14.9 ± 1.9	10.6 ± 1.2	-10.4 ± 1.2	25.3 ± 0.8	25.3 ± 0.7
tetrahydrofuran	5	15.7 ± 0.3	15.7 ± 0.3	16.6 ± 0.2	16.6 ± 0.2	3.6 ± 0.4	-3.5 ± 0.4	20.1 ± 0.3	20.1 ± 0.3
thiophene	1	21.8	21.8	15.9	15.9	-7.5	-7.5	23.4	23.4
toluene	17	19.3 ± 0.5	19.3 ± 0.5	17.5 ± 0.6	17.3 ± 0.6	6.5 ± 0.3	-6.3 ± 0.4	23.8 ± 0.7	23.6 ± 0.8
triethyl phosphate	1	24.9	24.9	36.4	36.4	-15.1	-15.1	51.4	51.4
triethylamine	3	28.0 ± 1.7	27.8 ± 1.7	24.9 ± 0.6	24.9 ± 0.6	0.8 ± 0.2	0.7 ± 0.2	24.2 ± 0.7	24.2 ± 0.7

Table S17: Root mean square deviation (RMSD) and mean signed error (MSE) of B3LYP/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
1-butanol	6	4.90 ± 1.14	-3.80 ± 1.26	2.98 ± 0.76	-2.09 ± 0.87
1-chlorobutane	4	8.77 ± 0.50	-8.71 ± 0.51	10.39 ± 0.79	-10.27 ± 0.81
1-octanol	1	1.18	1.18	4.69	4.69
1-pentanol	4	5.79 ± 1.53	-4.75 ± 1.65	3.01 ± 0.74	-1.66 ± 1.25
1,2-dichloroethane	3	7.43 ± 1.97	-6.65 ± 1.90	7.18 ± 2.17	-6.24 ± 2.06
2-hexanone	3	8.36 ± 2.12	-7.38 ± 2.27	4.05 ± 1.06	-3.59 ± 1.09
2-methyl-2-butanol	1	-8.84	-8.84	-0.36	-0.36
2-methyl-2-propanol	2	7.78 ± 1.79	-7.37 ± 1.80	2.80 ± 1.12	-2.33 ± 1.09
2-methylpyridine	1	1.04	1.04	-0.97	-0.97
3-methylpyridine	1	-4.86	-4.86	-7.25	-7.25
N-methylformamide	2	4.37 ± 0.33	-4.34 ± 0.34	6.77 ± 0.10	-6.77 ± 0.10
N,N-dimethylacetamide	1	0.05	0.05	0.88	0.88
N,N-dimethylformamide	6	5.24 ± 0.64	-5.00 ± 0.62	2.02 ± 0.51	-1.66 ± 0.47
acetone	17	7.57 ± 0.57	-7.00 ± 0.70	6.66 ± 0.44	-6.03 ± 0.68
acetonitrile	12	8.20 ± 0.64	-7.89 ± 0.65	9.50 ± 0.53	-9.29 ± 0.58
acetophenone	2	6.00 ± 1.23	-5.75 ± 1.23	4.73 ± 2.47	-3.32 ± 2.38
anisole	2	2.76 ± 0.17	-2.75 ± 0.17	2.29 ± 1.13	-1.71 ± 1.08
benzaldehyde	1	-2.57	-2.57	-0.68	-0.68
benzonitrile	3	4.27 ± 1.53	-3.40 ± 1.50	3.69 ± 1.85	-2.42 ± 1.61
chloroform	15	2.93 ± 0.43	-2.09 ± 0.53	4.71 ± 0.52	-4.14 ± 0.58
cyclohexanone	1	-9.04	-9.04	-7.44	-7.44

Table S17: Root mean square deviation (RMSD) and mean signed error (MSE) of B3LYP/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
dibromomethane	1	-5.19	-5.19	-6.08	-6.08
dibutyl ether	2	6.04 ± 1.77	-5.49 ± 1.78	4.93 ± 1.82	-4.25 ± 1.77
dichloromethane	14	5.63 ± 0.50	-5.28 ± 0.53	7.13 ± 0.54	-6.77 ± 0.59
diethyl sulfide	1	4.47	4.47	-2.25	-2.25
diethylamine	3	0.75 ± 0.18	0.16 ± 0.43	2.82 ± 1.20	-1.04 ± 1.52
diisopropyl ether	3	9.81 ± 0.65	-9.75 ± 0.63	5.23 ± 1.27	-2.76 ± 2.58
dimethyl ether	2	2.12 ± 0.82	-1.79 ± 0.81	3.41 ± 1.05	-3.07 ± 1.05
dimethyl sulfoxide	5	13.01 ± 2.02	-12.16 ± 2.05	8.60 ± 1.07	-8.20 ± 1.16
ethanol	19	4.11 ± 0.60	-2.56 ± 0.73	4.09 ± 0.47	-1.50 ± 0.88
ethyl acetate	8	3.91 ± 0.54	-2.20 ± 1.13	4.36 ± 1.14	2.94 ± 1.13
ethylbenzene	6	2.88 ± 0.43	0.79 ± 1.14	1.33 ± 0.21	-0.42 ± 0.51
formaldehyde	1	-8.30	-8.30	2.55	2.55
isopropylbenzene	1	-0.83	-0.83	-1.31	-1.31
methanol	17	3.07 ± 0.48	0.54 ± 0.73	4.18 ± 0.63	1.39 ± 0.95
methyl acetate	4	7.01 ± 1.97	-1.73 ± 3.41	7.75 ± 1.01	2.97 ± 3.58
morpholine	1	-0.34	-0.34	2.34	2.34
n-butylamine	3	2.42 ± 0.55	-1.25 ± 1.19	1.51 ± 0.23	-0.26 ± 0.85
nitrobenzene	1	-0.14	-0.14	8.45	8.45
nitromethane	12	3.03 ± 0.48	-2.36 ± 0.55	7.59 ± 0.62	7.27 ± 0.63
o-xylene	3	1.90 ± 0.51	0.54 ± 1.05	0.93 ± 0.06	0.24 ± 0.52
phenol	1	-2.41	-2.41	-5.32	-5.32

Table S17: Root mean square deviation (RMSD) and mean signed error (MSE) of B3LYP/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
pyridine	3	0.97 ± 0.26	-0.10 ± 0.56	2.43 ± 0.73	-2.00 ± 0.80
tetrahydrofuran	5	6.31 ± 0.70	-6.14 ± 0.66	5.51 ± 0.83	-5.19 ± 0.85
thiophene	1	5.23	5.23	-0.70	-0.70
toluene	17	4.56 ± 0.51	3.98 ± 0.55	3.06 ± 0.39	2.06 ± 0.55
triethyl phosphate	1	7.43	7.43	18.84	18.84
triethylamine	3	4.18 ± 1.97	-2.96 ± 1.68	6.03 ± 0.72	-5.88 ± 0.76

Table S18: Root mean square deviation (RMSD) and mean signed error (MSE) of HF/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
1-butanol	6	6.01 ± 1.52	-4.75 ± 1.48	4.08 ± 1.08	-3.04 ± 1.13
1-chlorobutane	4	9.96 ± 0.54	-9.90 ± 0.56	11.60 ± 0.86	-11.47 ± 0.87
1-octanol	1	-2.42	-2.42	1.09	1.09
1-pentanol	4	7.15 ± 1.91	-6.00 ± 1.94	4.23 ± 1.19	-2.90 ± 1.54
1,2-dichloroethane	3	9.04 ± 2.17	-8.25 ± 2.10	8.76 ± 2.38	-7.85 ± 2.24
2-hexanone	3	13.42 ± 3.26	-11.93 ± 3.53	9.11 ± 2.22	-8.14 ± 2.37
2-methyl-2-butanol	1	-11.30	-11.30	-2.82	-2.82
2-methyl-2-propanol	2	9.10 ± 2.27	-8.53 ± 2.24	4.13 ± 1.59	-3.49 ± 1.55
2-methylpyridine	1	-1.10	-1.10	-3.11	-3.11

Table S18: Root mean square deviation (RMSD) and mean signed error (MSE) of HF/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
3-methylpyridine	1	-3.17	-3.17	-5.56	-5.56
N-methylformamide	2	9.85 ± 1.39	-9.65 ± 1.39	12.30 ± 1.60	-12.08 ± 1.63
N,N-dimethylacetamide	1	-7.90	-7.90	-7.07	-7.07
N,N-dimethylformamide	6	9.87 ± 1.24	-9.40 ± 1.23	6.41 ± 0.78	-6.06 ± 0.85
acetone	17	9.95 ± 0.96	-9.02 ± 1.03	8.86 ± 0.70	-8.05 ± 0.90
acetonitrile	12	10.85 ± 0.67	-10.59 ± 0.68	12.18 ± 0.57	-11.99 ± 0.63
acetophenone	2	10.97 ± 1.90	-10.63 ± 1.88	9.28 ± 3.08	-8.21 ± 3.05
anisole	2	4.12 ± 2.00	-2.72 ± 2.19	2.14 ± 0.96	-1.68 ± 0.94
benzaldehyde	1	-6.90	-6.90	-5.01	-5.01
benzonitrile	3	8.39 ± 1.76	-7.88 ± 1.65	7.60 ± 2.00	-6.90 ± 1.82
chloroform	15	4.11 ± 0.49	-3.51 ± 0.55	6.06 ± 0.58	-5.56 ± 0.63
cyclohexanone	1	-11.10	-11.10	-9.50	-9.50
dibromomethane	1	-6.54	-6.54	-7.43	-7.43
dibutyl ether	2	7.36 ± 1.99	-6.80 ± 1.98	6.22 ± 2.01	-5.57 ± 1.95
dichloromethane	14	7.42 ± 0.54	-7.09 ± 0.58	8.94 ± 0.60	-8.59 ± 0.65
diethyl sulfide	1	3.50	3.50	-3.22	-3.22
diethylamine	3	1.24 ± 0.51	-0.83 ± 0.53	3.50 ± 1.73	-2.03 ± 1.63
diisopropyl ether	3	8.69 ± 0.85	-8.57 ± 0.83	4.96 ± 1.13	-1.58 ± 2.72
dimethyl ether	2	2.93 ± 1.09	-2.51 ± 1.09	4.22 ± 1.32	-3.79 ± 1.32
dimethyl sulfoxide	5	20.63 ± 3.11	-19.44 ± 3.10	16.16 ± 2.02	-15.49 ± 2.06
ethanol	19	5.14 ± 0.84	-3.45 ± 0.88	4.94 ± 0.70	-2.39 ± 0.99

Table S18: Root mean square deviation (RMSD) and mean signed error (MSE) of HF/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
ethyl acetate	8	7.28 ± 1.08	-6.22 ± 1.35	3.51 ± 0.41	-1.08 ± 1.18
ethylbenzene	6	3.70 ± 0.91	-2.69 ± 1.06	4.09 ± 0.50	-3.90 ± 0.50
formaldehyde	1	-12.26	-12.26	-1.41	-1.41
isopropylbenzene	1	-4.58	-4.58	-5.06	-5.06
methanol	17	3.43 ± 0.58	-0.38 ± 0.82	4.31 ± 0.58	0.48 ± 1.05
methyl acetate	4	10.01 ± 3.00	-7.81 ± 3.19	6.42 ± 1.64	-3.12 ± 2.76
morpholine	1	-1.92	-1.92	0.76	0.76
n-butylamine	3	2.88 ± 0.75	-1.83 ± 1.28	1.81 ± 0.24	-0.84 ± 0.92
nitrobenzene	1	-3.72	-3.72	4.87	4.87
nitromethane	12	8.49 ± 0.52	-8.28 ± 0.54	2.61 ± 0.50	1.34 ± 0.64
o-xylene	3	2.14 ± 0.53	-1.53 ± 0.86	1.88 ± 0.23	-1.84 ± 0.24
phenol	1	-5.10	-5.10	-8.01	-8.01
pyridine	3	3.29 ± 1.01	-2.85 ± 0.94	5.19 ± 1.17	-4.75 ± 1.21
tetrahydrofuran	5	7.28 ± 0.87	-7.01 ± 0.88	6.58 ± 1.07	-6.06 ± 1.15
thiophene	1	2.94	2.94	-2.99	-2.99
toluene	17	4.85 ± 0.49	-4.26 ± 0.56	6.62 ± 0.58	-6.18 ± 0.59
triethyl phosphate	1	1.65	1.65	13.06	13.06
triethylamine	3	1.42 ± 0.68	-0.71 ± 0.70	3.99 ± 1.02	-3.63 ± 0.95

Table S19: Root mean square deviation (RMSD) and mean signed error (MSE) of M06-2X/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
1-butanol	6	5.48 ± 1.35	-4.26 ± 1.41	3.57 ± 0.92	-2.55 ± 1.03
1-chlorobutane	4	8.44 ± 0.50	-8.38 ± 0.51	10.07 ± 0.80	-9.94 ± 0.82
1-octanol	1	-2.87	-2.87	0.64	0.64
1-pentanol	4	5.49 ± 1.48	-4.55 ± 1.51	2.69 ± 0.72	-1.46 ± 1.12
1,2-dichloroethane	3	6.71 ± 1.92	-5.89 ± 1.86	6.47 ± 2.11	-5.49 ± 1.98
2-hexanone	3	9.83 ± 2.27	-8.85 ± 2.46	5.52 ± 1.18	-5.07 ± 1.28
2-methyl-2-butanol	1	-9.73	-9.73	-1.25	-1.25
2-methyl-2-propanol	2	7.39 ± 1.59	-7.04 ± 1.59	2.38 ± 0.92	-2.01 ± 0.91
2-methylpyridine	1	0.05	0.05	-1.96	-1.96
3-methylpyridine	1	1.03	1.03	-1.36	-1.36
N-methylformamide	2	4.76 ± 0.08	-4.76 ± 0.08	7.19 ± 0.15	-7.19 ± 0.16
N,N-dimethylacetamide	1	-2.92	-2.92	-2.09	-2.09
N,N-dimethylformamide	6	5.08 ± 0.65	-4.82 ± 0.65	1.90 ± 0.55	-1.48 ± 0.49
acetone	17	9.49 ± 0.58	-9.09 ± 0.67	8.54 ± 0.48	-8.12 ± 0.64
acetonitrile	12	7.47 ± 0.64	-7.15 ± 0.62	8.76 ± 0.51	-8.55 ± 0.56
acetophenone	2	7.19 ± 1.48	-6.87 ± 1.50	5.81 ± 2.74	-4.45 ± 2.63
anisole	2	4.04 ± 0.21	-4.03 ± 0.21	3.34 ± 1.05	-2.99 ± 1.05
benzaldehyde	1	-3.02	-3.02	-1.13	-1.13
benzonitrile	3	4.28 ± 1.54	-3.40 ± 1.48	3.70 ± 1.89	-2.41 ± 1.61
chloroform	15	3.10 ± 0.45	-2.29 ± 0.54	4.91 ± 0.53	-4.34 ± 0.59
cyclohexanone	1	-8.59	-8.59	-6.99	-6.99

Table S19: Root mean square deviation (RMSD) and mean signed error (MSE) of M06-2X/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
dibromomethane	1	-5.51	-5.51	-6.40	-6.40
dibutyl ether	2	8.72 ± 2.10	-8.19 ± 2.13	7.55 ± 2.10	-6.96 ± 2.09
dichloromethane	14	5.88 ± 0.51	-5.53 ± 0.54	7.38 ± 0.55	-7.02 ± 0.61
diethyl sulfide	1	0.76	0.76	-5.96	-5.96
diethylamine	3	1.51 ± 0.57	-1.20 ± 0.53	3.75 ± 1.80	-2.40 ± 1.66
diisopropyl ether	3	9.19 ± 0.73	-9.10 ± 0.71	4.98 ± 1.17	-2.12 ± 2.63
dimethyl ether	2	2.30 ± 0.56	-2.16 ± 0.56	3.62 ± 0.80	-3.44 ± 0.80
dimethyl sulfoxide	5	14.97 ± 2.29	-14.06 ± 2.28	10.54 ± 1.25	-10.11 ± 1.34
ethanol	19	4.58 ± 0.70	-2.93 ± 0.81	4.49 ± 0.57	-1.88 ± 0.93
ethyl acetate	8	6.83 ± 0.87	-6.01 ± 1.15	3.33 ± 0.51	-0.87 ± 1.13
ethylbenzene	6	3.06 ± 0.72	-1.77 ± 1.00	3.21 ± 0.50	-2.98 ± 0.48
formaldehyde	1	-8.43	-8.43	2.42	2.42
isopropylbenzene	1	-3.86	-3.86	-4.34	-4.34
methanol	17	3.25 ± 0.51	0.14 ± 0.79	4.26 ± 0.61	1.00 ± 1.00
methyl acetate	4	4.95 ± 1.27	-2.79 ± 2.07	4.26 ± 0.96	1.91 ± 1.89
morpholine	1	-0.51	-0.51	2.17	2.17
n-butylamine	3	2.67 ± 0.68	-1.64 ± 1.22	1.65 ± 0.23	-0.65 ± 0.87
nitrobenzene	1	-0.26	-0.26	8.32	8.32
nitromethane	12	10.12 ± 0.65	-9.88 ± 0.64	2.45 ± 0.44	-0.25 ± 0.70
o-xylene	3	2.07 ± 0.60	-1.59 ± 0.77	1.92 ± 0.20	-1.90 ± 0.19
phenol	1	-4.38	-4.38	-7.29	-7.29

Table S19: Root mean square deviation (RMSD) and mean signed error (MSE) of M06-2X/6-31+G(d,p) calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
pyridine	3	1.54 ± 0.74	-0.98 ± 0.69	3.30 ± 0.89	-2.88 ± 0.94
tetrahydrofuran	5	5.93 ± 0.59	-5.78 ± 0.58	5.17 ± 0.76	-4.83 ± 0.82
thiophene	1	4.14	4.14	-1.79	-1.79
toluene	17	4.10 ± 0.46	-3.40 ± 0.56	5.81 ± 0.57	-5.32 ± 0.57
triethyl phosphate	1	6.52	6.52	17.93	17.93
triethylamine	3	2.62 ± 0.61	-2.29 ± 0.73	5.50 ± 0.94	-5.21 ± 1.04

Table S20: Root mean square deviation (RMSD) and mean signed error (MSE) of M06-2X/cc-pVTZ calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
1-butanol	6	3.02 ± 0.66	-1.62 ± 1.05	1.49 ± 0.18	0.09 ± 0.60
1-chlorobutane	4	7.24 ± 0.46	-7.18 ± 0.46	8.89 ± 0.78	-8.75 ± 0.79
1-octanol	1	1.52	1.52	5.03	5.03
1-pentanol	4	1.94 ± 0.66	-0.91 ± 0.86	2.43 ± 0.53	2.18 ± 0.53
1,2-dichloroethane	3	5.19 ± 1.75	-4.32 ± 1.68	5.00 ± 1.97	-3.91 ± 1.79
2-hexanone	3	7.87 ± 1.88	-7.07 ± 2.02	3.57 ± 0.79	-3.29 ± 0.80
2-methyl-2-butanol	1	-7.21	-7.21	1.27	1.27
2-methyl-2-propanol	2	4.47 ± 0.89	-4.29 ± 0.88	0.80 ± 0.21	0.75 ± 0.20
2-methylpyridine	1	1.77	1.77	-0.24	-0.24

Table S20: Root mean square deviation (RMSD) and mean signed error (MSE) of M06-2X/cc-pVTZ calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
3-methylpyridine	1	3.01	3.01	0.62	0.62
N-methylformamide	2	1.35 ± 0.41	-1.23 ± 0.40	3.66 ± 0.17	-3.65 ± 0.16
N,N-dimethylacetamide	1	1.68	1.68	2.51	2.51
N,N-dimethylformamide	6	2.56 ± 0.53	-2.25 ± 0.51	1.57 ± 0.23	1.10 ± 0.46
acetone	17	8.30 ± 0.47	-8.00 ± 0.52	7.41 ± 0.44	-7.04 ± 0.57
acetonitrile	12	7.33 ± 0.64	-7.01 ± 0.61	8.62 ± 0.51	-8.41 ± 0.56
acetophenone	2	5.20 ± 1.31	-4.86 ± 1.30	4.24 ± 1.77	-2.44 ± 2.46
anisole	2	3.38 ± 0.02	-0.03 ± 2.39	1.89 ± 0.72	1.01 ± 1.14
benzaldehyde	1	-1.16	-1.16	0.73	0.73
benzonitrile	3	3.53 ± 1.33	-2.48 ± 1.45	3.07 ± 1.52	-1.49 ± 1.55
chloroform	15	2.07 ± 0.29	-0.49 ± 0.52	3.31 ± 0.46	-2.54 ± 0.55
cyclohexanone	1	-7.06	-7.06	-5.46	-5.46
dibromomethane	1	-4.42	-4.42	-5.31	-5.31
dibutyl ether	2	2.80 ± 1.03	-1.43 ± 1.71	2.38 ± 0.14	-0.20 ± 1.68
dichloromethane	14	3.86 ± 0.46	-3.42 ± 0.48	5.32 ± 0.50	-4.92 ± 0.54
diethyl sulfide	1	3.50	3.50	-3.22	-3.22
diethylamine	3	0.69 ± 0.16	-0.11 ± 0.39	2.87 ± 1.35	-1.31 ± 1.47
diisopropyl ether	3	7.26 ± 0.49	-7.22 ± 0.47	3.99 ± 0.91	-0.23 ± 2.27
dimethyl ether	2	0.35 ± 0.14	0.29 ± 0.14	1.12 ± 0.39	-0.99 ± 0.38
dimethyl sulfoxide	5	8.87 ± 1.74	-7.88 ± 1.84	4.45 ± 0.80	-3.92 ± 0.95
ethanol	19	2.69 ± 0.39	-0.27 ± 0.62	3.45 ± 0.53	0.79 ± 0.78

Table S20: Root mean square deviation (RMSD) and mean signed error (MSE) of M06-2X/cc-pVTZ calculations from the calculations with explicit solvent model or from experimental data (kJ/mol) per solute

		$\Delta G_{Exper.}$		$\Delta G_{Expl.}$	
Solute	N	RMSD	MSE	RMSD	MSE
ethyl acetate	8	5.40 ± 0.77	-4.47 ± 1.05	3.23 ± 0.75	0.67 ± 1.13
ethylbenzene	6	2.74 ± 0.53	-1.02 ± 1.02	2.52 ± 0.48	-2.23 ± 0.48
formaldehyde	1	-6.94	-6.94	3.91	3.91
isopropylbenzene	1	-3.32	-3.32	-3.80	-3.80
methanol	17	3.89 ± 0.63	2.87 ± 0.64	5.18 ± 0.87	3.73 ± 0.87
methyl acetate	4	3.48 ± 0.47	-0.71 ± 1.70	5.17 ± 1.28	3.98 ± 1.65
morpholine	1	2.42	2.42	5.10	5.10
n-butylamine	3	1.73 ± 0.53	0.30 ± 0.98	1.76 ± 0.67	1.29 ± 0.69
nitrobenzene	1	2.08	2.08	10.66	10.66
nitromethane	12	6.81 ± 0.53	-6.54 ± 0.55	3.75 ± 0.54	3.09 ± 0.62
o-xylene	3	1.61 ± 0.47	-0.71 ± 0.83	1.17 ± 0.37	-1.02 ± 0.33
phenol	1	-2.07	-2.07	-4.98	-4.98
pyridine	3	1.01 ± 0.22	0.71 ± 0.41	1.62 ± 0.51	-1.19 ± 0.64
tetrahydrofuran	5	3.78 ± 0.41	-3.69 ± 0.37	2.92 ± 0.47	-2.74 ± 0.45
thiophene	1	5.16	5.16	-0.77	-0.77
toluene	17	3.28 ± 0.42	-2.39 ± 0.55	4.88 ± 0.55	-4.31 ± 0.55
triethyl phosphate	1	3.77	3.77	15.18	15.18
triethylamine	3	1.26 ± 0.24	-0.61 ± 0.63	3.91 ± 0.91	-3.53 ± 0.96

4 Boltzmann-enhanced discrimination of receiver-operating characteristic (BEDROC) metric

Table S21: BEDROC values for solvents (N $\geq$ 10), compared to what would be expected for a uniform distribution of the same number of compounds ($BEDROC_{unif}$), calculated by using the unsigned error in solvation free energies calculated with SMD model with four levels of theory from experimental data [a]

Solvent	N	$BEDROC_{unif}$	B3LYP/6-31+G(d,p)	HF/6-31+G(d,p)	M06-2X/6-31+G(d,p)	M06-2X/cc-pVTZ
1-octanol	29	0.44	**0.56 ± 0.06**	**0.56 ± 0.06**	**0.52 ± 0.05**	0.43 ± 0.06
acetone	12	0.43	**0.56 ± 0.08**	**0.53 ± 0.10**	**0.57 ± 0.10**	**0.53 ± 0.09**
chloroform	28	0.44	0.28 ± 0.04	0.33 ± 0.05	0.26 ± 0.04	0.33 ± 0.04
ethanol	13	0.43	**0.61 ± 0.08**	**0.54 ± 0.09**	**0.59 ± 0.07**	0.49 ± 0.09
ethyl acetate	13	0.43	0.39 ± 0.06	0.38 ± 0.07	0.40 ± 0.07	0.42 ± 0.08
methanol	20	0.43	**0.67 ± 0.07**	**0.58 ± 0.08**	**0.62 ± 0.06**	**0.51 ± 0.07**
nitromethane	10	0.43	0.46 ± 0.07	0.39 ± 0.09	0.49 ± 0.07	**0.51 ± 0.08**
toluene	11	0.43	0.08 ± 0.02	0.12 ± 0.03	0.10 ± 0.03	0.17 ± 0.04

[a] N is the number of solutes tested.

Table S22: BEDROC values for solutes (N $\geq$ 10), compared to what would be expected for a uniform distribution of the same number of compounds ($BEDROC_{unif}$), calculated by using the unsigned error in solvation free energies calculated with SMD model with four levels of theory from experimental data [a]

Solute	N	$BEDROC_{unif}$	B3LYP/6-31+G(d,p)	HF/6-31+G(d,p)	M06-2X/6-31+G(d,p)	M06-2X/cc-pVTZ
acetone	17	0.43	**0.64 ± 0.07**	**0.69 ± 0.07**	**0.78 ± 0.06**	**0.86 ± 0.04**
acetonitrile	12	0.43	**0.77 ± 0.05**	**0.76 ± 0.05**	**0.61 ± 0.06**	**0.76 ± 0.05**
chloroform	15	0.43	0.23 ± 0.04	0.22 ± 0.05	0.20 ± 0.04	0.19 ± 0.04
dichloromethane	14	0.43	**0.51 ± 0.05**	**0.52 ± 0.06**	0.47 ± 0.05	0.41 ± 0.06
ethanol	19	0.43	0.27 ± 0.06	0.32 ± 0.06	0.30 ± 0.06	0.24 ± 0.05
methanol	17	0.43	0.17 ± 0.04	0.22 ± 0.05	0.20 ± 0.04	0.36 ± 0.07
nitromethane	12	0.43	**0.60 ± 0.05**	0.24 ± 0.05	**0.83 ± 0.05**	**0.73 ± 0.05**
toluene	17	0.43	0.28 ± 0.04	0.39 ± 0.06	0.29 ± 0.05	0.32 ± 0.05

[a] N is the number of solvents tested.

Table S23: BEDROC values for solvents ($N \geq 10$), compared to what would be expected for a uniform distribution of the same number of compounds ($BEDROC_{unif}$), calculated by using the unsigned error in ΔG_{polar}[a]

Solvent	N	$BEDROC_{unif}$	PB	Still	HCT	OBC-I	OBC-II
1-octanol	29	0.44	**0.66 ± 0.05**	**0.54 ± 0.06**	**0.53 ± 0.06**	**0.51 ± 0.06**	**0.51 ± 0.06**
acetone	12	0.43	**0.56 ± 0.09**	**0.52 ± 0.11**	**0.53 ± 0.11**	**0.53 ± 0.10**	**0.53 ± 0.11**
chloroform	28	0.44	0.40 ± 0.05	0.46 ± 0.05	0.46 ± 0.05	0.45 ± 0.05	0.45 ± 0.05
ethanol	13	0.43	**0.54 ± 0.07**	0.44 ± 0.09	0.45 ± 0.08	0.45 ± 0.09	0.44 ± 0.09
ethyl acetate	13	0.43	0.34 ± 0.07	0.44 ± 0.10	0.45 ± 0.09	0.45 ± 0.10	0.45 ± 0.09
methanol	20	0.43	0.31 ± 0.05	0.35 ± 0.07	0.33 ± 0.07	0.34 ± 0.06	0.33 ± 0.07
nitromethane	10	0.43	0.22 ± 0.07	0.38 ± 0.10	0.38 ± 0.09	0.39 ± 0.10	0.39 ± 0.09
toluene	11	0.43	0.20 ± 0.03	0.32 ± 0.04	0.35 ± 0.05	0.34 ± 0.04	0.35 ± 0.05

[a]N is the number of solutes tested.

Table S24: BEDROC values for solutes (N $\geq$ 10), compared to what would be expected for a uniform distribution of the same number of compounds ($BEDROC_{unif}$), calculated by using the unsigned error in ΔG_{polar}[a]

Solute	N	$BEDROC_{unif}$	PB	Still	HCT	OBC-I	OBC-II
acetone	17	0.43	**0.55 ± 0.06**	**0.70 ± 0.04**	**0.66 ± 0.04**	**0.66 ± 0.04**	**0.66 ± 0.04**
acetonitrile	12	0.43	**0.59 ± 0.07**	**0.65 ± 0.05**	**0.80 ± 0.04**	**0.77 ± 0.04**	**0.80 ± 0.03**
chloroform	15	0.43	0.14 ± 0.03	0.08 ± 0.02	0.07 ± 0.02	0.06 ± 0.01	0.07 ± 0.02
dichloromethane	14	0.43	0.13 ± 0.03	0.18 ± 0.02	0.17 ± 0.03	0.15 ± 0.02	0.17 ± 0.03
ethanol	19	0.43	0.46 ± 0.06	0.37 ± 0.04	0.31 ± 0.04	0.34 ± 0.04	0.32 ± 0.04
methanol	17	0.43	**0.56 ± 0.07**	0.48 ± 0.05	0.44 ± 0.05	0.46 ± 0.05	0.46 ± 0.05
nitromethane	12	0.43	**0.75 ± 0.08**	**0.98 ± 0.01**	**0.97 ± 0.01**	**0.98 ± 0.01**	**0.98 ± 0.01**
toluene	17	0.43	0.25 ± 0.05	0.05 ± 0.01	0.19 ± 0.03	0.20 ± 0.03	0.21 ± 0.03

[a]N is the number of solvents tested.

5 Student's *t* test

Table S25: Student's *t* test of the unsigned error in solvation free energies calculated using SMD model with four levels of theory from experimental data per solvent[a]

		B3LYP/6-31+G(d,p)		HF/6-31+G(d,p)		M06-2X/6-31+G(d,p)		M06-2X/cc-pVTZ	
Solvent	N	*t* value	*p* value	*t* value	*p* value	*t* value	*p* value	*t* value	*p* value
1-octanol	29	1.7e+00	1.0e-01	1.7e+00	1.0e-01	1.2e+00	2.4e-01	6.9e-03	9.9e-01
acetone	12	1.5e+00	1.7e-01	1.1e+00	2.8e-01	1.5e+00	1.7e-01	1.1e+00	3.0e-01
chloroform	28	-3.4e+00	**1.3e-03**	-2.2e+00	**3.3e-02**	-3.8e+00	**4.7e-04**	-2.7e+00	**8.9e-03**
ethanol	13	2.0e+00	6.9e-02	1.2e+00	2.7e-01	2.1e+00	5.4e-02	6.5e-01	5.3e-01
ethyl acetate	13	-6.9e-01	5.0e-01	-9.1e-01	3.8e-01	-4.7e-01	6.4e-01	-3.8e-01	7.1e-01
methanol	20	2.7e+00	**1.3e-02**	1.6e+00	1.1e-01	2.4e+00	**2.7e-02**	1.1e+00	3.0e-01
nitromethane	10	4.3e-01	6.7e-01	-4.3e-01	6.7e-01	8.0e-01	4.4e-01	6.6e-01	5.2e-01
toluene	11	-1.1e+01	**4.0e-12**	-7.5e+00	**4.1e-07**	-8.3e+00	**7.2e-08**	-6.3e+00	**5.6e-06**

[a]N is the number of solutes tested.

Table S26: Student's t test of the unsigned error in solvation free energies calculated using SMD models from experimental data per solute[a]

		B3LYP/6-31+G(d,p)		HF/6-31+G(d,p)		M06-2X/6-31+G(d,p)		M06-2X/cc-pVTZ	
Solute	N	t value	p value	t value	p value	t value	p value	t value	p value
acetone	17	2.5e+00	**2.0e-02**	3.3e+00	**3.6e-03**	5.5e+00	**2.1e-05**	7.2e+00	**5.9e-07**
acetonitrile	12	5.6e+00	**4.5e-05**	4.8e+00	**3.0e-04**	2.9e+00	**1.2e-02**	4.7e+00	**4.3e-04**
chloroform	15	-4.2e+00	**3.6e-04**	-4.2e+00	**4.0e-04**	-4.9e+00	**7.3e-05**	-6.0e+00	**2.0e-06**
dichloromethane	14	1.3e+00	2.2e-01	1.3e+00	2.0e-01	6.2e-01	5.4e-01	-8.3e-01	4.2e-01
ethanol	19	-2.7e+00	**1.1e-02**	-1.9e+00	**6.4e-02**	-2.2e+00	**3.9e-02**	-4.0e+00	**3.9e-04**
methanol	17	-5.7e+00	**5.2e-06**	-4.0e+00	**6.5e-04**	-4.6e+00	**1.2e-04**	-1.2e+00	2.5e-01
nitromethane	12	3.2e+00	**4.9e-03**	-3.7e+00	**2.1e-03**	6.6e+00	**1.0e-05**	4.5e+00	**5.6e-04**
toluene	17	-3.0e+00	**5.8e-03**	-8.6e-01	4.0e-01	-2.8e+00	**1.0e-02**	-2.3e+00	**3.3e-02**

[a]N is the number of solvents tested.

Table S27: Student's t test of the unsigned error per solvent calculated by using the unsigned error in ΔG_{polar}[a]

		PB		Still		HCT		OBC-I		OBC-II	
Solvent	N	t value	p value	t value	p value	t value	p value	t value	p value	t value	p value
1-octanol	29	3.2e+00	**3.3e-03**	1.5e+00	1.3e-01	1.4e+00	1.8e-01	1.1e+00	2.6e-01	1.2e+00	2.5e-01
acetone	12	1.3e+00	2.1e-01	1.1e+00	3.0e-01	1.1e+00	3.0e-01	1.0e+00	3.2e-01	1.1e+00	3.1e-01
chloroform	28	-9.6e-01	3.4e-01	1.3e-01	9.0e-01	2.1e-01	8.4e-01	2.5e-02	9.8e-01	-2.3e-02	9.8e-01
ethanol	13	1.1e+00	2.9e-01	2.9e-01	7.8e-01	2.7e-01	8.0e-01	2.5e-01	8.0e-01	2.2e-01	8.3e-01
ethyl acetate	13	-1.4e+00	2.0e-01	1.4e-01	8.9e-01	1.8e-01	8.6e-01	1.6e-01	8.7e-01	2.0e-01	8.4e-01
methanol	20	-2.5e+00	**1.8e-02**	-1.0e+00	3.2e-01	-1.4e+00	1.8e-01	-1.3e+00	2.1e-01	-1.4e+00	1.8e-01
nitromethane	10	-3.4e+00	**5.5e-03**	-5.4e-01	6.0e-01	-5.3e-01	6.1e-01	-3.3e-01	7.5e-01	-4.3e-01	6.8e-01
toluene	11	-7.9e+00	**2.5e-10**	-1.9e+00	7.1e-02	-2.0e+00	5.9e-02	-2.2e+00	**4.4e-02**	-2.1e+00	5.2e-02

[a]N is the number of solutes tested.

Table S28: Student's t test of the unsigned error per solute calculated by using the unsigned error in ΔG_{polar}[a]

		PB		Still		HCT		OBC-I		OBC-II	
Solute	N	t value	p value	t value	p value	t value	p value	t value	p value	t value	p value
acetone	17	1.3e+00	2.0e-01	6.6e+00	**3.6e-08**	6.4e+00	**6.5e-08**	6.3e+00	**8.6e-08**	6.4e+00	**7.0e-08**
acetonitrile	12	1.7e+00	1.2e-01	4.7e+00	**1.3e-04**	8.5e+00	**7.5e-08**	7.9e+00	**9.6e-08**	8.6e+00	**5.3e-08**
chloroform	15	-7.9e+00	**1.5e-09**	-1.3e+01	**2.2e-16**	-1.3e+01	**2.2e-16**	-1.4e+01	**2.2e-16**	-1.3e+01	**2.2e-16**
dichloromethane	14	-8.1e+00	**1.8e-09**	-9.3e+00	**1.8e-14**	-9.1e+00	**1.5e-13**	-9.9e+00	**9.3e-16**	-9.1e+00	**1.0e-13**
ethanol	19	6.3e-02	9.5e-01	-1.3e+00	1.9e-01	-3.2e+00	**3.0e-03**	-2.4e+00	**2.2e-02**	-2.9e+00	**6.5e-03**
methanol	17	1.5e+00	1.4e-01	1.1e+00	2.9e-01	-1.4e-01	8.9e-01	7.3e-01	4.7e-01	4.2e-01	6.8e-01
nitromethane	12	3.2e+00	**7.7e-03**	1.4e+01	**5.4e-11**	1.3e+01	**4.7e-10**	1.4e+01	**3.5e-11**	1.3e+01	**2.4e-10**
toluene	17	-4.6e+00	**6.7e-05**	-1.5e+01	**2.2e-16**	-8.3e+00	**4.7e-12**	-8.2e+00	**1.5e-12**	-7.7e+00	**4.7e-11**

[a]N is the number of solvents tested.

6 Polar contribution

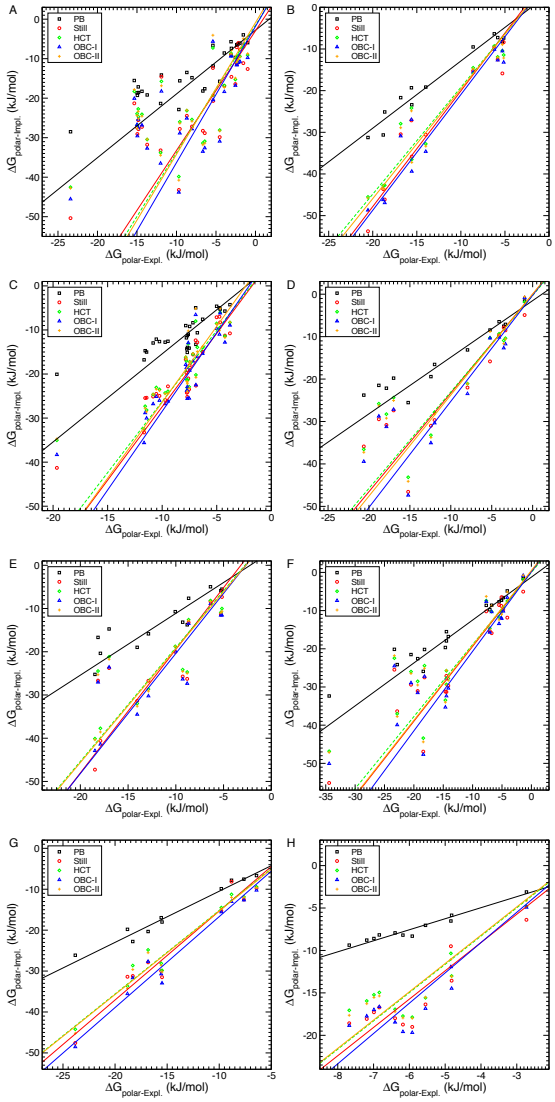

Figure S1: Correlation between polar contribution to solvation free energy calculated with explicit solvent ($\Delta G_{\text{polar-Expl.}}$) and that with PB (black), Still (red), HCT (green), OBC-I (blue) and OBC-II (orange) ($\Delta G_{\text{polar-Impl.}}$) per solvent: (A) 1-octanol, (B) acetone, (C) chloroform, (D) ethanol, (E) ethyl acetate, (F) methanol, (G) nitromethane, and (H) toluene.

Table S29: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{polar-Expl.}}$) and that with PB model ($\Delta G_{\text{polar-Impl.}}$) per solvent

Solvent	N	R[a]	m[b]	b[c]
1-octanol	29	0.83 ± 0.04	0.62 ± 0.10	1.74 ± 0.81
acetone	12	0.98 ± 0.01	0.62 ± 0.05	-2.01 ± 0.81
chloroform	28	0.77 ± 0.08	0.50 ± 0.08	-2.29 ± 0.76
ethanol	13	0.96 ± 0.02	0.75 ± 0.08	1.14 ± 0.83
ethyl acetate	13	0.90 ± 0.05	0.70 ± 0.07	-2.21 ± 0.90
methanol	20	0.97 ± 0.01	0.89 ± 0.07	1.10 ± 0.65
nitromethane	10	0.98 ± 0.02	0.80 ± 0.06	-1.61 ± 0.78
toluene	11	0.97 ± 0.04	0.77 ± 0.08	-0.18 ± 0.61

Table S30: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{polar-Expl.}}$) and that with Still ($\Delta G_{\text{polar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.73 ± 0.05	0.33 ± 0.06	0.97 ± 1.00
acetone	12	0.96 ± 0.02	0.36 ± 0.03	-2.78 ± 0.97
chloroform	28	0.85 ± 0.05	0.30 ± 0.04	-1.77 ± 0.70
ethanol	13	0.92 ± 0.05	0.43 ± 0.08	0.01 ± 1.10
ethyl acetate	13	0.85 ± 0.08	0.35 ± 0.04	-3.19 ± 0.87
methanol	20	0.94 ± 0.02	0.51 ± 0.06	-0.12 ± 0.86
nitromethane	10	0.98 ± 0.02	0.46 ± 0.04	-2.95 ± 1.00

[a]Number of solutes tested
[b]Slope of the linear fits of $\Delta G_{\text{polar-Exol.}}$ with respect to $\Delta G_{\text{polar-Impl.}}$
[c]y-Intercept of the linear fits of $\Delta G_{\text{polar-Expl.}}$ with respect to $\Delta G_{\text{polar-Impl.}}$

Table S30: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{polar-Expl.}}$) and that with Still ($\Delta G_{\text{polar-Impl.}}$) per solvent

Solvent	N	R	m	b
toluene	11	0.86 ± 0.15	0.30 ± 0.09	-1.28 ± 1.46

Table S31: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{polar-Expl.}}$) and that with HCT ($\Delta G_{\text{polar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.69 ± 0.06	0.31 ± 0.07	0.48 ± 0.96
acetone	12	0.96 ± 0.03	0.39 ± 0.03	-2.51 ± 0.87
chloroform	28	0.87 ± 0.04	0.31 ± 0.04	-1.86 ± 0.68
ethanol	13	0.91 ± 0.05	0.44 ± 0.08	0.13 ± 1.06
ethyl acetate	13	0.83 ± 0.09	0.38 ± 0.04	-2.76 ± 1.07
methanol	20	0.92 ± 0.02	0.53 ± 0.07	0.01 ± 0.85
nitromethane	10	0.98 ± 0.02	0.49 ± 0.03	-2.56 ± 0.76
toluene	11	0.83 ± 0.18	0.30 ± 0.11	-1.51 ± 1.67

Table S32: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{polar-Expl.}}$) and that with OBC-I ($\Delta G_{\text{polar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.70 ± 0.06	0.29 ± 0.06	0.53 ± 0.96
acetone	12	0.96 ± 0.03	0.36 ± 0.03	-2.46 ± 0.84

Table S32: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{polar-Expl.}}$) and that with OBC-I ($\Delta G_{\text{polar-Impl.}}$) per solvent

Solvent	N	R	m	b
chloroform	28	0.85 ± 0.05	0.28 ± 0.04	-2.03 ± 0.76
ethanol	13	0.91 ± 0.04	0.40 ± 0.07	0.10 ± 1.22
ethyl acetate	13	0.84 ± 0.09	0.36 ± 0.04	-2.66 ± 1.04
methanol	20	0.92 ± 0.02	0.48 ± 0.06	-0.08 ± 0.91
nitromethane	10	0.98 ± 0.02	0.45 ± 0.03	-2.49 ± 0.70
toluene	11	0.84 ± 0.17	0.28 ± 0.09	-1.46 ± 1.56

Table S33: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{polar-Expl.}}$) and that with OBC-II ($\Delta G_{\text{polar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.69 ± 0.07	0.30 ± 0.07	0.26 ± 0.93
acetone	12	0.96 ± 0.03	0.38 ± 0.03	-2.55 ± 0.87
chloroform	28	0.83 ± 0.05	0.29 ± 0.04	-2.34 ± 0.76
ethanol	13	0.91 ± 0.05	0.42 ± 0.07	-0.02 ± 1.11
ethyl acetate	13	0.84 ± 0.09	0.38 ± 0.04	-2.66 ± 1.09
methanol	20	0.92 ± 0.02	0.51 ± 0.07	-0.25 ± 0.89
nitromethane	10	0.98 ± 0.02	0.49 ± 0.03	-2.49 ± 0.79
toluene	11	0.85 ± 0.17	0.30 ± 0.09	-1.54 ± 1.46

Table S34: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with explicit solvent model and 2(ε-1)/(2ε+1) per solute

Solute	N[a]	R	m[b]	b[c]
acetone	17	0.87 ± 0.07	-14.11 ± 2.61	1.03 ± 2.24
acetonitrile	12	0.67 ± 0.17	-14.47 ± 15.18	-1.66 ± 14.15
chloroform	15	0.39 ± 0.22	-5.12 ± 5.16	-1.14 ± 4.79
dichloromethane	14	0.63 ± 0.28	-6.70 ± 5.48	-2.43 ± 5.09
ethanol	19	0.77 ± 0.15	-24.04 ± 8.15	6.73 ± 7.36
methanol	17	0.77 ± 0.16	-25.40 ± 9.61	6.75 ± 8.75
nitromethane	12	0.31 ± 0.21	-9.62 ± 25.61	-10.25 ± 23.78
toluene	17	0.67 ± 0.16	-9.76 ± 7.13	3.20 ± 6.70

Table S35: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with PB and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	1.00 ± 0.00	-18.92 ± 0.25	1.25 ± 0.22
acetonitrile	12	1.00 ± 0.00	-20.62 ± 0.07	-0.01 ± 0.06
chloroform	15	1.00 ± 0.00	-8.39 ± 0.39	1.41 ± 0.36
dichloromethane	14	1.00 ± 0.00	-11.25 ± 0.40	0.94 ± 0.38
ethanol	19	1.00 ± 0.00	-26.37 ± 1.27	5.10 ± 1.17
methanol	17	1.00 ± 0.00	-28.73 ± 1.16	4.97 ± 1.06
nitromethane	12	1.00 ± 0.00	-30.39 ± 0.55	3.05 ± 0.50
toluene	17	1.00 ± 0.00	-10.98 ± 0.66	2.79 ± 0.62

[a]Number of solvents tested
[b]Slope of linear fits of ΔG_{polar} with respect to 2(ε-1)/(2ε+1)
[c]y-Intercept of linear fits of ΔG_{polar} with respect to 2(ε-1)/(2ε+1)

Table S36: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation (ΔG_{polar}) calculated with Still and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	1.00 ± 0.00	-24.33 ± 0.52	-6.78 ± 0.47
acetonitrile	12	1.00 ± 0.00	-23.91 ± 0.35	-8.42 ± 0.32
chloroform	15	1.00 ± 0.00	-7.71 ± 0.26	-2.36 ± 0.24
dichloromethane	14	1.00 ± 0.01	-12.54 ± 0.59	-3.51 ± 0.55
ethanol	19	1.00 ± 0.00	-22.35 ± 0.65	-6.33 ± 0.59
methanol	17	1.00 ± 0.00	-25.49 ± 0.81	-6.82 ± 0.74
nitromethane	12	1.00 ± 0.00	-35.82 ± 1.10	-12.90 ± 1.01
toluene	17	0.92 ± 0.10	-6.68 ± 0.85	-2.07 ± 0.79

Table S37: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with HCT and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	1.00 ± 0.00	-22.66 ± 0.52	-6.51 ± 0.47
acetonitrile	12	1.00 ± 0.00	-25.57 ± 0.49	-9.08 ± 0.45
chloroform	15	0.99 ± 0.01	-7.36 ± 0.40	-2.39 ± 0.37
dichloromethane	14	1.00 ± 0.02	-11.90 ± 0.56	-3.36 ± 0.51
ethanol	19	1.00 ± 0.00	-19.77 ± 0.55	-5.75 ± 0.51
methanol	17	1.00 ± 0.00	-23.33 ± 0.83	-6.31 ± 0.76
nitromethane	12	0.99 ± 0.01	-33.28 ± 1.68	-11.84 ± 1.54
toluene	17	0.95 ± 0.08	-9.11 ± 0.95	-2.87 ± 0.89

Table S38: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with OBC-I and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	1.00 ± 0.00	-24.79 ± 0.55	-7.05 ± 0.50
acetonitrile	12	1.00 ± 0.00	-26.98 ± 0.45	-9.58 ± 0.41
chloroform	15	0.99 ± 0.01	-8.02 ± 0.47	-2.60 ± 0.44
dichloromethane	14	1.00 ± 0.01	-12.76 ± 0.64	-3.60 ± 0.59
ethanol	19	1.00 ± 0.00	-22.07 ± 0.63	-6.37 ± 0.58
methanol	17	1.00 ± 0.00	-25.81 ± 0.95	-6.97 ± 0.87
nitromethane	12	0.99 ± 0.01	-36.51 ± 1.71	-13.05 ± 1.57
toluene	17	0.96 ± 0.07	-10.54 ± 0.92	-3.30 ± 0.85

Table S39: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with OBC-II and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	1.00 ± 0.00	-23.04 ± 0.52	-6.62 ± 0.47
acetonitrile	12	1.00 ± 0.00	-25.98 ± 0.52	-9.24 ± 0.48
chloroform	15	0.99 ± 0.01	-7.49 ± 0.46	-2.46 ± 0.42
dichloromethane	14	1.00 ± 0.02	-12.12 ± 0.58	-3.43 ± 0.54
ethanol	19	1.00 ± 0.00	-20.30 ± 0.57	-5.92 ± 0.52
methanol	17	1.00 ± 0.00	-24.11 ± 0.90	-6.54 ± 0.82
nitromethane	12	0.99 ± 0.01	-33.99 ± 1.72	-12.15 ± 1.58
toluene	17	0.96 ± 0.07	-9.68 ± 0.98	-3.06 ± 0.92

Table S40: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with SMD at B3LYP/6-31+G(d,p) level of theory and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	0.82 ± 0.08	-37.74 ± 5.60	11.11 ± 4.10
acetonitrile	12	1.00 ± 0.00	-37.24 ± 0.32	1.66 ± 0.29
chloroform	15	1.00 ± 0.00	-16.00 ± 0.44	2.67 ± 0.41
dichloromethane	14	1.00 ± 0.00	-20.69 ± 0.55	1.94 ± 0.51
ethanol	19	0.60 ± 0.12	-30.11 ± 8.33	7.65 ± 6.80
methanol	17	0.57 ± 0.15	-25.44 ± 7.60	4.96 ± 6.18
nitromethane	12	0.60 ± 0.20	-46.92 ± 22.01	16.03 ± 19.97
toluene	17	1.00 ± 0.00	-20.30 ± 0.58	8.52 ± 0.54

Table S41: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with SMD model at HF/6-31+G(d,p) level of theory and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	0.78 ± 0.09	-43.60 ± 7.39	13.95 ± 5.29
acetonitrile	12	1.00 ± 0.00	-40.02 ± 0.36	1.45 ± 0.33
chloroform	15	1.00 ± 0.00	-17.95 ± 0.35	2.96 ± 0.33
dichloromethane	14	1.00 ± 0.00	-23.12 ± 0.65	2.26 ± 0.60
ethanol	19	0.58 ± 0.12	-31.72 ± 9.89	8.13 ± 8.24
methanol	17	0.56 ± 0.15	-26.66 ± 8.55	5.05 ± 6.98
nitromethane	12	0.54 ± 0.20	-57.34 ± 32.46	19.44 ± 29.45
toluene	17	1.00 ± 0.00	-24.23 ± 0.59	3.90 ± 0.55

Table S42: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with SMD model at M06-2X/6-31+G(d,p) level of theory and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	0.81 ± 0.08	-36.70 ± 5.46	8.16 ± 3.89
acetonitrile	12	1.00 ± 0.00	-35.98 ± 0.28	1.27 ± 0.25
chloroform	15	1.00 ± 0.00	-16.43 ± 0.44	2.83 ± 0.41
dichloromethane	14	1.00 ± 0.00	-21.03 ± 0.54	1.99 ± 0.51
ethanol	19	0.58 ± 0.13	-30.65 ± 9.41	7.74 ± 7.76
methanol	17	0.55 ± 0.15	-25.76 ± 8.04	4.85 ± 6.52
nitromethane	12	0.63 ± 0.19	-49.04 ± 20.60	10.41 ± 18.65
toluene	17	1.00 ± 0.00	-23.10 ± 0.61	3.69 ± 0.57

Table S43: Correlation (R) and regression to a straight line $y = mx + b$ of polar contribution to solvation free energy (ΔG_{polar}) calculated with SMD model at M06-2X/cc-pVTZ level of theory and 2(ε-1)/(2ε+1) per solute

Solute	N	R	m	b
acetone	17	0.79 ± 0.09	-32.80 ± 5.20	5.97 ± 3.76
acetonitrile	12	1.00 ± 0.00	-35.56 ± 0.29	1.11 ± 0.26
chloroform	15	1.00 ± 0.00	-13.71 ± 0.34	2.19 ± 0.32
dichloromethane	14	1.00 ± 0.00	-18.45 ± 0.53	1.78 ± 0.50
ethanol	19	0.59 ± 0.12	-26.13 ± 7.75	6.50 ± 6.32
methanol	17	0.55 ± 0.15	-21.54 ± 6.84	3.98 ± 5.54
nitromethane	12	0.58 ± 0.19	-43.99 ± 21.25	9.19 ± 19.20
toluene	17	1.00 ± 0.00	-21.84 ± 0.59	3.65 ± 0.55

7 Apolar contribution

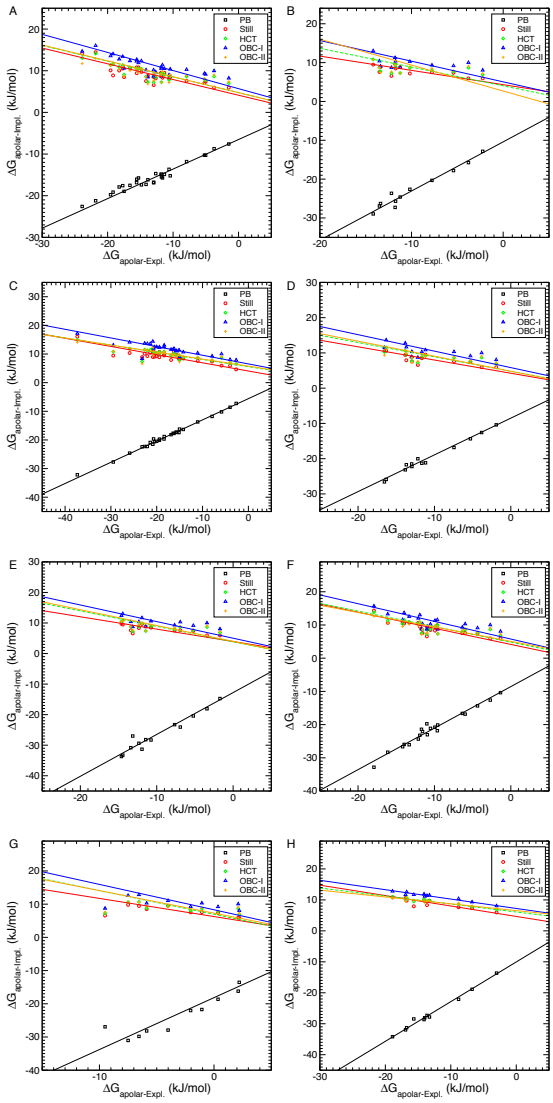

Figure S2: Correlation between apolar contribution to solvation free energy calculated with explicit solvent ($\Delta G_{\text{apolar-Expl.}}$) and that with PB (black), Still (red), HCT (green), OBC-I (blue), and OBC-II (orange) models ($\Delta G_{\text{apolar-Impl.}}$) per solvent: (A) 1-octanol, (B) acetone, (C) chloroform, (D) ethanol, (E) ethyl acetate, (F) methanol, (G) nitromethane, and (H) toluene

Table S44: Correlation (R) and regression to a straight line $y = mx+b$ of apolar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{apolar-Expl.}}$) and that with PB ($\Delta G_{\text{apolar-Impl.}}$) per solvent

Solvent	N	R[a]	m[b]	b[c]
1-octanol	29	0.98 ± 0.01	1.41 ± 0.05	9.18 ± 0.64
acetone	12	0.99 ± 0.03	0.79 ± 0.05	8.22 ± 1.20
chloroform	28	1.00 ± 0.00	1.35 ± 0.02	7.54 ± 0.37
ethanol	13	0.99 ± 0.01	0.96 ± 0.04	8.17 ± 0.68
ethyl acetate	13	0.97 ± 0.05	0.73 ± 0.05	9.33 ± 1.25
methanol	20	0.99 ± 0.01	0.80 ± 0.03	6.85 ± 0.71
nitromethane	10	0.92 ± 0.06	0.64 ± 0.11	11.62 ± 2.11
toluene	11	1.00 ± 0.02	0.78 ± 0.03	7.83 ± 0.71

Table S45: Correlation (R) and regression to a straight line $y = mx+b$ of apolar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{apolar-Expl.}}$) and that with Still ($\Delta G_{\text{apolar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.81 ± 0.08	-2.65 ± 0.46	10.92 ± 4.25
acetone	12	0.79 ± 0.17	-2.72 ± 0.70	11.78 ± 5.86
chloroform	28	0.91 ± 0.06	-3.50 ± 0.36	14.25 ± 3.03
ethanol	13	0.78 ± 0.15	-2.67 ± 0.64	11.31 ± 5.64
ethyl acetate	13	0.67 ± 0.23	-2.47 ± 0.89	9.72 ± 7.63
methanol	20	0.83 ± 0.11	-2.06 ± 0.44	8.54 ± 4.18
nitromethane	10	0.57 ± 0.28	-1.83 ± 0.85	11.46 ± 7.25

[a]Number of solutes tested
[b]Slope of the linear fits of $\Delta G_{\text{apolar-Expl.}}$ with respect to $\Delta G_{\text{apolar-Impl.}}$
[c]y-Intercept of the linear fits of $\Delta G_{\text{apolar-Expl.}}$ with respect to $\Delta G_{\text{apolar-Impl.}}$

Table S45: Correlation (R) and regression to a straight line $y = mx+b$ of apolar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{apolar-Expl.}}$) and that with Still ($\Delta G_{\text{apolar-Impl.}}$) per solvent

Solvent	N	R	m	b
toluene	11	0.91 ± 0.13	-2.97 ± 0.56	13.83 ± 5.25

Table S46: Correlation (R) and regression to a straight line $y = mx+b$ of apolar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{apolar-Expl.}}$) and that with HCT ($\Delta G_{\text{apolar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.71 ± 0.10	-2.65 ± 0.54	12.58 ± 5.47
acetone	12	0.47 ± 0.23	-2.07 ± 1.36	8.31 ± 11.50
chloroform	28	0.88 ± 0.09	-3.98 ± 0.48	22.18 ± 4.97
ethanol	13	0.63 ± 0.21	-2.46 ± 0.98	11.87 ± 8.98
ethyl acetate	13	0.48 ± 0.25	-1.98 ± 1.19	7.63 ± 10.60
methanol	20	0.75 ± 0.13	-2.14 ± 0.52	10.30 ± 5.27
nitromethane	10	0.38 ± 0.29	-1.40 ± 1.36	9.73 ± 11.98
toluene	11	0.98 ± 0.07	-3.87 ± 0.35	23.57 ± 3.32

Table S47: Correlation (R) and regression to a straight line $y = mx+b$ of apolar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{apolar-Expl.}}$) and that with OBC-I ($\Delta G_{\text{apolar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.72 ± 0.10	-2.30 ± 0.44	13.10 ± 5.24
acetone	12	0.52 ± 0.22	-1.88 ± 1.11	9.50 ± 11.13

Table S47: Correlation (R) and regression to a straight line $y = mx+b$ of apolar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{apolar-Expl.}}$) and that with OBC-I ($\Delta G_{\text{apolar-Impl.}}$) per solvent

Solvent	N	R	m	b
chloroform	28	0.88 ± 0.10	-3.31 ± 0.46	21.66 ± 5.61
ethanol	13	0.65 ± 0.20	-2.14 ± 0.77	12.48 ± 8.51
ethyl acetate	13	0.53 ± 0.24	-1.84 ± 0.92	9.24 ± 9.84
methanol	20	0.75 ± 0.13	-1.88 ± 0.46	10.84 ± 5.41
nitromethane	10	0.43 ± 0.28	-1.31 ± 1.10	10.88 ± 11.45
toluene	11	0.98 ± 0.05	-3.30 ± 0.31	23.88 ± 3.48

Table S48: Correlation (R) and regression to a straight line $y = mx+b$ of apolar contribution to solvation free energy calculated with explicit solvent model ($\Delta G_{\text{apolar-Expl.}}$) and that with OBC-II ($\Delta G_{\text{apolar-Impl.}}$) per solvent

Solvent	N	R	m	b
1-octanol	29	0.63 ± 0.13	-2.62 ± 0.66	12.39 ± 6.49
acetone	12	0.34 ± 0.22	-1.50 ± 1.48	4.03 ± 12.81
chloroform	28	0.81 ± 0.13	-4.07 ± 0.81	23.47 ± 8.27
ethanol	13	0.54 ± 0.23	-2.34 ± 1.20	11.21 ± 10.95
ethyl acetate	13	0.44 ± 0.24	-1.93 ± 1.29	7.68 ± 11.73
methanol	20	0.67 ± 0.16	-2.30 ± 0.70	11.64 ± 6.84
nitromethane	10	0.37 ± 0.29	-1.47 ± 1.48	10.70 ± 13.36
toluene	11	0.97 ± 0.09	-4.54 ± 0.54	29.68 ± 5.10

8 Distribution of single-conformation solvation free energy

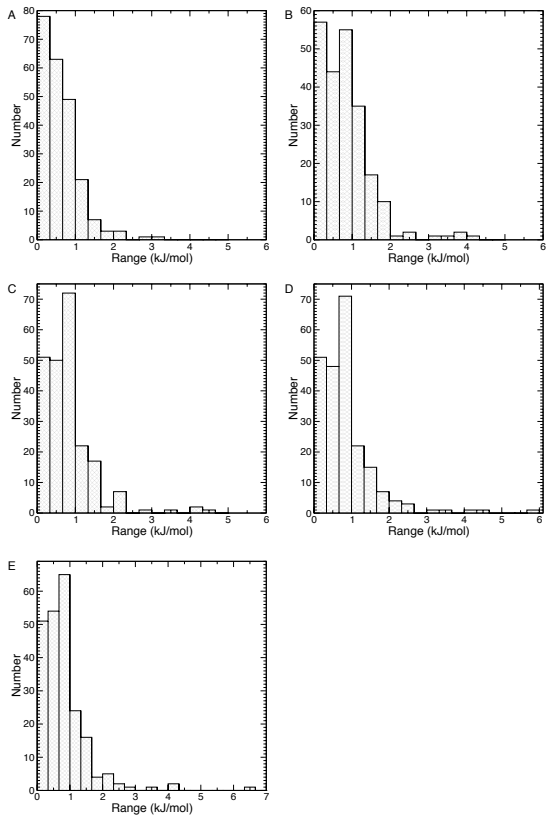

Figure S3: Distribution of range of standard deviation of single-conformation solvation free energy for (A) PB, (B) Still, (C) HCT, (D) OBC-I, (E) OBC-II

9 Optimization of apolar contribution

Table S49: Correlation (R) and regression to a straight line $y = mx + b$ of optimized implicit solvation free energies with explicit ones ($\Delta G_{Expl.}$) and with experimental numbers ($\Delta G_{Exper.}$). Explicit data from ref.[5,6]

	$\Delta G_{Expl.}$			$\Delta G_{Exper.}$		
	R	m	b	R	m	b
PB	0.92 ± 0.01	0.88 ± 0.04	-3.5 ± 0.8	0.77 ± 0.04	1.03 ± 0.06	0.5 ± 1.2
Still	0.81 ± 0.03	0.55 ± 0.04	-10.1 ± 0.7	0.63 ± 0.05	1.18 ± 0.12	3.5 ± 2.4
HCT	0.71 ± 0.04	0.50 ± 0.04	-11.0 ± 0.8	0.57 ± 0.06	1.03 ± 0.10	0.5 ± 2.2
OBC-I	0.70 ± 0.04	0.45 ± 0.04	-12.1 ± 0.8	0.55 ± 0.05	1.09 ± 0.11	1.8 ± 2.4
OBC-II	0.65 ± 0.04	0.45 ± 0.05	-12.1 ± 0.9	0.52 ± 0.06	0.96 ± 0.11	-0.8 ± 2.5

Table S50: Root mean square deviation (RMSD) and mean signed error (MSE) from the calculations with explicit solvent model ($\Delta G_{Expl.}$) or from experimental solvation energy ($\Delta G_{Exper.}$) per solvent (kJ/mol) for calculations with implicit solvent models

	$\Delta G_{Expl.}$		$\Delta G_{Exper.}$	
PB	3.04 ± 0.15	1.04 ± 0.19	4.51 ± 0.24	-0.02 ± 0.30
Still	6.11 ± 0.30	1.06 ± 0.41	7.88 ± 0.34	0.00 ± 0.53
HCT	6.83 ± 0.30	1.06 ± 0.45	7.87 ± 0.29	0.00 ± 0.53
OBC-I	7.64 ± 0.33	1.06 ± 0.50	8.82 ± 0.33	0.00 ± 0.58
OBC-II	7.60 ± 0.37	1.06 ± 0.50	8.47 ± 0.36	0.00 ± 0.57

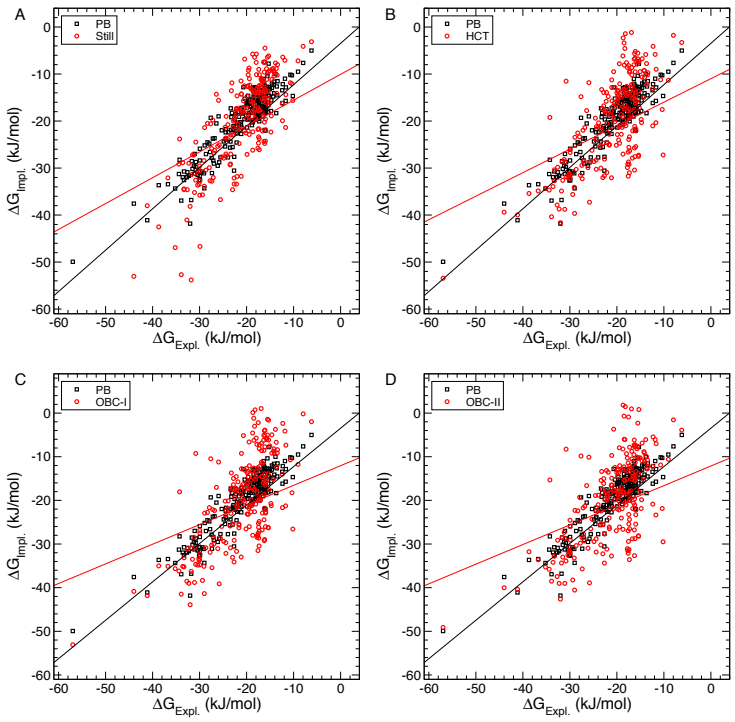

Figure S4: Correlation between calculated solvation free energies obtained using explicit solvent model ($\Delta G_{Expl.}$) and that obtained using optimized PB (black) and GB (red) models ($\Delta G_{Impl.}$): (A) Still, (B) HCT, (C) OBC-I (D) OBC-II

Table S51: Scale factor to optimize apolar contribution calculated with PB obtained by fitting to a straight line $\Delta G_{Exper.}$ - ΔG_{polar} = m·ΔG_{apolar} + b, root mean square deviation (RMSD) and mean signed error (MSE) of the optimized PB calculations from experimental data, and correlation (R) between the optimized PB calculations and experimental data per solvent[a]

Solvent	N	m	b	RMSD	MSE	R
1-octanol	29	1.30	14.28	5.0 ± 0.9	0.0 ± 0.9	0.73 ± 0.13
benzonitrile	6	0.87	19.59	5.3 ± 1.5	-0.1 ± 2.2	0.76 ± 0.23
acetone	12	0.94	17.59	4.5 ± 0.7	-0.1 ± 1.3	0.92 ± 0.10
acetonitrile	6	1.35	22.54	1.9 ± 0.3	-0.0 ± 0.8	0.85 ± 0.14
chloroform	28	1.24	10.02	4.8 ± 0.6	-0.0 ± 0.9	0.82 ± 0.08
acetophenone	8	0.97	13.97	5.5 ± 1.6	-0.1 ± 1.9	0.70 ± 0.22

[a]N is the number of solutes tested.

Table S51: Scale factor to optimize apolar contribution calculated with PB obtained by fitting to a straight line $\Delta G_{Exper.}$ - ΔG_{polar} = m·ΔG_{apolar} + b, root mean square deviation (RMSD) and mean signed error (MSE) of the optimized PB calculations from experimental data, and correlation (R) between the optimized PB calculations and experimental data per solvent[a]

Solvent	N	m	b	RMSD	MSE	R
cyclohexanone	9	0.78	9.03	5.6 ± 1.0	-0.0 ± 1.9	0.36 ± 0.19
dibutyl ether	5	1.59	16.69	1.9 ± 0.6	-0.0 ± 0.8	0.84 ± 0.14
dimethyl sulfoxide	9	-0.26	-4.67	6.0 ± 0.6	-0.0 ± 2.0	0.70 ± 0.26
ethanol	13	1.20	18.50	4.7 ± 1.3	-0.0 ± 1.3	0.61 ± 0.25
ethyl acetate	13	0.59	9.30	4.0 ± 0.5	-0.0 ± 1.1	0.79 ± 0.18
methanol	20	0.99	14.72	4.5 ± 0.8	-0.0 ± 1.0	0.78 ± 0.14
methyl acetate	7	0.70	11.69	3.7 ± 0.9	0.0 ± 1.4	0.68 ± 0.28
nitromethane	10	0.71	14.52	4.5 ± 0.6	-0.0 ± 1.4	0.70 ± 0.23
N-methylformamide	9	1.83	17.15	3.1 ± 0.9	-0.0 ± 1.0	0.96 ± 0.21
N,N-dimethylacetamide	9	1.13	9.98	4.6 ± 1.2	-0.1 ± 1.5	0.16 ± 0.20
N,N-dimethylformamide	9	0.76	7.34	5.0 ± 1.1	-0.0 ± 1.7	0.84 ± 0.11
o-xylene	5	0.95	11.38	1.9 ± 0.4	0.1 ± 0.8	0.83 ± 0.15
pyridine	8	0.73	12.09	4.7 ± 1.3	-0.1 ± 1.7	0.62 ± 0.20
toluene	11	0.71	8.92	2.0 ± 0.4	-0.0 ± 0.6	0.86 ± 0.12

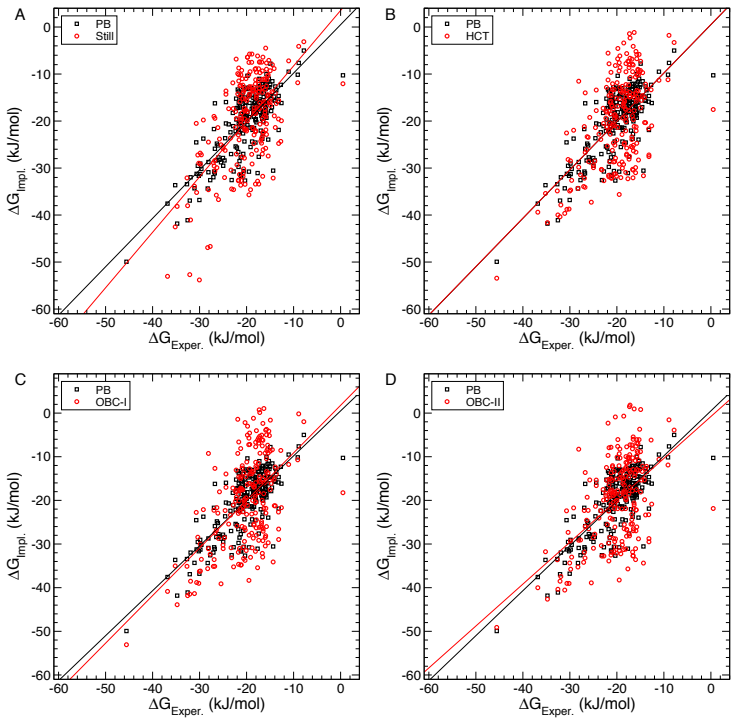

Figure S5: Correlation between experimental solvation free energies ($\Delta G_{Exper.}$) and that calculated using optimized PB (black) and GB (red) models ($\Delta G_{Impl.}$): (A) Still, (B) HCT, (C) OBC-I (D) OBC-II

Table S52: Optimal surface tension parameters for Still obtained by fitting to a straight line $\Delta G_{Exper.}$ - $\Delta G_{polar} = \gamma \cdot A + c$, root mean square deviation (RMSD) and mean signed error (MSE) of the optimized Still calculations from experimental data, and correlation (R) between the optimized Still calculations and experimental data per solvent[a]

Solvent	N	γ	c	RMSD	MSE	R
1-octanol	29	-7.01	33.52	8.3 ± 1.1	-0.0 ± 1.6	0.61 ± 0.15
benzonitrile	6	-18.22	74.63	6.0 ± 1.1	-0.0 ± 2.5	0.87 ± 0.12
acetone	12	-12.37	53.19	9.3 ± 2.4	-0.0 ± 2.7	0.83 ± 0.10
acetonitrile	6	-16.70	65.60	4.8 ± 0.9	-0.0 ± 2.0	0.55 ± 0.23
chloroform	28	-5.02	18.35	7.6 ± 0.7	0.0 ± 1.4	0.64 ± 0.17
acetophenone	8	-13.28	54.80	7.3 ± 1.3	-0.0 ± 2.5	0.83 ± 0.23
cyclohexanone	9	-9.71	43.14	9.7 ± 1.4	-0.0 ± 3.3	0.29 ± 0.20

[a]N is the number of solutes tested. γ is in kJ/(mol·nm^2), and c is in kJ/mol

Table S52: Optimal surface tension parameters for Still obtained by fitting to a straight line $\Delta G_{Exper.}$ - $\Delta G_{polar} = \gamma \cdot A + c$, root mean square deviation (RMSD) and mean signed error (MSE) of the optimized Still calculations from experimental data, and correlation (R) between the optimized Still calculations and experimental data per solvent[a]

Solvent	N	γ	c	RMSD	MSE	R
dibutyl ether	5	-16.34	61.63	4.5 ± 1.0	0.0 ± 2.0	0.43 ± 0.32
dimethyl sulfoxide	9	-5.77	27.25	11.3 ± 1.9	-0.0 ± 3.7	0.69 ± 0.26
ethanol	13	-14.00	58.68	6.7 ± 1.2	-0.0 ± 1.9	0.52 ± 0.24
ethyl acetate	13	-8.05	35.32	8.9 ± 1.6	0.0 ± 2.5	0.68 ± 0.23
methanol	20	-8.22	37.56	9.1 ± 0.9	0.0 ± 2.0	0.68 ± 0.19
methyl acetate	7	-16.14	61.55	6.4 ± 0.8	-0.0 ± 2.4	0.50 ± 0.26
nitromethane	10	-10.25	45.81	8.3 ± 1.4	-0.0 ± 2.6	0.62 ± 0.21
N-methylformamide	9	-9.62	40.98	6.8 ± 1.1	0.0 ± 2.2	0.64 ± 0.25
N,N-dimethylacetamide	9	-6.87	29.45	8.6 ± 1.7	0.0 ± 2.9	0.38 ± 0.23
N,N-dimethylformamide	9	-13.00	54.55	5.8 ± 1.1	0.0 ± 1.9	0.76 ± 0.17
o-xylene	5	-8.30	30.94	5.8 ± 0.9	0.0 ± 2.6	0.24 ± 0.31
pyridine	8	-13.82	56.30	7.9 ± 1.0	0.0 ± 2.8	0.68 ± 0.24
toluene	11	-5.89	23.81	4.1 ± 0.8	0.0 ± 1.2	0.57 ± 0.21

Table S53: Optimal surface tension parameters for HCT obtained by fitting to a straight line $\Delta G_{Exper.}$ - $\Delta G_{polar} = \gamma \cdot A + c$, root mean square deviation (RMSD) and mean signed error (MSE) of the optimized HCT calculations from experimental data, and correlation (R) between the optimized HCT calculations and experimental data per solvent[a]

Solvent	N	γ	c	RMSD	MSE	R
1-octanol	29	-7.37	31.85	8.2 ± 0.9	-0.0 ± 1.6	0.54 ± 0.15
benzonitrile	6	-8.25	38.15	7.5 ± 1.2	-0.0 ± 3.1	0.83 ± 0.22
acetone	12	-12.86	52.22	8.8 ± 1.2	-0.0 ± 2.6	0.76 ± 0.16
acetonitrile	6	-11.19	43.74	5.7 ± 1.3	0.0 ± 2.3	0.41 ± 0.27
chloroform	28	-5.96	20.96	8.0 ± 0.9	-0.0 ± 1.5	0.59 ± 0.16
acetophenone	8	-10.52	44.92	8.0 ± 1.2	-0.0 ± 2.8	0.73 ± 0.21
cyclohexanone	9	-8.54	37.83	9.5 ± 1.2	0.0 ± 3.2	0.13 ± 0.17
dibutyl ether	5	-12.44	46.39	5.5 ± 1.8	0.0 ± 2.5	0.22 ± 0.29
dimethyl sulfoxide	9	-5.88	25.28	8.5 ± 1.5	0.0 ± 2.8	0.54 ± 0.24
ethanol	13	-12.91	52.37	9.2 ± 1.3	0.0 ± 2.5	0.32 ± 0.21
ethyl acetate	13	-10.07	41.49	7.0 ± 1.0	0.0 ± 1.9	0.59 ± 0.17
methanol	20	-8.57	35.33	9.3 ± 1.1	0.0 ± 2.0	0.46 ± 0.19
methyl acetate	7	-13.97	54.38	7.6 ± 1.0	0.0 ± 2.8	0.50 ± 0.25
nitromethane	10	-9.27	41.43	8.1 ± 1.1	0.0 ± 2.5	0.79 ± 0.13
N-methylformamide	9	-8.59	35.46	5.8 ± 1.4	0.0 ± 1.9	0.82 ± 0.30
N,N-dimethylacetamide	9	-1.95	9.33	9.1 ± 1.1	-0.0 ± 3.0	0.08 ± 0.21
N,N-dimethylformamide	9	-14.20	59.10	6.8 ± 0.6	0.0 ± 2.3	0.81 ± 0.16
o-xylene	5	-8.42	30.04	4.4 ± 0.7	-0.0 ± 2.0	0.36 ± 0.31
pyridine	8	-12.98	50.79	7.0 ± 1.2	0.0 ± 2.5	0.51 ± 0.24
toluene	11	-7.76	29.53	3.9 ± 0.6	0.0 ± 1.2	0.62 ± 0.17

[a]N is the number of solutes tested. γ is in kJ/(mol·nm^2), and c is in kJ/mol

Table S54: Optimal surface tension parameters for OBC-I obtained by fitting to a straight line $\Delta G_{Exper.}$ - $\Delta G_{polar} = \gamma \cdot A + c$, root mean square deviation (RMSD) and mean signed error (MSE) of the optimized OBC-I calculations from experimental data, and correlation (R) between the optimized OBC-I calculations and experimental data per solvent[a]

Solvent	N	γ	c	RMSD	MSE	R
1-octanol	29	-6.51	34.75	9.1 ± 1.0	0.0 ± 1.7	0.52 ± 0.15
benzonitrile	6	-6.74	39.82	8.6 ± 1.6	0.0 ± 3.5	0.79 ± 0.22
acetone	12	-10.78	53.87	9.9 ± 1.3	0.0 ± 2.9	0.77 ± 0.14
acetonitrile	6	-8.87	43.13	6.8 ± 1.4	0.0 ± 2.8	0.37 ± 0.28
chloroform	28	-4.72	21.12	8.7 ± 1.0	0.0 ± 1.6	0.56 ± 0.16
acetophenone	8	-8.80	46.66	8.8 ± 1.5	0.0 ± 3.1	0.72 ± 0.21
cyclohexanone	9	-6.90	38.34	10.5 ± 1.4	0.0 ± 3.5	0.09 ± 0.17
dibutyl ether	5	-9.99	45.65	6.2 ± 2.1	-0.0 ± 2.8	0.11 ± 0.31
dimethyl sulfoxide	9	-4.97	27.51	9.3 ± 1.7	0.0 ± 3.1	0.54 ± 0.24
ethanol	13	-10.73	53.34	10.7 ± 1.7	-0.0 ± 3.0	0.32 ± 0.20
ethyl acetate	13	-8.70	44.28	7.8 ± 1.2	-0.0 ± 2.2	0.59 ± 0.17
methanol	20	-7.88	39.75	10.5 ± 1.4	-0.0 ± 2.4	0.44 ± 0.18
methyl acetate	7	-12.62	59.55	8.5 ± 1.1	-0.0 ± 3.2	0.50 ± 0.26
nitromethane	10	-7.84	43.61	9.1 ± 1.3	0.0 ± 2.9	0.79 ± 0.13
N-methylformamide	9	-7.43	37.75	6.8 ± 1.4	0.0 ± 2.3	0.83 ± 0.26
N,N-dimethylacetamide	9	-1.53	10.72	9.8 ± 1.1	0.0 ± 3.3	0.06 ± 0.21
N,N-dimethylformamide	9	-12.82	64.52	8.3 ± 0.9	-0.0 ± 2.8	0.82 ± 0.15
o-xylene	5	-6.45	28.01	5.0 ± 0.8	0.0 ± 2.2	0.27 ± 0.31
pyridine	8	-10.58	51.37	8.2 ± 1.5	-0.0 ± 2.9	0.49 ± 0.23
toluene	11	-7.00	33.07	4.2 ± 0.7	-0.0 ± 1.3	0.61 ± 0.17

[a]N is the number of solutes tested. γ is in kJ/(mol·nm^2), and c is in kJ/mol

Table S55: Optimal surface tension parameters for OBC-II obtained by fitting to a straight line $\Delta G_{Exper.}$ - $\Delta G_{polar} = \gamma \cdot A + c$, root mean square deviation (RMSD) and mean signed error (MSE) of the optimized OBC-II calculations from experimental data, and correlation (R) between the optimized OBC-II calculations and experimental data per solvent[a]

Solvent	N	γ	c	RMSD	MSE	R
1-octanol	29	-7.09	30.20	9.2 ± 1.1	-0.0 ± 1.7	0.44 ± 0.15
benzonitrile	6	-8.39	40.35	7.8 ± 1.2	-0.0 ± 3.2	0.81 ± 0.23
acetone	12	-11.65	49.02	9.6 ± 1.6	0.0 ± 2.8	0.73 ± 0.17
acetonitrile	6	-13.44	54.39	5.1 ± 1.2	0.0 ± 2.0	0.49 ± 0.26
chloroform	28	-4.91	16.23	9.0 ± 1.1	-0.0 ± 1.7	0.48 ± 0.17
acetophenone	8	-12.79	55.60	7.6 ± 1.1	-0.0 ± 2.7	0.75 ± 0.19
cyclohexanone	9	-9.77	43.77	9.6 ± 1.0	-0.0 ± 3.2	0.02 ± 0.16
dibutyl ether	5	-14.24	55.19	4.9 ± 1.5	-0.0 ± 2.1	0.35 ± 0.30
dimethyl sulfoxide	9	-7.49	32.53	8.3 ± 1.6	0.0 ± 2.8	0.50 ± 0.24
ethanol	13	-11.38	46.71	10.9 ± 1.9	0.0 ± 3.0	0.23 ± 0.20
ethyl acetate	13	-11.95	50.19	6.7 ± 0.9	0.0 ± 1.9	0.56 ± 0.16
methanol	20	-8.93	36.18	10.5 ± 1.4	0.0 ± 2.4	0.37 ± 0.19
methyl acetate	7	-15.46	62.64	7.3 ± 0.9	0.0 ± 2.8	0.56 ± 0.24
nitromethane	10	-10.81	48.95	8.2 ± 1.1	0.0 ± 2.6	0.81 ± 0.11
N-methylformamide	9	-11.53	47.87	6.0 ± 1.1	0.0 ± 2.0	0.86 ± 0.24
N,N-dimethylacetamide	9	-1.65	8.65	9.4 ± 1.0	0.0 ± 3.1	0.03 ± 0.21
N,N-dimethylformamide	9	-14.37	60.49	8.7 ± 1.4	-0.0 ± 2.9	0.77 ± 0.16
o-xylene	5	-12.69	48.48	4.1 ± 0.9	-0.0 ± 1.9	0.44 ± 0.32
pyridine	8	-15.75	63.35	6.5 ± 1.0	0.0 ± 2.3	0.47 ± 0.24
toluene	11	-8.79	33.74	4.4 ± 0.6	-0.0 ± 1.3	0.52 ± 0.17

[a]N is the number of solutes tested. γ is in kJ/(mol·nm^2), and c is in kJ/mol

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