solvents - implicit

MN15/6-311++G***/auto				**SCF energies in a.u.**			
Enthalpy values	**$CHCl_3$**	**NEt_3**	**MeOEtOH**	**GBL**	**THF**	**DMSO**	**H_2O**
gas phase	-1419.0194	-292.1008	-269.3321	-306.1286	-232.1075	-552.8762	-76.3507
protonation		-292.4844	-269.6508	-306.4461		-553.2189	-76.6144
PCM solv	-1419.0217	-292.1018	-269.3384	-306.1401	-232.1112	-552.8908	-76.3590
+non-electrostatic	-1419.0188			**-306.1317**	-232.1028	-552.8834	-76.3548
protonation		-292.5303	-269.7364	-306.5317		-553.3077	-76.7373
+non-electrostatic				**-306.5233**		-553.2995	-76.7327
CPCM solv	-1419.0220	-292.1022	-269.3385	-306.1401	-232.1115	-552.8909	-76.3591
+non-electrostatic	-1419.0191			**-306.1317**	-232.1031	-552.8836	-76.3548
protonation		-292.5300	-269.7366	-306.5317		-553.3078	-76.7373
+non-electrostatic				**-306.5233**		-553.2996	-76.7327
SMD solv already w/non-electrostatic	-1419.0273	-292.1061	-269.3423	-306.1450	-232.1146	-552.8910	-76.3650
protonation		-292.5434	-269.7548	-306.5440		-553.3158	-76.7672

Heat of solvation of the solvents, kJ mol^{-1}

PCM solv	-6	-3	-16	-30	-10	-38	-22
+non-electrostatic	2			-8	12	-19	-11
CPCM solv	-7	-4	-17	-30	-10	-38	-22
+non-electrostatic	1			-8	12	-19	-11
SMD solv	-21	-14	-27	-43	-19	-39	-37

Heat of protonation, kJ mol^{-1}

gas phase	-1006	-836	-833		-899	-692
PCM solv	-1127	-1060	-1057		-1132	-1014
+non-electrostatic			-1036		-1110	-1002
CPCM solv	-1126	-1061	-1057		-1132	-1014
+non-electrostatic			-1036		-1111	-1002
SMD solv	-1161	-1109	-1090		-1153	-1093

solute - gas phase

Enthalpy

numbering scheme of the molecules are adopted from *JOC* 78 7674.

Sum of electronic and thermal Enthalpies, a.u.

		keto tautomer			enol tautomer	
Level of theory		**0HB – 15**	**1HB – 19**	**2HB – 17**	**1HB – 16**	**2HB – 18**
Rung 2	BP86	-765.1806	-765.2040	-765.2250	-765.1876	-765.2003
	BLYP	-764.9303	-764.9516	-764.9715	-764.9358	-764.9480
	PBE	-764.2702	-764.2934	-764.3141	-764.2770	-764.2893
Rung 3	TPSSTPSS	-765.2960	-765.3186	-765.3394	-765.3009	-765.3135
	revTPSSrevTPSS	-765.0691	-765.0912	-765.1114	-765.0719	-765.0840
	M06L	-765.0733	-765.0942	-765.1136	-765.0767	-765.0877
Rung 4	MN15	-764.2765	-764.2961	-764.3153	-764.2825	-764.2952
	wB97XD	-764.9063	-764.9258	-764.9451	-764.9056	-764.9181
	B3LYP	-765.1709	-765.1915	-765.2114	-765.1759	-765.1895
	CAM-B3LYP	-764.2702	-764.2934	-764.3141	-764.2770	-764.2893
	CAM-B3LYP+ED	-764.8215	-764.8422	-764.8625	-764.8240	-764.8374

relative enthalpies of tautomerization, kJ mol^{-1}

		keto tautomer			enol tautomer	
Level of theory		**0HB – 15**	**1HB – 19**	**2HB – 17**	**1HB – 16**	**2HB – 18**
Rung 2	BP86	116	55	0	98	65
	BLYP	108	52	0	94	62
	PBE	115	54	0	97	65
Rung 3	TPSSTPSS	114	54	0	101	68
	revTPSSrevTPSS	111	53	0	104	72
	M06L	106	51	0	97	68
Rung 4	MN15	102	50	0	86	53
	wB97XD	102	51	0	104	71
	B3LYP	106	52	0	93	58
	CAM-B3LYP	115	54	0	97	65
	CAM-B3LYP+ED	108	53	0	101	66
CBS-QB3 (*JOC* 78 7674)		95	47	0	84	52

deviation from CBS-QB3 reference, kJ mol^{-1}

		keto tautomer			enol tautomer		r.m.s.
Level of theory		**0HB – 15**	**1HB – 19**	**2HB – 17**	**1HB – 16**	**2HB – 18**	deviation
Rung 2	BP86	21	8		14	13	15.0
	BLYP	13	5		10	10	9.8
	PBE	20	7		13	13	14.2
Rung 3	TPSSTPSS	19	7		17	16	15.5
	revTPSSrevTPSS	16	6		20	20	16.3
	M06L	11	4		13	16	11.6
Rung 4	**MN15 (HFX 44%)**	**7**	**3**		**2**	**1**	**4.0**
	wB97XD (HFX 100%)	7	4		20	19	14.3
	B3LYP	11	5		9	6	8.2
	CAM-B3LYP	20	7		13	13	14.2
	CAM-B3LYP+ED	13	6		17	14	13.1

Gibbs free energy (gas phase)

Sum of electronic and thermal Enthalpies, a.u.

		keto tautomer			enol tautomer	
Level of theory		**0HB – 15**	**1HB – 19**	**2HB – 17**	**1HB – 16**	**2HB – 18**
Rung 2	BP86	-765.2351	-765.2577	-765.2778	-765.2416	-765.2540
	BLYP	-764.9847	-765.0053	-765.0243	-764.9899	-765.0018
	PBE	-764.3246	-764.3470	-764.3668	-764.3309	-764.3431
Rung 3	TPSSTPSS	-765.3502	-765.3721	-765.3919	-765.3546	-765.3670
	revTPSSrevTPSS	-765.1234	-765.1446	-765.1639	-765.1257	-765.1378
	M06L	-765.1268	-765.1471	-765.1658	-765.1317	-765.1412
Rung 4	MN15	-764.3303	-764.3492	-764.3678	-764.3364	-764.3484
	wB97XD	-764.9598	-764.9786	-764.9973	-764.9599	-764.9711
	B3LYP	-765.2245	-765.2446	-765.2637	-765.2296	-765.2409
	CAM-B3LYP	-764.8453	-764.8653	-764.8847	-764.8485	-764.8605
	CAM-B3LYP+ED	-764.8748	-764.8949	-764.9145	-764.8782	-764.8903

relative enthalpies of tautomerization, kJ mol^{-1}

		keto tautomer			enol tautomer	
Level of theory		**0HB – 15**	**1HB – 19**	**2HB – 17**	**1HB – 16**	**2HB – 18**
Rung 2	BP86	112	53	0	95	62
	BLYP	104	50	0	90	59
	PBE	111	52	0	94	62
Rung 3	TPSSTPSS	109	52	0	98	65
	revTPSSrevTPSS	106	51	0	100	68
	M06L	102	49	0	89	64
Rung 4	MN15	98	49	0	82	51
	wB97XD	98	49	0	98	69
	B3LYP	103	50	0	89	60
	CAM-B3LYP	103	51	0	95	64
	CAM-B3LYP+ED	104	51	0	95	63