

water model	charge model	all compounds	subset by functionalities		
			alkanes (6)	arenes (6)	alcohols (6)
implicit ²⁵	AM1BCC	1.35	0.26	0.29	1.41
	AMSOL	2.46	0.31	1.34	2.08
	RESP (SCF/6-31G*)	1.28	0.49	0.23	2.00
explicit TIP3P	AM1BCC	0.92	0.51	0.30	1.43
	AMSOL	1.38	0.41	0.73	1.49
	RESP (SCF/6-31G*)	0.82	0.47	1.05	0.84
	RESP (B3LYP/cc-pVTZ+SCRF)	0.78	0.47	0.60	0.46
explicit TIP4P-Ew	AM1 BCC	1.24	1.09	0.75	1.06
	AMSOL	1.55	1.09	0.99	1.41
	RESP (SCF/6-31G*)	1.27	0.89	0.85	1.41
	RESP (B3LYP/cc-pVTZ+SCRF)	1.45	0.87	1.08	1.04