LogTW SAMPL9 prediction using Fast Growth Nonequilibrium Alchemy

1	2.92	0.51
2	3.73	0.60
3	5.64	0.40
4	5.97	0.44
5	4.04	0.52
6	-2.02	0.40
7	5.61	0.78
8	-0.93	3.06
9	5.67	0.49
10	3.67	0.30
11	1.37	0.63
12	-0.96	0.64
13	2.10	0.54
14	3.87	0.38
15	-1.12	0.95
16	1.88	1.02

Method: Force field for solute is GAFF2 with AM1-BCC charges (generated with PrimaDORAC www1.chim.unifi.it/orac/primadorac); Starting nonequilibrium state
is prepared by combining 96 confs of the gas-phase solute sampled with H-REM (min scale → 0.1) combined with 96 confs of solvent in standard conditions (NPT). Solute molecules are in their neutral state. For the solvent, we used 344 Toluene molecules in a cubic box (GAFF2-AM1-BCC) with a mean side-length of 39.72 Angs and 1728 OPC3 water molecules in a cubic box with a mean side-length of 37.45 Angs. In the 100 NE alchemy runs, the solute was recoupled in the solvent (NPT condition) in 450 ps. The solvation free energies DG_w and DG_t are evaluated using the Gaussian estimate if the p-value of the Andreson-Darling test of the work distribution is greater than 50% or with the Jarzynski estimate DG=-RT ln(e^{-\beta W} with bias estimated from the variance. Errors (confidence interval 95%) are computed with bootstrap with resampling. The Toluene-water partition coefficient is computed as

LogTW= -(DG_t -DG_w)/RT/log(10).

Calculation were done on the ENEA-CRESCO6 cluster in Portici (NA), Italy using the program ORAC (www1.chim.unifi.it/orac). Wall-clock time for a full LogTW calculation, on a per solute basis, was ~ 2 hour using 12 48-cores nodes (Skylake Intel(R) Xeon(R) Platinum 8160 2.10GHz).