

Table 1. *Atomic solvation parameters determined with different surface descriptors^a*

Type of surface	C	N/O	O ⁻	N ⁺	S
MS	24 ± 2	-28 ± 3	-71 ± 6	-83 ± 5	-14 ± 5
SAS	12 ± 1	-13 ± 4	-38 ± 6	-29 ± 5	-9 ± 5
VV	24 ± 2	-14 ± 3	-61 ± 8	-73 ± 7	-14 ± 5
EM	18 ± 1	-9 ± 3	-37 ± 7	-38 ± 4	-5 ± 6

^a Atomic solvation parameters calculated using solvent-accessible surfaces (SAS), molecular surfaces (MS), and Voronoi volumes (VV). The values used in calculating association energies are those of Eisenberg and McLaughlin (EM).