

I have taken this table from AMBER 12 / Examples /TEMPLATE_INPUT_SCRIPTS / SURFTEN_SURFOFF_Recommendations.pdf file

Table 2: Input parameters recommended for nonpolar solvation free energy calculations for protein systems

$G_{pb gb}$ ¹⁾	Flags affecting nonpolar solvation energy calculation			Calculation of G_{np} ²⁾	Radii ³⁾	SURFTEN	SURFOFF
IGB = 1	MS=0 1	GBSA=1		$G_{np}=\gamma A + b$	mbondi	0.00720	0.0000
IGB = 2	MS=0 1	GBSA=1 2		$G_{np}=\gamma A + b$	mbondi2	0.00500	0.0000
IGB = 5	MS=0 1	GBSA=1 2		$G_{np}=\gamma A + b$	mbondi2	0.00500	0.0000
PB	MS=0	INP=1	RADIOPT=0	$G_{np}=\gamma A + b$	Parse	0.00542	0.9200
	MS=0	INP=2 ⁴⁾	RADIOPT=1	$G_{np}=\gamma A + b + G_{disp}$	R_{min}	0.03780	-0.5692
	MS=1	IVCAP > 0	RADIOPT=1	$G_{np} = G_{cavity} + E_{vdw}$	bondi	⁵⁾ 0.06900	⁵⁾ 0.0000

¹⁾ Procedure used for the calculation of the polar solvation free energy

²⁾ Method employed for determination of the nonpolar solvation free energy

³⁾ Radii used for calculation of the nonpolar solvation free energy (G_{np}).

⁴⁾ Calculation procedure for INP=2 changed in mm_pbsa.pl of AMBER12 according to the recommendations of Dr. Luo.

New parameters: DECOMPOPT = 2 (σ decomposition scheme)

USE_RMIN = 1 (vdW R_{min} values)

USE_SAV = 1 (Molecular volume enclosed by SASA (SAV) used for estimation of G_{cavity})

SPROB = 0.557 (Solvent probe radius for SASA used for calculation of $G_{dispersion}$)

VPROB = 1.3 (Solvent probe radius for molecular volume used for computation of G_{cavity})

RHOW_EFFECT = 1.129 (Effective water density used for calculation of $G_{dispersion}$)

DPROB = 1.6 (Solvent probe radius for molecular surface used to define the dielectric boundary between solute and solvent)

Parameters up to AMBER11: DECOMPOPT = 1 (6/12 decomposition scheme)

USE_RMIN = 0 (vdW σ values)

USE_SAV = 0 (SASA used for estimation of G_{cavity})

SPROB = 1.6 (Solvent probe radius for SASA used for calculation of G_{cavity} , $G_{dispersion}$ and polar solvation free energy (DPROB = SPROB))

⁵⁾ These parameters should only be applied when calculations according to the hybrid model are conducted (IVCAP > 0) or when an analogous calculation procedure as in [4] is intended. The nonpolar solvation free energy is calculated as the sum of the cavity free energy $G_{cavity} = \gamma MSA + b$ (where MSA = molecular surface area) and the van der Waals interaction energy between solute and solvent atoms (E_{vdw}).

G pb/gb	Flag affecting nonpolar solvation energy calculation	Calculation of G_{np}	RADII	SURFTEN	SURFOFF
IGB=1	MS=0 GBSA=1	$G_{np} = \gamma A + b$	mbondi	default	default
IGB=2	MS=0 GBSA=1	$G_{np} = \gamma A + b$	mbondi2	default	default
IGB=5	MS=0 GBSA=1	$G_{np} = \gamma A + b$	mbondi2	default	default
IGB=8	MS=0 GBSA=1	$G_{np} = \gamma A + b$	mbondi3	default	default
PB	MS=0 INP=1 RADIOPT=0	$G_{np} = \gamma A + b$	mbondi, mbondi2, mbondi3	default	default
PB*	MS=0 INP=1 RADIOPT=0	$G_{np} = \gamma A + b$	Parse	0.00542	0.9200
PB	MS=0 INP=2 RADIOPT=1 prbrad=1.4	$G_{np} = \gamma A + b$ + G_{disp}	mbondi, mbondi2, mbondi3	default	default
PB*	MS=0 INP=2 RADIOPT=1 prbrad=1.4	$G_{np} = \gamma A + b$ + G_{disp}	Rmin	0.03780 (default)	- 0.5692 (default)
PB*	MS=1 IVCAP=1 RADIOPT=1 prbrad=1.4	$G_{np} = G_{cavity}$ + E_{vdW}	bondi	0.06900	0.0000
PB*	MS=1 IVCAP=5 RADIOPT=1 prbrad=1.4	$G_{np} = G_{cavity}$ + E_{vdW}	bondi	0.06900	0.0000

* Input parameters were taken from the Recommendations.pdf file.