
List of MM-PB/GBSA [GB1] Result (kcal/mol)

LIG

BOND	0.0000	0.0000	0.0000
ANGLE	0.0000	0.0001	0.0000
DIHED	-0.0000	0.0000	0.0000
VDWAALS	-59.3049	4.1538	0.3392
EEL	-267.9998	18.3507	1.4983
1-4 VDW	0.0000	0.0001	0.0000
1-4 EEL	-0.0000	0.0000	0.0000
EGB	254.7026	16.2796	1.3292
ESURF	-8.0508	0.4014	0.0328
DELTA G gas	-327.3047	18.9933	1.5508
DELTA G solv	246.6518	16.1607	1.3195
DELTA TOTAL	-80.6529	5.3642	0.4380
TdeltaS	-50.5890	(from quasi-harmonic analysis in project2)	
DELTA TOTAL -TdeltaS	-30.0639		

ZINC19169954

BOND	0.0000	0.0001	0.0000
ANGLE	-0.0000	0.0000	0.0000
DIHED	0.0000	0.0000	0.0000
VDWAALS	-30.7485	2.2155	0.1809
EEL	-10.9899	4.3608	0.3561
1-4 VDW	0.0000	0.0001	0.0000
1-4 EEL	0.0000	0.0000	0.0000
EGB	24.9730	3.6955	0.3017
ESURF	-3.1342	0.2133	0.0174
DELTA G gas	-41.7384	5.3152	0.4340
DELTA G solv	21.8388	3.6047	0.2943
DELTA TOTAL	-19.8995	2.5159	0.2054
TdeltaS	-41.1650	(from quasi-harmonic analysis in project2)	
DELTA TOTAL -TdeltaS	21.2655		

ZINC19369903

BOND	-0.0000	0.0001	0.0000
ANGLE	0.0000	0.0000	0.0000
DIHED	0.0000	0.0000	0.0000
VDWAALS	-40.8662	3.6531	0.2983
EEL	-3.8997	4.6646	0.3809
1-4 VDW	0.0000	0.0001	0.0000
1-4 EEL	0.0000	0.0000	0.0000
EGB	18.7486	4.3236	0.3530
ESURF	-4.9355	0.3607	0.0295
DELTA G gas	-44.7659	6.2830	0.5130
DELTA G solv	13.8131	4.2039	0.3432
DELTA TOTAL	-30.9528	3.1236	0.2550
TdeltaS	-36.7320	(from quasi-harmonic analysis in project2)	
DELTA TOTAL -TdeltaS	5.7792		

ZINC19369905

BOND	0.0000	0.0001	0.0000
ANGLE	-0.0000	0.0001	0.0000

mmpbsa_gb1.summary

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DIHED	-0.0000	0.0000	0.0000
VDWAALS	-43.3572	3.6836	0.3008
EEL	-7.3048	6.2394	0.5094
1-4 VDW	0.0000	0.0001	0.0000
1-4 EEL	0.0000	0.0000	0.0000
EGB	20.4958	5.5782	0.4555
ESURF	-5.2132	0.2967	0.0242
DELTA G gas	-50.6620	8.8392	0.7217
DELTA G solv	15.2826	5.3894	0.4400
DELTA TOTAL	-35.3794	4.3310	0.3536
TdeltaS	-36.2300	(from quasi-harmonic analysis in project2	
DELTA TOTAL -TdeltaS	0.8506		
