
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	274.3668	16.3402	1.3342
ESURF	-8.0508	0.4014	0.0328
DELTA G gas	-327.3047	18.9933	1.5508
DELTA G solv	266.3160	16.2224	1.3246
DELTA TOTAL	-60.9887	5.3502	0.4368
TdeltaS	-50.5890	(from quasi-harmonic analysis in project2)	
DELTA TOTAL -TdeltaS	-10.3997		

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	28.1636	4.0348	0.3294
ESURF	-3.1342	0.2133	0.0174
DELTA G gas	-41.7384	5.3152	0.4340
DELTA G solv	25.0294	3.9397	0.3217
DELTA TOTAL	-16.7090	2.4720	0.2018
TdeltaS	-41.1650	(from quasi-harmonic analysis in project2)	
DELTA TOTAL -TdeltaS	24.4560		

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	22.7664	4.6502	0.3797
ESURF	-4.9355	0.3607	0.0295
DELTA G gas	-44.7659	6.2830	0.5130
DELTA G solv	17.8309	4.5015	0.3675
DELTA TOTAL	-26.9350	2.7531	0.2248
TdeltaS	-36.7320	(from quasi-harmonic analysis in project2)	
DELTA TOTAL -TdeltaS	9.7970		

ZINC19369905

BOND	0.0000	0.0001	0.0000
ANGLE	-0.0000	0.0001	0.0000
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	24.0021	5.7873	0.4725
ESURF	-5.2132	0.2967	0.0242

DELTA G gas	-50.6620	8.8392	0.7217
DELTA G solv	18.7889	5.5962	0.4569

DELTA TOTAL	-31.8731	4.2121	0.3439
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TdeltaS	-36.2300	(from quasi-harmonic analysis in project2)	
DELTA TOTAL -TdeltaS	4.3569		
