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

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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 282.2021 16.1957 1.3224  
ESURF -8.0508 0.4014 0.0328  
  
DELTA G gas -327.3047 18.9933 1.5508  
DELTA G solv 274.1513 16.0813 1.3130  
  
DELTA TOTAL -53.1534 5.9511 0.4859  
TdeltaS -50.5890 (from quasi-harmonic analysis in project2)  
DELTA TOTAL -TdeltaS -2.5644  
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## ZINC19169954

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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 25.6357 4.1639 0.3400  
ESURF -3.1342 0.2133 0.0174  
  
DELTA G gas -41.7384 5.3152 0.4340  
DELTA G solv 22.5015 4.0745 0.3327  
  
DELTA TOTAL -19.2368 2.6887 0.2195  
TdeltaS -41.1650 (from quasi-harmonic analysis in project2)  
DELTA TOTAL -TdeltaS 21.9282  
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## ZINC19369903

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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 23.3478 4.7082 0.3844  
ESURF -4.9355 0.3607 0.0295  
  
DELTA G gas -44.7659 6.2830 0.5130  
DELTA G solv 18.4124 4.5433 0.3710  
  
DELTA TOTAL -26.3535 2.6691 0.2179  
  
TdeltaS -36.7320 (from quasi-harmonic analysis in project2)  
DELTA TOTAL -TdeltaS 10.3785  
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## ZINC19369905

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mmpbsa\_gb5.summary

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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	23.1341	5.5616	0.4541
ESURF	-5.2132	0.2967	0.0242

DELTA G gas	-50.6620	8.8392	0.7217
DELTA G solv	17.9209	5.3738	0.4388

DELTA TOTAL	-32.7412	4.4615	0.3643
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TdeltaS -36.2300 (from quasi-harmonic analysis in project2)

DELTA TOTAL -TdeltaS 3.4888

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