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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
EPB           265.5030         17.5780          1.4352
ENPOLAR      -44.7120           2.3964          0.1957
EDISPER       76.9352           3.5161          0.2871

DELTA G gas   -327.3047         18.9933          1.5508
DELTA G solv  297.7262         18.3106          1.4951

DELTA TOTAL   -29.5785           6.0371          0.4929

TdeltaS      -50.5890 (from quasi-harmonic analysis in project2)
DELTA TOTAL -TdeltaS  21.0105
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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
EPB           33.9655          6.5902          0.5381
ENPOLAR      -18.5739          1.3047          0.1065
EDISPER       35.9640          1.4285          0.1166

DELTA G gas   -41.7384          5.3152          0.4340
DELTA G solv  51.3556          6.7471          0.5509

DELTA TOTAL    9.6173          4.6115          0.3765

TdeltaS      -41.1650 (from quasi-harmonic analysis in project2)
DELTA TOTAL -TdeltaS  50.7823
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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
EPB           27.3705          6.4503          0.5267
ENPOLAR      -29.1536          2.1401          0.1747
EDISPER       51.1048          2.9964          0.2447

DELTA G gas   -44.7659          6.2830          0.5130
DELTA G solv  49.3216          7.3667          0.6015

DELTA TOTAL    4.5558          5.1471          0.4203
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TdeltaS -36.7320 (from quasi-harmonic analysis in project2)  
DELTA TOTAL -TdeltaS 41.2878

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ZINC19369905

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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
EPB	23.7297	5.8727	0.4795
ENPOLAR	-30.8625	1.8613	0.1520
EDISPER	52.2079	2.1571	0.1761
DELTA G gas	-50.6620	8.8392	0.7217
DELTA G solv	45.0751	6.2835	0.5130
DELTA TOTAL	-5.5870	4.9825	0.4068

TdeltaS -36.2300 (from quasi-harmonic analysis in project2)  
DELTA TOTAL -TdeltaS 30.6430

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