

bond

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0.030	18.84700
0.040	18.79600
0.050	18.74500
0.060	18.69400
0.070	18.64300
0.080	18.59200
0.090	18.54100
0.100	18.49000
0.110	18.43900
0.120	18.38800
0.130	18.33700
0.140	18.28600
0.150	18.23500
0.160	18.18400
0.170	18.13300
0.180	18.08200
0.190	18.03100
0.200	17.98000
0.210	17.92900
0.220	17.87800
0.230	17.82700
0.240	17.77600
0.250	17.72500
0.260	17.67400
0.270	17.62300
0.280	17.57200
0.290	17.52100
0.300	17.47000
0.310	17.41900
0.320	17.36800
0.330	17.31700
0.340	17.26600
0.350	17.21500
0.360	17.16400
0.370	17.11300
0.380	17.06200
0.390	17.01100
0.400	16.96000
0.410	16.90900
0.420	16.85800
0.430	16.80700
0.440	16.75600
0.450	16.70500
0.460	16.65400
0.470	16.60300
0.480	16.55200
0.490	16.50100
0.500	16.45000
0.510	16.39900
0.520	16.34800
0.530	16.29700
0.540	16.24600
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0.560	16.14400
0.570	16.09300
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0.590	15.99100
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0.610	15.88900
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0.630	15.78700
0.640	15.73600
0.650	15.68500
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0.670	15.58300
0.680	15.53200
0.690	15.48100
0.700	15.43000
0.710	15.37900
0.720	15.32800
0.730	15.27700
0.740	15.22600
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0.880	14.51200
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5.960	15.29600
5.970	15.34700
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5.990 15.44900
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angle

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nonbonded AA

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nonbonded AB

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