```
    ##############################
    ##                          ##
    ## Glycerol Parameters New! vdw, bond, angle       ##
    ## from analogy to Ethanol and isopropanol in amoeba.prm       ##
    ##                          ##
    ## some dmso parameters     (bond and angle) taken  ##
    ## from MM3 forcefield.         ##
    ##############################

atom       294   60    C     "Glycerol CH2"           6     12.000    4
atom       295   57    H     "Glycerol H2C"           1      1.008    1
atom       296   58    O     "Glycerol O"             8     15.995    2
atom       297   59    H     "Glycerol HO"            1      1.008    1
atom       298   63    C     "Glycerol >CH-"          6     12.000    4
atom       299   57    H     "Glycerol >CH-"          1      1.008    1
atom       300   58    O     "Glycerol central O"     8     15.995    2
atom       301   59    H     "Glycerol central HO"    1      1.008    1

atom       310   79    S     "DiMeSulfoxide S"       16     31.972    4
atom       311   73    C     "DiMeSulfoxide CH3"      6     12.000    4
atom       312   78    H     "DiM Sulfoxide H3C"      1      1.000    1
atom       313   80    O     "DMSO    O"              8     15.995    1
atom       314   81    M     "LONE PAIR "             1      1.000    1

    ################################
    ##                            ##
    ##  Van der Waals Parameters  ##
    ##                            ##
    ################################


vdw        57           2.980    0.0240    0.94
vdw        58           3.405    0.1100
vdw        59           2.655    0.0135    0.91
vdw        60           3.820    0.1010
vdw        63           3.650    0.1010
vdw        73           3.820    0.1060
vdw        79           3.910    0.3850
vdw        78           2.910    0.0330    0.90
vdw        80           3.300    0.1120
vdw        81           0.000    0.0000


    ###################################
    ##                               ##
    ##  Bond Stretching Parameters   ##
    ##                               ##
    ###################################


bond       57   60        341.0    1.1120
bond       57   63        341.0    1.1120
```

```
bond      58  59      548.9    0.9470
bond      58  60      410.1    1.4130
bond      58  63      410.1    1.4130
bond      60  60      323.0    1.5247
bond      60  63      323.0    1.5247
bond      73  78      341.0    1.1120
bond      73  79      211.5    1.8000
bond      80  79      510.8    1.4870
bond      81  79      211.5    0.9500


   ##################################
   ##                              ##
   ##  Angle Bending Parameters    ##
   ##                              ##
   ##################################


angle     59  58  60   53.96   106.80
angle     59  58  63   53.96   106.80
angle     60  58  60   58.99   106.00
angle     57  60  57   39.57   107.60   107.80   109.47
angle     57  60  58   58.99   110.00   108.90   108.70
angle     57  60  60   42.44   109.80   109.31   110.70
angle     57  60  63   42.44   109.80   109.31   110.70
angle     58  60  60   59.71   107.50   107.00   107.90
angle     58  60  63   59.71   107.50   107.00   107.90
angle     60  60  60   48.20   109.50   110.20   111.00
angle     57  63  57   39.57   107.60   107.80   109.47
angle     57  63  58   58.99   110.00   108.90   108.70
angle     57  63  60   42.44   109.80   109.31   110.70
angle     58  63  60   59.71   107.50   107.00   107.90
angle     60  63  60   48.20   109.50   110.20   111.00
angle     78  73  79   51.43   105.00   105.00   107.70
angle     73  79  80   57.55   105.60   107.80
angle     73  79  73   86.33    94.40
angle     78  73  78   39.57   107.60   107.80   109.47
angle     81  79  73   86.33   113.60
angle     81  79  80   57.55   115.39


   ##################################
   ##                              ##
   ##  Stretch-Bend Parameters     ##
   ##                              ##
   ##################################


strbnd    58          14.40    12.95    0.00
strbnd    60          18.70    11.50    0.00
strbnd    63          18.70    11.50    0.00
strbnd    73          18.70    11.50    0.00
strbnd    79          -5.75     1.45    0.00
```

```
    ##############################
    ##                          ##
    ##  Torsional Parameters    ##
    ##                          ##
    ##############################


torsion     59   58   60   57     -0.130 0.0 1   0.110 180.0 2   0.210 0.0 3
torsion     59   58   60   60      0.400 0.0 1   0.000 180.0 2   0.100 0.0 3
torsion     59   58   60   60      0.400 0.0 1   0.000 180.0 2   0.100 0.0 3
torsion     59   58   63   57      0.300 0.0 1  -0.300 180.0 2   0.600 0.0 3
torsion     59   58   63   60     -0.900 0.0 1   0.300 180.0 2   0.200 0.0 3
torsion     57   60   60   60      0.000 0.0 1   0.000 180.0 2   0.280 0.0 3
torsion     58   60   60   60      0.200 0.0 1   0.000 180.0 2   0.300 0.0 3
torsion     60   60   60   60      0.185 0.0 1   0.170 180.0 2   0.520 0.0 3
torsion     57   60   63   57      0.400 0.0 1   0.200 180.0 2   0.238 0.0 3
torsion     57   60   63   58      0.200 0.0 1   0.000 180.0 2   0.300 0.0 3
torsion     57   60   63   60      0.100 0.0 1   0.000 180.0 2   0.480 0.0 3
torsion     58   60   63   60      0.700 0.0 1   0.200 180.0 2   0.300 0.0 3
torsion     58   60   63   57      0.000 0.0 1   0.000 180.0 2   0.300 0.0 3
torsion     59   58   60   63      0.585 0.0 1   0.500 180.0 2   0.370 0.0 3
torsion     58   60   63   58      0.200 0.0 1   0.000 180.0 2   0.300 0.0 3
torsion     78   73   79   73     -0.200 0.0 1   0.000 180.0 2   0.600 0.0 3
torsion     78   73   79   80      0.000 0.0 1   0.000 180.0 2   0.075 0.0 3
torsion     78   73   79   81      0.000 0.0 1   0.000 180.0 2   0.000 0.0 3


    ####################################
    ##                                ##
    ##  Atomic Multipole Parameters   ##
    ##                                ##
    ####################################


multipole   294  296  298          0.05632
                      0.22202   -0.00617   -0.09479
                      0.05001
                     -0.03826   -0.05908
                     -0.04711    0.02065    0.00906
multipole   295  294  296          0.08878
                      0.02543    0.00022    0.14344
                     -0.02959
                     -0.00198   -0.07956
                     -0.00428   -0.00549    0.10915
multipole   296  294  297         -0.45981
                      0.26419   -0.01508    0.40896
                      0.40038
                      0.02027   -0.97332
                     -0.42686   -0.02467    0.57294
multipole   297  296  294          0.25345
                      0.03112   -0.00086    0.11539
                     -0.02858
                      0.00035   -0.11378
```

```
                    0.00767   -0.00069    0.14236
multipole   298  298  300          0.03652
                    0.03576   -0.20813   -0.09796
                    0.14363
                    0.07582   -0.04569
                    0.01873    0.01213   -0.09795
multipole   299  296  298          0.10581
                    0.02396    0.00634    0.19818
                   -0.05517
                    0.00051   -0.02112
                   -0.01326   -0.00452    0.07629
multipole   300  298  301         -0.47028
                    0.25083   -0.02100    0.44696
                    0.40312
                   -0.00366   -1.02102
                   -0.40948   -0.06889    0.61790
multipole   301  300  298          0.27294
                    0.03342   -0.00880    0.13492
                   -0.01897
                   -0.01747   -0.11264
                   -0.00767    0.00817    0.13161

multipole   310  313  314          1.16119
                   -0.79796    0.00000    0.87605
                   -1.21585
                    0.00000    0.68562
                    1.29767    0.00000    0.53023
multipole   311  310  313         -0.32373
                    0.00255    0.00000   -0.12382
                    0.24226
                    0.00000    0.09536
                    0.12479    0.00000   -0.33762
multipole   312  311  310          0.07449
                    0.05338    0.00000    0.18850
                   -0.06353
                    0.00000   -0.10468
                   -0.00279    0.00000    0.16821
multipole   313  310  314         -0.96063
                    0.01649    0.00000   -0.15813
                   -0.53285
                    0.00000   -0.39611
                   -0.15449    0.00000    0.92896
multipole   314  310  313          0.00000
                    0.00000    0.00000    0.00000
                    0.00000
                    0.00000    0.00000
                    0.00000    0.00000    0.00000
```

```
##########################################
##                                      ##
##  Dipole Polarizability Parameters    ##
##                                      ##
##########################################


polarize   294          1.334     0.390    295
polarize   295          0.496     0.390    294
polarize   296          0.834     0.390    297
polarize   297          0.496     0.390    296
polarize   298          1.334     0.390    299
polarize   299          0.496     0.390    298
polarize   300          0.834     0.390    301
polarize   301          0.496     0.390    300
polarize   310          3.300     0.390    313 314
polarize   311          1.334     0.390    312
polarize   312          0.496     0.390    311
polarize   313          0.834     0.390    310 314
polarize   314          0.000     0.390    310 313
```