1.1 Decanol (DeOH)

```
;
;
;       This file was generated by PRODRG version AA081006.0504
;       PRODRG written/copyrighted by Daan van Aalten
;       and Alexander Schuettelkopf
;
;       Questions/comments to dava@davapc1.bioch.dundee.ac.uk
;
;       When using this software in a publication, cite:
;       A. W. Schuettelkopf and D. M. F. van Aalten (2004).
;       PRODRG - a tool for high-throughput crystallography
;       of protein-ligand complexes.
;       Acta Crystallogr. D60, 1355--1363.
;
;       Nombre: decanol

[ moleculetype ]
; Name nrexcl
DOH      3

[ atoms ]
;   nr      type  resnr resid  atom  cgnr   charge     mass
     1       LP3     1  DOH     CAA     1    0.000  15.0350
     2       LP2     1  DOH     CAB     2    0.000  14.0270
     3       LP2     1  DOH     CAC     3    0.000  14.0270
     4       LP2     1  DOH     CAD     4    0.000  14.0270
     5       LP2     1  DOH     CAE     5    0.000  14.0270
     6       LP2     1  DOH     CAF     6    0.000  14.0270
     7       LP2     1  DOH     CAG     7    0.000  14.0270
     8       LP2     1  DOH     CAH     8    0.000  14.0270
     9       LP2     1  DOH     CAI     9    0.000  14.0270
    10       LP2     1  DOH     CAJ    10    0.156  14.0270
    11        OA     1  DOH     OAK    10   -0.563  15.9994
    12         H     1  DOH     HAV    10    0.407   1.0080
;sum of charge = 0

[ bonds ]
; ai  aj  fu    c0, c1, ...
   2   1    1     0.153   0.33470E+06 ;   CAB  CAA
   2   3    1     0.153   0.33470E+06 ;   CAB  CAC
   3   4    1     0.153   0.33470E+06 ;   CAC  CAD
   4   5    1     0.153   0.33470E+06 ;   CAD  CAE
   5   6    1     0.153   0.33470E+06 ;   CAE  CAF
   6   7    1     0.153   0.33470E+06 ;   CAF  CAG
   7   8    1     0.153   0.33470E+06 ;   CAG  CAH
   8   9    1     0.153   0.33470E+06 ;   CAH  CAI
   9  10    1     0.153   0.33470E+06 ;   CAI  CAJ
  10  11    1     0.123   0.50210E+06 ;   CAJ  OAK
  11  12    1     0.100   15700000.0    ;   OAK  HAV

[ pairs ]
; ai  aj  fu    c0, c1, ...
   1   4   1                                ;   CAA  CAD
   2   5   1                                ;   CAB  CAE
   3   6   1                                ;   CAC  CAF
   4   7   1                                ;   CAD  CAG
   5   8   1                                ;   CAE  CAH
   6   9   1                                ;   CAF  CAI
   7  10   1                                 ;   CAG  CAJ
   8  11   1                                 ;   CAH  OAK
   9  12   1                                 ;   CAI  HAV

[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   1   2   3    1    0.11100E+03 0.46020E+03 ;   CAA  CAB  CAC
   2   3   4    1    0.11100E+03 0.46020E+03 ;   CAB  CAC  CAD
   3   4   5    1    0.11100E+03 0.46020E+03 ;   CAC  CAD  CAE
   4   5   6    1    0.11100E+03 0.46020E+03 ;   CAD  CAE  CAF
   5   6   7    1    0.11100E+03 0.46020E+03 ;   CAE  CAF  CAG
```

```
  6   7   8    1    0.11100E+03 0.46020E+03 ;   CAF  CAG  CAH
  7   8   9    1    0.11100E+03 0.46020E+03 ;   CAG  CAH  CAI
  8   9  10    1    0.11100E+03 0.46020E+03 ;   CAH  CAI  CAJ
  9  10  11    1    0.12100E+03 0.50210E+03 ;   CAI  CAJ  OAK
 10  11  12    1     0.10950E+03 0.39748E+03 ;   CAJ  OAK  HAV

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
  4   3   2   1     3     ;0.0    5.9 3    ; dih   CAD  CAC  CAB  CAA
  5   4   3   2     3     ;0.0    5.9 3    ; dih   CAE  CAD  CAC  CAB
  6   5   4   3     3     ;0.0    5.9 3    ; dih   CAF  CAE  CAD  CAC
  7   6   5   4     3     ;0.0    5.9 3    ; dih   CAG  CAF  CAE  CAD
  8   7   6   5     3     ;0.0    5.9 3    ; dih   CAH  CAG  CAF  CAE
  9   8   7   6     3     ;0.0    5.9 3    ; dih   CAI  CAH  CAG  CAF
 10   9   8   7     3     ;0.0    5.9 3    ; dih   CAJ  CAI  CAH  CAG
 11  10   9   8    1      0.0    1.255 3  ; dih   OAK  CAJ  CAI  CAH
  9  10  11  12   1      0.0    1.255 3  ; dih   CAI  CAJ  OAK  HAV
```