# (+/-) - [1S-(1«beta»,4«beta»,4a«beta»,6«alpha»,8a«alpha»,8a-decahydro-1,6-naphthalenediol

**Inchi:** InChI=1S/C15H28O2/c1-10(2)11-5-8-15(4,17)13-6-7-14(3,16)9-12(11)13/h10-13,16-17H,5-9H2,1-4H3/t11-,12+,13+,14+,15+/m1/s1

**InchiKey:** PNPPFTXWBZJPGW-AHDPXTMNSA-N

**Formula:** C15H28O2

**SMILES:** CC(C)C1CCC(C)(O)C2CCC(C)(O)CC12

**Mol. weight [g/mol]:** 240.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -161.67 | kJ/mol | Joback Method |
| hf | -572.25 | kJ/mol | Joback Method |
| hfus | 17.75 | kJ/mol | Joback Method |
| hvap | 79.24 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 2.971 | | Crippen Method |
| mcvol | 212.230 | ml/mol | McGowan Method |
| pc | 2235.52 | kPa | Joback Method |
| rinpol | 1740.00 | | NIST Webbook |
| tb | 743.55 | K | Joback Method |
| tc | 942.30 | K | Joback Method |
| tf | 422.33 | K | Joback Method |
| vc | 0.782 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 691.30 | J/mol×K | 743.55 | Joback Method |
| cpg | 709.90 | J/mol×K | 776.67 | Joback Method |
| cpg | 728.06 | J/mol×K | 809.80 | Joback Method |
| cpg | 745.95 | J/mol×K | 842.92 | Joback Method |
| cpg | 763.74 | J/mol×K | 876.05 | Joback Method |
| cpg | 781.60 | J/mol×K | 909.17 | Joback Method |
| cpg | 799.70 | J/mol×K | 942.30 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R496541&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |