# 1,15-Pentadecanediol

**Inchi:** InChI=1S/C15H32O2/c16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-17/h16-17H,1-15H2
**InchiKey:** ZBPYFGWSQQFVCJ-UHFFFAOYSA-N
**Formula:** C15H32O2
**SMILES:** OCCCCCCCCCCCCCCCO
**Mol. weight [g/mol]:** 244.41
**CAS:** 14722-40-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -198.22 | kJ/mol | Joback Method |
| hf | -657.39 | kJ/mol | Joback Method |
| hfus | 42.78 | kJ/mol | Joback Method |
| hvap | 82.34 | kJ/mol | Joback Method |
| log10ws | -4.63 | | Crippen Method |
| logp | 4.042 | | Crippen Method |
| mcvol | 233.950 | ml/mol | McGowan Method |
| pc | 1633.81 | kPa | Joback Method |
| tb | 726.96 | K | Joback Method |
| tc | 892.82 | K | Joback Method |
| tf | 359.90 ± 1.50 | K | NIST Webbook |
| tf | 361.20 | K | Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect |
| vc | 0.913 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 708.97 | J/mol×K | 726.96 | Joback Method |
| cpg | 723.91 | J/mol×K | 754.60 | Joback Method |
| cpg | 738.21 | J/mol×K | 782.25 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 751.86 | J/mol×K | 809.89 | Joback Method |
| cpg | 764.91 | J/mol×K | 837.54 | Joback Method |
| cpg | 777.37 | J/mol×K | 865.18 | Joback Method |
| cpg | 789.27 | J/mol×K | 892.82 | Joback Method |
| dvisc | 0.0053326 | Pa×s | 380.45 | Joback Method |
| dvisc | 0.0008919 | Pa×s | 438.20 | Joback Method |
| dvisc | 0.0002263 | Pa×s | 495.95 | Joback Method |
| dvisc | 0.0000764 | Pa×s | 553.71 | Joback Method |
| dvisc | 0.0000317 | Pa×s | 611.46 | Joback Method |
| dvisc | 0.0000153 | Pa×s | 669.21 | Joback Method |
| dvisc | 0.0000083 | Pa×s | 726.96 | Joback Method |
| hfust | 23.60 | kJ/mol | 361.40 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 2.64185e+01 |
| Coeff. B | -9.95723e+03 |
| Coeff. C | -1.19668e+02 |
| Temperature range (K), min. | 500.72 |
| Temperature range (K), max. | 591.42 |

# Sources

| | |
|---|---|
| **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=C14722408&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect:** | https://www.doi.org/10.1016/j.jct.2013.08.019 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |