# 2-epi-Prezizanoic acid

**Inchi:** InChI=1S/C15H22O2/c1-9-10-6-7-15(8-10)11(13(16)17)4-5-12(15)14(9,2)3/h10-12H,1,4-
**InchiKey:** ANQAQROTXVSMMN-OZTPJHRESA-N
**Formula:** C15H22O2
**SMILES:** C=C1C2CCC3(C2)C(C(=O)O)CCC3C1(C)C
**Mol. weight [g/mol]:** 234.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -5.59 | kJ/mol | Joback Method |
| hf | -337.62 | kJ/mol | Joback Method |
| hfus | 18.89 | kJ/mol | Joback Method |
| hvap | 69.73 | kJ/mol | Joback Method |
| log10ws | -3.53 | | Crippen Method |
| logp | 3.480 | | Crippen Method |
| mcvol | 192.770 | ml/mol | McGowan Method |
| pc | 2450.74 | kPa | Joback Method |
| rinpol | 1884.00 | | NIST Webbook |
| rinpol | 1884.00 | | NIST Webbook |
| tb | 707.71 | K | Joback Method |
| tc | 921.86 | K | Joback Method |
| tf | 469.34 | K | Joback Method |
| vc | 0.734 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 596.02 | J/mol×K | 707.71 | Joback Method |
| cpg | 613.45 | J/mol×K | 743.40 | Joback Method |
| cpg | 630.39 | J/mol×K | 779.09 | Joback Method |
| cpg | 647.10 | J/mol×K | 814.78 | Joback Method |
| cpg | 663.83 | J/mol×K | 850.48 | Joback Method |
| cpg | 680.83 | J/mol×K | 886.17 | Joback Method |
| cpg | 698.35 | J/mol×K | 921.86 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=R516219&Units=SI |

# 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 |