# «beta»-Acorenol

**Inchi:** InChI=1S/C15H26O/c1-11-7-9-15(10-8-11)12(2)5-6-13(15)14(3,4)16/h12-13,16H,1,5-10H
**InchiKey:** ZHMYLLJMCGLTQY-PZORYLMUSA-N
**Formula:** C15H26O
**SMILES:** C=C1CCC2(CC1)C(C)CCC2C(C)(C)O
**Mol. weight [g/mol]:** 222.37

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 54.42 | kJ/mol | Joback Method |
| hf | -313.81 | kJ/mol | Joback Method |
| hfus | 12.76 | kJ/mol | Joback Method |
| hvap | 63.58 | kJ/mol | Joback Method |
| log10ws | -4.39 | | Crippen Method |
| logp | 3.920 | | Crippen Method |
| mcvol | 202.060 | ml/mol | McGowan Method |
| pc | 2151.31 | kPa | Joback Method |
| rinpol | 1639.00 | | NIST Webbook |
| rinpol | 1635.00 | | NIST Webbook |
| rinpol | 1636.00 | | NIST Webbook |
| rinpol | 1636.00 | | NIST Webbook |
| rinpol | 1637.00 | | NIST Webbook |
| rinpol | 1637.00 | | NIST Webbook |
| rinpol | 1615.00 | | NIST Webbook |
| rinpol | 1635.00 | | NIST Webbook |
| rinpol | 1637.00 | | NIST Webbook |
| rinpol | 1633.00 | | NIST Webbook |
| rinpol | 1634.00 | | NIST Webbook |
| rinpol | 1633.00 | | NIST Webbook |
| rinpol | 1588.00 | | NIST Webbook |
| ripol | 2212.00 | | NIST Webbook |
| ripol | 2212.00 | | NIST Webbook |
| ripol | 2149.00 | | NIST Webbook |
| ripol | 2149.00 | | NIST Webbook |
| tb | 656.84 | K | Joback Method |
| tc | 868.05 | K | Joback Method |
| tf | 377.19 | K | Joback Method |
| vc | 0.747 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 597.18 | J/mol×K | 656.84 | Joback Method |
| cpg | 617.32 | J/mol×K | 692.04 | Joback Method |
| cpg | 636.34 | J/mol×K | 727.24 | Joback Method |
| cpg | 654.38 | J/mol×K | 762.45 | Joback Method |
| cpg | 671.60 | J/mol×K | 797.65 | Joback Method |
| cpg | 688.14 | J/mol×K | 832.85 | Joback Method |
| cpg | 704.15 | J/mol×K | 868.05 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R286087&Units=SI
**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

# 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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume