# humulan-1,6-dien-3-ol

**Inchi:** InChI=1S/C15H26O/c1-12-6-5-10-15(3,4)11-9-13(2)14(16)8-7-12/h7,9,11,13-14,16H,5-6,
**InchiKey:** DRAXKQKWFHOAHF-WEYIAPCQSA-N
**Formula:** C15H26O
**SMILES:** CC1=CCC(O)C(C)C=CC(C)(C)CCC1
**Mol. weight [g/mol]:** 222.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -68.07 | kJ/mol | Joback Method |
| hf | -402.99 | kJ/mol | Joback Method |
| hfus | 17.93 | kJ/mol | Joback Method |
| hvap | 66.43 | kJ/mol | Joback Method |
| log10ws | -4.60 | | Crippen Method |
| logp | 4.086 | | Crippen Method |
| mcvol | 208.620 | ml/mol | McGowan Method |
| pc | 2066.12 | kPa | Joback Method |
| rinpol | 1655.00 | | NIST Webbook |
| tb | 669.88 | K | Joback Method |
| tc | 884.88 | K | Joback Method |
| tf | 338.87 | K | Joback Method |
| vc | 0.755 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 599.52 | J/mol×K | 669.88 | Joback Method |
| cpg | 621.01 | J/mol×K | 705.71 | Joback Method |
| cpg | 641.36 | J/mol×K | 741.55 | Joback Method |
| cpg | 660.64 | J/mol×K | 777.38 | Joback Method |
| cpg | 678.92 | J/mol×K | 813.22 | Joback Method |
| cpg | 696.28 | J/mol×K | 849.05 | Joback Method |
| cpg | 712.77 | J/mol×K | 884.88 | 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=R285400&Units=SI |

# Legend

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|---|---|
| **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 |