

6-Hydroxycaryophyllene

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| Other names: | Caryophyllene, 6-hydroxy- |
| Inchi: | InChI=1S/C15H24O/c1-10-5-6-14-13(9-15(14,3)4)11(2)8-12(16)7-10/h7,12-14,16H,2,5-6 |
| InchiKey: | DJGZASXOWNHOFE-MNUBBZDBSA-N |
| Formula: | C15H24O |
| SMILES: | <chem>C=C1CC(O)C=C(C)CCC2C1CC2(C)C</chem> |
| Mol. weight [g/mol]: | 220.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 52.10 | kJ/mol | Joback Method |
| hf | -285.25 | kJ/mol | Joback Method |
| hfus | 19.98 | kJ/mol | Joback Method |
| hvap | 65.69 | kJ/mol | Joback Method |
| log10ws | -4.25 | | Crippen Method |
| logp | 3.696 | | Crippen Method |
| mcvol | 197.760 | ml/mol | McGowan Method |
| pc | 2139.38 | kPa | Joback Method |
| rinpol | 1643.00 | | NIST Webbook |
| rinpol | 1649.00 | | NIST Webbook |
| ripol | 2346.00 | | NIST Webbook |
| ripol | 2346.00 | | NIST Webbook |
| ripol | 2346.00 | | NIST Webbook |
| tb | 663.81 | K | Joback Method |
| tc | 872.81 | K | Joback Method |
| tf | 380.29 | K | Joback Method |
| vc | 0.735 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 576.12 | J/molxK | 663.81 | Joback Method |
| cpg | 595.62 | J/molxK | 698.64 | Joback Method |
| cpg | 614.14 | J/molxK | 733.48 | Joback Method |
| cpg | 631.79 | J/molxK | 768.31 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 648.66 | J/mol×K | 803.14 | Joback Method |
| cpg | 664.87 | J/mol×K | 837.98 | Joback Method |
| cpg | 680.52 | J/mol×K | 872.81 | Joback Method |

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=R275037&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| mvol: | 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 |

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<https://www.chemeo.com/cid/44-809-5/6-Hydroxycaryophyllene.pdf>

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