# 14-Hydroxy-«beta»-caryophyllene acetate

**Inchi:** InChI=1S/C17H26O2/c1-12-6-5-7-14(11-19-13(2)18)8-9-16-15(12)10-17(16,3)4/h7,15-16
**InchiKey:** XLKYRVILZQUEJC-IAGRGRHTSA-N
**Formula:** C17H26O2
**SMILES:** C=C1CCC=C(COC(C)=O)CCC2C1CC2(C)C
**Mol. weight [g/mol]:** 262.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -20.45 | kJ/mol | Joback Method |
| hf | -398.76 | kJ/mol | Joback Method |
| hfus | 22.79 | kJ/mol | Joback Method |
| hvap | 62.93 | kJ/mol | Joback Method |
| log10ws | -4.57 | | Crippen Method |
| logp | 4.268 | | Crippen Method |
| mcvol | 227.510 | ml/mol | McGowan Method |
| pc | 1784.86 | kPa | Joback Method |
| rinpol | 1807.00 | | NIST Webbook |
| rinpol | 1807.00 | | NIST Webbook |
| tb | 698.35 | K | Joback Method |
| tc | 919.73 | K | Joback Method |
| tf | 418.41 | K | Joback Method |
| vc | 0.853 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 669.66 | J/mol×K | 698.35 | Joback Method |
| cpg | 691.18 | J/mol×K | 735.25 | Joback Method |
| cpg | 711.58 | J/mol×K | 772.14 | Joback Method |
| cpg | 730.98 | J/mol×K | 809.04 | Joback Method |
| cpg | 749.50 | J/mol×K | 845.93 | Joback Method |
| cpg | 767.26 | J/mol×K | 882.83 | Joback Method |
| cpg | 784.38 | J/mol×K | 919.73 | Joback Method |

# Sources

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|---|---|
| **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=R618969&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |