# Desoxycohumulone

**Inchi:** InChI=1S/C20H28O4/c1-11(2)7-9-14-18(22)15(10-8-12(3)4)20(24)16(19(14)23)17(21)13
**InchiKey:** KKFIZYKKQLWBKH-UHFFFAOYSA-N
**Formula:** C20H28O4
**SMILES:** CC(C)=CCc1c(O)c(CC=C(C)C)c(O)c(C(=O)C(C)C)c1O
**Mol. weight [g/mol]:** 332.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -241.21 | kJ/mol | Joback Method |
| hf | -677.47 | kJ/mol | Joback Method |
| hfus | 54.03 | kJ/mol | Joback Method |
| hvap | 109.19 | kJ/mol | Joback Method |
| log10ws | -5.20 | | Crippen Method |
| logp | 4.660 | | Crippen Method |
| mcvol | 279.480 | ml/mol | McGowan Method |
| pc | 2056.76 | kPa | Joback Method |
| rinpol | 2317.00 | | NIST Webbook |
| rinpol | 2317.00 | | NIST Webbook |
| tb | 997.01 | K | Joback Method |
| tc | 1235.35 | K | Joback Method |
| tf | 698.63 | K | Joback Method |
| vc | 0.907 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 920.20 | J/mol×K | 997.01 | Joback Method |
| cpg | 939.76 | J/mol×K | 1036.73 | Joback Method |
| cpg | 960.15 | J/mol×K | 1076.46 | Joback Method |
| cpg | 981.61 | J/mol×K | 1116.18 | Joback Method |
| cpg | 1004.42 | J/mol×K | 1155.91 | Joback Method |
| cpg | 1028.84 | J/mol×K | 1195.63 | Joback Method |
| cpg | 1055.11 | J/mol×K | 1235.35 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R97036&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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