# 3«beta»-hydroxy-manool

**Inchi:** InChI=1S/C20H34O2/c1-7-19(5,22)11-9-15-8-10-18(3,4)17-12-16(21)14(2)13-20(15,17)6
**InchiKey:** PHBWMJAQSYRNTB-LSUMQRJUSA-N
**Formula:** C20H34O2
**SMILES:** C=CC(C)(O)CCC1CCC(C)(C)C2CC(O)C(=C)CC12C
**Mol. weight [g/mol]:** 306.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 26.63 | kJ/mol | Joback Method |
| hf | -469.25 | kJ/mol | Joback Method |
| hfus | 24.37 | kJ/mol | Joback Method |
| hvap | 88.95 | kJ/mol | Joback Method |
| log10ws | -5.48 | | Crippen Method |
| logp | 4.473 | | Crippen Method |
| mcvol | 274.080 | ml/mol | McGowan Method |
| pc | 1570.96 | kPa | Joback Method |
| rinpol | 2295.00 | | NIST Webbook |
| tb | 851.00 | K | Joback Method |
| tc | 1054.41 | K | Joback Method |
| tf | 508.02 | K | Joback Method |
| vc | 1.022 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 936.83 | J/mol×K | 851.00 | Joback Method |
| cpg | 957.92 | J/mol×K | 884.90 | Joback Method |
| cpg | 979.01 | J/mol×K | 918.80 | Joback Method |
| cpg | 1000.30 | J/mol×K | 952.71 | Joback Method |
| cpg | 1022.02 | J/mol×K | 986.61 | Joback Method |
| cpg | 1044.37 | J/mol×K | 1020.51 | Joback Method |
| cpg | 1067.56 | J/mol×K | 1054.41 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R333465&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |