# 3,6-dihydroxy-megastigm-7-en-9-ol

**Inchi:** InChI=1S/C13H24O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-6,9-11,14-16H,7-8H
**InchiKey:** OJGKTHCXUFNMIQ-AATRIKPKSA-N
**Formula:** C13H24O3
**SMILES:** CC(O)C=CC1(O)C(C)CC(O)CC1(C)C
**Mol. weight [g/mol]:** 228.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -283.76 | kJ/mol | Joback Method |
| hf | -632.62 | kJ/mol | Joback Method |
| hfus | 20.82 | kJ/mol | Joback Method |
| hvap | 91.34 | kJ/mol | Joback Method |
| log10ws | -2.66 | | Crippen Method |
| logp | 1.472 | | Crippen Method |
| mcvol | 196.480 | ml/mol | McGowan Method |
| pc | 2673.54 | kPa | Joback Method |
| ripol | 3100.00 | | NIST Webbook |
| ripol | 3100.00 | | NIST Webbook |
| tb | 783.12 | K | Joback Method |
| tc | 972.86 | K | Joback Method |
| tf | 441.11 | K | Joback Method |
| vc | 0.721 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 630.58 | J/mol×K | 783.12 | Joback Method |
| cpg | 645.42 | J/mol×K | 814.74 | Joback Method |
| cpg | 660.20 | J/mol×K | 846.37 | Joback Method |
| cpg | 675.06 | J/mol×K | 877.99 | Joback Method |
| cpg | 690.13 | J/mol×K | 909.61 | Joback Method |
| cpg | 705.57 | J/mol×K | 941.23 | Joback Method |
| cpg | 721.51 | J/mol×K | 972.86 | Joback Method |

# Sources

| | |
|---|---|
| **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=R332917&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |