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

**Inchi:** InChI=1S/C13H22O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-6,9,11,15-16H,7-8H
**InchiKey:** CWLKAPCFJXJCEO-AATRIKPKSA-N
**Formula:** C13H22O3
**SMILES:** CC(=O)C=CC1(O)C(C)CC(O)CC1(C)C
**Mol. weight [g/mol]:** 226.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -273.42 | kJ/mol | Joback Method |
| hf | -587.69 | kJ/mol | Joback Method |
| hfus | 21.86 | kJ/mol | Joback Method |
| hvap | 81.79 | kJ/mol | Joback Method |
| log10ws | -2.56 | | Crippen Method |
| logp | 1.680 | | Crippen Method |
| mcvol | 192.180 | ml/mol | McGowan Method |
| pc | 2574.11 | kPa | Joback Method |
| ripol | 3118.00 | | NIST Webbook |
| ripol | 3118.00 | | NIST Webbook |
| tb | 745.25 | K | Joback Method |
| tc | 942.41 | K | Joback Method |
| tf | 445.22 | K | Joback Method |
| vc | 0.714 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 587.14 | J/mol×K | 745.25 | Joback Method |
| cpg | 602.16 | J/mol×K | 778.11 | Joback Method |
| cpg | 616.96 | J/mol×K | 810.97 | Joback Method |
| cpg | 631.69 | J/mol×K | 843.83 | Joback Method |
| cpg | 646.51 | J/mol×K | 876.69 | Joback Method |
| cpg | 661.56 | J/mol×K | 909.55 | Joback Method |
| cpg | 677.01 | J/mol×K | 942.41 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R332922&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |