# megastigman-3,9-diol

**Inchi:** InChI=1S/C13H26O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h9-12,14-15H,5-8H2,1-4H
**InchiKey:** YLDOBTZIBQRAPU-UHFFFAOYSA-N
**Formula:** C13H26O2
**SMILES:** CC(O)CCC1C(C)CC(O)CC1(C)C
**Mol. weight [g/mol]:** 214.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -221.67 | kJ/mol | Joback Method |
| hf | -612.85 | kJ/mol | Joback Method |
| hfus | 22.83 | kJ/mol | Joback Method |
| hvap | 75.85 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 2.581 | | Crippen Method |
| mcvol | 194.910 | ml/mol | McGowan Method |
| pc | 2218.71 | kPa | Joback Method |
| ripol | 2651.00 | | NIST Webbook |
| ripol | 2651.00 | | NIST Webbook |
| tb | 686.54 | K | Joback Method |
| tc | 868.74 | K | Joback Method |
| tf | 361.47 | K | Joback Method |
| vc | 0.724 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 594.74 | J/mol×K | 686.54 | Joback Method |
| cpg | 611.14 | J/mol×K | 716.91 | Joback Method |
| cpg | 626.87 | J/mol×K | 747.27 | Joback Method |
| cpg | 641.99 | J/mol×K | 777.64 | Joback Method |
| cpg | 656.57 | J/mol×K | 808.01 | Joback Method |
| cpg | 670.66 | J/mol×K | 838.37 | Joback Method |
| cpg | 684.34 | J/mol×K | 868.74 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R333054&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

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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 |