# Modhephen-8«beta»-ol

**Inchi:** InChI=1S/C15H24O/c1-11-10-12(2,3)14-6-5-7-15(11,14)13(4,16)8-9-14/h10,16H,5-9H2,1
**InchiKey:** WAFFJCDTFBFQCN-KKUMJFAQSA-N
**Formula:** C15H24O
**SMILES:** CC1=CC(C)(C)C23CCCC12C(C)(O)CC3
**Mol. weight [g/mol]:** 220.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 87.31 | kJ/mol | Joback Method |
| hf | -212.15 | kJ/mol | Joback Method |
| hfus | 5.61 | kJ/mol | Joback Method |
| hvap | 61.79 | kJ/mol | Joback Method |
| log10ws | -4.29 | | Crippen Method |
| logp | 3.674 | | Crippen Method |
| mcvol | 191.200 | ml/mol | McGowan Method |
| pc | 2608.40 | kPa | Joback Method |
| rinpol | 1514.00 | | NIST Webbook |
| tb | 663.97 | K | Joback Method |
| tc | 887.90 | K | Joback Method |
| tf | 471.05 | K | Joback Method |
| vc | 0.727 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 565.30 | J/mol×K | 663.97 | Joback Method |
| cpg | 583.16 | J/mol×K | 701.29 | Joback Method |
| cpg | 600.73 | J/mol×K | 738.61 | Joback Method |
| cpg | 618.48 | J/mol×K | 775.94 | Joback Method |
| cpg | 636.91 | J/mol×K | 813.26 | Joback Method |
| cpg | 656.50 | J/mol×K | 850.58 | Joback Method |
| cpg | 677.73 | J/mol×K | 887.90 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R641444&Units=SI |

# 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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