# 6,10-epoxybisabol-3-en-12-al

**Inchi:** InChI=1S/C15H24O2/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)17-15(13)8-10/h4,9,11-15H,5-
**InchiKey:** NPSHXIOPYGVQEX-SHIHICALSA-N
**Formula:** C15H24O2
**SMILES:** CC1=CCC2C(C)CCC(C(C)C=O)OC2C1
**Mol. weight [g/mol]:** 236.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -46.75 | kJ/mol | Joback Method |
| hf | -455.36 | kJ/mol | Joback Method |
| hfus | 30.10 | kJ/mol | Joback Method |
| hvap | 60.85 | kJ/mol | Joback Method |
| log10ws | -3.61 | | Crippen Method |
| logp | 3.361 | | Crippen Method |
| mcvol | 203.630 | ml/mol | McGowan Method |
| pc | 1984.12 | kPa | Joback Method |
| rinpol | 1675.00 | | NIST Webbook |
| rinpol | 1675.00 | | NIST Webbook |
| tb | 647.40 | K | Joback Method |
| tc | 867.03 | K | Joback Method |
| tf | 335.46 | K | Joback Method |
| vc | 0.765 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 592.44 | J/mol×K | 647.40 | Joback Method |
| cpg | 689.69 | J/mol×K | 830.42 | Joback Method |
| cpg | 672.93 | J/mol×K | 793.82 | Joback Method |
| cpg | 654.86 | J/mol×K | 757.21 | Joback Method |
| cpg | 635.44 | J/mol×K | 720.61 | Joback Method |
| cpg | 614.65 | J/mol×K | 684.00 | Joback Method |
| cpg | 705.18 | J/mol×K | 867.03 | Joback Method |
| dvisc | 0.0003630 | Pa×s | 647.40 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004488 | Pa×s | 595.41 | Joback Method |
| dvisc | 0.0005779 | Pa×s | 543.42 | Joback Method |
| dvisc | 0.0007849 | Pa×s | 491.43 | Joback Method |
| dvisc | 0.0011462 | Pa×s | 439.44 | Joback Method |
| dvisc | 0.0018530 | Pa×s | 387.45 | Joback Method |
| dvisc | 0.0034763 | Pa×s | 335.46 | 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=R233548&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |