# 1-Butyn-3-one, 1-(6,6-dimethyl-1,2-epoxycyclohexyl)-

**Inchi:** InChI=1S/C12H16O2/c1-9(13)6-8-12-10(14-12)5-4-7-11(12,2)3/h10H,4-5,7H2,1-3H3
**InchiKey:** ITPNMZLJZQEEOU-UHFFFAOYSA-N
**Formula:** C12H16O2
**SMILES:** CC(=O)C#CC12OC1CCCC2(C)C
**Mol. weight [g/mol]:** 192.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 128.63 | kJ/mol | Joback Method |
| hf | -113.71 | kJ/mol | Joback Method |
| hfus | 22.18 | kJ/mol | Joback Method |
| hvap | 53.10 | kJ/mol | Joback Method |
| log10ws | -2.78 | | Crippen Method |
| logp | 1.926 | | Crippen Method |
| mcvol | 157.060 | ml/mol | McGowan Method |
| pc | 3038.96 | kPa | Joback Method |
| rinpol | 1462.00 | | NIST Webbook |
| rinpol | 1462.00 | | NIST Webbook |
| tb | 577.34 | K | Joback Method |
| tc | 821.61 | K | Joback Method |
| tf | 483.52 | K | Joback Method |
| vc | 0.598 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 404.63 | J/mol×K | 577.34 | Joback Method |
| cpg | 421.77 | J/mol×K | 618.05 | Joback Method |
| cpg | 437.67 | J/mol×K | 658.76 | Joback Method |
| cpg | 452.69 | J/mol×K | 699.47 | Joback Method |
| cpg | 467.14 | J/mol×K | 740.18 | Joback Method |
| cpg | 481.38 | J/mol×K | 780.89 | Joback Method |
| cpg | 495.73 | J/mol×K | 821.61 | 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=U196972&Units=SI |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |