# 4-hydroxy-4-(3-oxo-1-butynyl)-3,5,5-trimethylcyclo

**Inchi:** InChI=1S/C13H16O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h7,16H,8H2,1-4H3
**InchiKey:** OIUCJUSKOSEUNB-UHFFFAOYSA-N
**Formula:** C13H16O3
**SMILES:** CC(=O)C#CC1(O)C(C)=CC(=O)CC1(C)C
**Mol. weight [g/mol]:** 220.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -100.86 | kJ/mol | Joback Method |
| hf | -331.09 | kJ/mol | Joback Method |
| hfus | 18.89 | kJ/mol | Joback Method |
| hvap | 73.13 | kJ/mol | Joback Method |
| log10ws | -2.50 | | Crippen Method |
| logp | 1.255 | | Crippen Method |
| mcvol | 179.280 | ml/mol | McGowan Method |
| pc | 2976.29 | kPa | Joback Method |
| rinpol | 1649.00 | | NIST Webbook |
| rinpol | 1649.00 | | NIST Webbook |
| tb | 739.21 | K | Joback Method |
| tc | 974.09 | K | Joback Method |
| tf | 585.56 | K | Joback Method |
| vc | 0.671 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 502.46 | J/mol×K | 739.21 | Joback Method |
| cpg | 517.77 | J/mol×K | 778.36 | Joback Method |
| cpg | 532.94 | J/mol×K | 817.50 | Joback Method |
| cpg | 548.17 | J/mol×K | 856.65 | Joback Method |
| cpg | 563.66 | J/mol×K | 895.80 | Joback Method |
| cpg | 579.63 | J/mol×K | 934.95 | Joback Method |
| cpg | 596.28 | J/mol×K | 974.09 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R218772&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |