# 2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-4-(3-oxo-1-butenyl)-

**Other names:** 4-Hydroxy-3,5,5-trimethyl-4-[3-oxo-1-butenyl]-2-cyclohexen-1-one
2-Cyclohexen-1-one-4-ol, 3,5,5-trimethyl-4-(3-oxo-1-butenyl)
4-Hydroxy-4-(3-oxo-1-butenyl)-3,5,5-trimethylcyclohex-2-en-1-one

**Inchi:** InChI=1S/C13H18O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-7,16H,8H2,1-4H3/b

**InchiKey:** JJRYPZMXNLLZFH-AATRIKPKSA-N

**Formula:** C13H18O3

**SMILES:** CC(=O)C=CC1(O)C(C)=CC(=O)CC1(C)C

**Mol. weight [g/mol]:** 222.28

**CAS:** 7070-24-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -223.44 | kJ/mol | Joback Method |
| hf | -486.17 | kJ/mol | Joback Method |
| hfus | 15.97 | kJ/mol | Joback Method |
| hvap | 70.93 | kJ/mol | Joback Method |
| log10ws | -2.56 | | Crippen Method |
| logp | 1.808 | | Crippen Method |
| mcvol | 183.580 | ml/mol | McGowan Method |
| pc | 2654.29 | kPa | Joback Method |
| rinpol | 1729.00 | | NIST Webbook |
| rinpol | 1729.00 | | NIST Webbook |
| rinpol | 1760.00 | | NIST Webbook |
| rinpol | 1757.00 | | NIST Webbook |
| rinpol | 1760.00 | | NIST Webbook |
| tb | 734.37 | K | Joback Method |
| tc | 955.11 | K | Joback Method |
| tf | 474.38 | K | Joback Method |
| vc | 0.690 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 525.71 | J/mol×K | 734.37 | Joback Method |

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|---|---|---|---|---|
| cpg | 540.92 | J/mol×K | 771.16 | Joback Method |
| cpg | 555.92 | J/mol×K | 807.95 | Joback Method |
| cpg | 570.90 | J/mol×K | 844.74 | Joback Method |
| cpg | 586.06 | J/mol×K | 881.53 | Joback Method |
| cpg | 601.58 | J/mol×K | 918.32 | Joback Method |
| cpg | 617.66 | J/mol×K | 955.11 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C7070248&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |