# 3-Oxa-2,2,4-trimethyl-4-vinylcyclohexanone

**Inchi:** InChI=1S/C11H16O2/c1-5-11(4)7-6-8(12)10(2,3)9(11)13/h5H,1,6-7H2,2-4H3
**InchiKey:** YLXCTKJCLZSLPF-UHFFFAOYSA-N
**Formula:** C11H16O2
**SMILES:** C=CC1(C)CCC(=O)C(C)(C)C1=O
**Mol. weight [g/mol]:** 180.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -109.84 | kJ/mol | Joback Method |
| hf | -355.88 | kJ/mol | Joback Method |
| hfus | 2.30 | kJ/mol | Joback Method |
| hvap | 45.72 | kJ/mol | Joback Method |
| log10ws | -2.25 | | Crippen Method |
| logp | 2.137 | | Crippen Method |
| mcvol | 153.830 | ml/mol | McGowan Method |
| pc | 2770.08 | kPa | Joback Method |
| rinpol | 1108.00 | | NIST Webbook |
| rinpol | 1108.00 | | NIST Webbook |
| tb | 598.76 | K | Joback Method |
| tc | 846.45 | K | Joback Method |
| tf | 399.35 | K | Joback Method |
| vc | 0.575 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 398.94 | J/mol×K | 598.76 | Joback Method |
| cpg | 417.41 | J/mol×K | 640.04 | Joback Method |
| cpg | 434.97 | J/mol×K | 681.32 | Joback Method |
| cpg | 451.85 | J/mol×K | 722.61 | Joback Method |
| cpg | 468.25 | J/mol×K | 763.89 | Joback Method |
| cpg | 484.37 | J/mol×K | 805.17 | Joback Method |
| cpg | 500.42 | J/mol×K | 846.45 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R432790&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 |