# 3-Buten-2-one, 4-(1,2,6,6-tetramethyl-2-cyclohexen-1-yl)-

**Other names:** 4-(1,2,6,6-Tetramethyl-2-cyclohexen-1-yl)-3-buten-2-one
6-Methyl-«alpha»-(E)-ionone

**Inchi:** InChI=1S/C14H22O/c1-11-7-6-9-13(3,4)14(11,5)10-8-12(2)15/h7-8,10H,6,9H2,1-5H3/b10

**InchiKey:** MOLZHSROFREFLG-CSKARUKUSA-N

**Formula:** C14H22O

**SMILES:** CC(=O)C=CC1(C)C(C)=CCCC1(C)C

**Mol. weight [g/mol]:** 206.32

**CAS:** 107815-05-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 44.39 | kJ/mol | Joback Method |
| hf | -216.88 | kJ/mol | Joback Method |
| hfus | 14.96 | kJ/mol | Joback Method |
| hvap | 52.23 | kJ/mol | Joback Method |
| log10ws | -4.08 | | Crippen Method |
| logp | 3.904 | | Crippen Method |
| mcvol | 190.230 | ml/mol | McGowan Method |
| pc | 2135.43 | kPa | Joback Method |
| rinpol | 1515.00 | | NIST Webbook |
| rinpol | 1497.00 | | NIST Webbook |
| rinpol | 1515.00 | | NIST Webbook |
| rinpol | 1497.00 | | NIST Webbook |
| tb | 597.25 | K | Joback Method |
| tc | 819.93 | K | Joback Method |
| tf | 356.61 | K | Joback Method |
| vc | 0.720 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 487.29 | J/mol×K | 597.25 | Joback Method |
| cpg | 506.21 | J/mol×K | 634.36 | Joback Method |
| cpg | 524.06 | J/mol×K | 671.48 | Joback Method |

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|---|---|---|---|---|
| cpg | 541.08 | J/mol×K | 708.59 | Joback Method |
| cpg | 557.51 | J/mol×K | 745.70 | Joback Method |
| cpg | 573.55 | J/mol×K | 782.81 | Joback Method |
| cpg | 589.46 | J/mol×K | 819.93 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C107815054&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 |