# Pent-4-yn-3-one, 2,2-dimethyl-

**Other names:** 4,4-Dimethyl-1-pentyne-3-one
**Inchi:** InChI=1S/C7H10O/c1-5-6(8)7(2,3)4/h1H,2-4H3
**InchiKey:** XRWYQSOYUZOEQH-UHFFFAOYSA-N
**Formula:** C7H10O
**SMILES:** C#CC(=O)C(C)(C)C
**Mol. weight [g/mol]:** 110.15
**CAS:** 5891-25-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 105.05 | kJ/mol | Joback Method |
| hf | -17.24 | kJ/mol | Joback Method |
| hfus | 11.05 | kJ/mol | Joback Method |
| hvap | 36.48 | kJ/mol | Joback Method |
| ie | 9.75 | eV | NIST Webbook |
| log10ws | -1.59 | | Crippen Method |
| logp | 1.235 | | Crippen Method |
| mcvol | 102.460 | ml/mol | McGowan Method |
| pc | 3628.97 | kPa | Joback Method |
| tb | 400.32 | K | Joback Method |
| tc | 602.82 | K | Joback Method |
| tf | 267.97 | K | Joback Method |
| vc | 0.385 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 191.25 | J/mol×K | 400.32 | Joback Method |
| cpg | 202.41 | J/mol×K | 434.07 | Joback Method |
| cpg | 212.87 | J/mol×K | 467.82 | Joback Method |
| cpg | 222.67 | J/mol×K | 501.57 | Joback Method |
| cpg | 231.84 | J/mol×K | 535.32 | Joback Method |
| cpg | 240.42 | J/mol×K | 569.07 | Joback Method |
| cpg | 248.45 | J/mol×K | 602.82 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5891258&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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |