# 2(5H)-Furanone, 3,5,5-trimethyl-

**Other names:** 2,4,4-Trimethyl-2-butenolide
3,5,5-trimethyl-2(5H)-furanone
**Inchi:** InChI=1S/C7H10O2/c1-5-4-7(2,3)9-6(5)8/h4H,1-3H3
**InchiKey:** OAVLYQLCBORARJ-UHFFFAOYSA-N
**Formula:** C7H10O2
**SMILES:** CC1=CC(C)(C)OC1=O
**Mol. weight [g/mol]:** 126.15
**CAS:** 50598-50-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -149.26 | kJ/mol | Joback Method |
| hf | -335.48 | kJ/mol | Joback Method |
| hfus | 9.84 | kJ/mol | Joback Method |
| hvap | 39.99 | kJ/mol | Joback Method |
| log10ws | -1.48 | | Crippen Method |
| logp | 1.268 | | Crippen Method |
| mcvol | 101.770 | ml/mol | McGowan Method |
| pc | 3819.82 | kPa | Joback Method |
| ripol | 2074.00 | | NIST Webbook |
| ripol | 2074.00 | | NIST Webbook |
| ripol | 2074.00 | | NIST Webbook |
| tb | 473.99 | K | Joback Method |
| tc | 701.21 | K | Joback Method |
| tf | 311.52 | K | Joback Method |
| vc | 0.381 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 219.58 | J/mol×K | 473.99 | Joback Method |
| cpg | 232.11 | J/mol×K | 511.86 | Joback Method |
| cpg | 243.87 | J/mol×K | 549.73 | Joback Method |
| cpg | 254.94 | J/mol×K | 587.60 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 265.41 | J/mol×K | 625.47 | Joback Method |
| cpg | 275.38 | J/mol×K | 663.34 | Joback Method |
| cpg | 284.92 | J/mol×K | 701.21 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C50598500&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |