# Methyl 4-chloro-2,2-dimethyl-4-pentenoate

**Inchi:** InChI=1S/C8H13ClO2/c1-6(9)5-8(2,3)7(10)11-4/h1,5H2,2-4H3
**InchiKey:** NMIYZQVNXZOOPF-UHFFFAOYSA-N
**Formula:** C8H13ClO2
**SMILES:** C=C(Cl)CC(C)(C)C(=O)OC
**Mol. weight [g/mol]:** 176.64
**CAS:** 86799-85-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -147.24 | kJ/mol | Joback Method |
| hf | -362.10 | kJ/mol | Joback Method |
| hfus | 13.46 | kJ/mol | Joback Method |
| hvap | 45.06 | kJ/mol | Joback Method |
| log10ws | -2.29 | | Crippen Method |
| logp | 2.328 | | Crippen Method |
| mcvol | 138.960 | ml/mol | McGowan Method |
| pc | 2738.28 | kPa | Joback Method |
| tb | 489.49 | K | Joback Method |
| tc | 689.10 | K | Joback Method |
| tf | 268.70 | K | Joback Method |
| vc | 0.527 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 293.06 | J/mol×K | 489.49 | Joback Method |
| cpg | 305.45 | J/mol×K | 522.76 | Joback Method |
| cpg | 317.15 | J/mol×K | 556.03 | Joback Method |
| cpg | 328.19 | J/mol×K | 589.29 | Joback Method |
| cpg | 338.60 | J/mol×K | 622.56 | Joback Method |
| cpg | 348.40 | J/mol×K | 655.83 | Joback Method |
| cpg | 357.61 | J/mol×K | 689.10 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C86799851&Units=SI |

# Legend

| | |
|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |