# 4-Methyl-4-heptanolide

**Inchi:** InChI=1S/C8H14O2/c1-3-5-8(2)6-4-7(9)10-8/h3-6H2,1-2H3
**InchiKey:** YSNGVCQTXRIIED-UHFFFAOYSA-N
**Formula:** C8H14O2
**SMILES:** CCCC1(C)CCC(=O)O1
**Mol. weight [g/mol]:** 142.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -161.17 | kJ/mol | Joback Method |
| hf | -402.43 | kJ/mol | Joback Method |
| hfus | 11.60 | kJ/mol | Joback Method |
| hvap | 41.27 | kJ/mol | Joback Method |
| log10ws | -2.04 | | Crippen Method |
| logp | 1.882 | | Crippen Method |
| mcvol | 120.160 | ml/mol | McGowan Method |
| pc | 3322.01 | kPa | Joback Method |
| rinpol | 1150.00 | | NIST Webbook |
| ripol | 1760.00 | | NIST Webbook |
| tb | 492.73 | K | Joback Method |
| tc | 712.64 | K | Joback Method |
| tf | 309.51 | K | Joback Method |
| vc | 0.451 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 277.93 | J/mol×K | 492.73 | Joback Method |
| cpg | 293.32 | J/mol×K | 529.38 | Joback Method |
| cpg | 307.79 | J/mol×K | 566.03 | Joback Method |
| cpg | 321.45 | J/mol×K | 602.68 | Joback Method |
| cpg | 334.37 | J/mol×K | 639.33 | Joback Method |
| cpg | 346.66 | J/mol×K | 675.98 | Joback Method |
| cpg | 358.40 | J/mol×K | 712.64 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R434721&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 |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |