# 3,6-Dimethyl-6-formyl-5,6-dihydropyran

**Inchi:** InChI=1S/C9H14O/c1-4-9(3)6-5-8(2)7-10-9/h4-5H,1,6-7H2,2-3H3
**InchiKey:** VBWAGXIOADKMRE-UHFFFAOYSA-N
**Formula:** C9H14O
**SMILES:** C=CC1(C)CC=C(C)CO1
**Mol. weight [g/mol]:** 138.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 65.91 | kJ/mol | Joback Method |
| hf | -119.79 | kJ/mol | Joback Method |
| hfus | 12.13 | kJ/mol | Joback Method |
| hvap | 39.70 | kJ/mol | Joback Method |
| log10ws | -2.39 | | Crippen Method |
| logp | 2.298 | | Crippen Method |
| mcvol | 124.080 | ml/mol | McGowan Method |
| pc | 3163.27 | kPa | Joback Method |
| ripol | 1709.00 | | NIST Webbook |
| ripol | 1709.00 | | NIST Webbook |
| tb | 452.88 | K | Joback Method |
| tc | 668.72 | K | Joback Method |
| tf | 260.56 | K | Joback Method |
| vc | 0.459 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 258.73 | J/mol×K | 452.88 | Joback Method |
| cpg | 274.74 | J/mol×K | 488.85 | Joback Method |
| cpg | 289.62 | J/mol×K | 524.83 | Joback Method |
| cpg | 303.49 | J/mol×K | 560.80 | Joback Method |
| cpg | 316.46 | J/mol×K | 596.78 | Joback Method |
| cpg | 328.62 | J/mol×K | 632.75 | Joback Method |
| cpg | 340.10 | J/mol×K | 668.72 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R560771&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |