# piperidinone

**Other names:** piperidone
**Inchi:** InChI=1S/C5H9NO/c7-5-3-1-2-4-6-5/h1-4H2,(H,6,7)
**InchiKey:** XUWHAWMETYGRKB-UHFFFAOYSA-N
**Formula:** C5H9NO
**SMILES:** O=C1CCCCN1
**Mol. weight [g/mol]:** 99.13
**CAS:** 27154-43-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -11.50 | kJ/mol | Joback Method |
| hf | -171.76 | kJ/mol | Joback Method |
| hfus | 8.57 | kJ/mol | Joback Method |
| hvap | 38.47 | kJ/mol | Joback Method |
| log10ws | -0.77 | | Crippen Method |
| logp | 0.287 | | Crippen Method |
| mcvol | 82.000 | ml/mol | McGowan Method |
| pc | 5102.04 | kPa | Joback Method |
| ripol | 2124.00 | | NIST Webbook |
| ripol | 2095.00 | | NIST Webbook |
| tb | 454.39 | K | Joback Method |
| tc | 692.75 | K | Joback Method |
| tf | 330.98 | K | Joback Method |
| tt | 342.30 ± 0.01 | K | NIST Webbook |
| vc | 0.293 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 160.54 | J/mol×K | 454.39 | Joback Method |
| cpg | 173.63 | J/mol×K | 494.12 | Joback Method |
| cpg | 186.19 | J/mol×K | 533.84 | Joback Method |
| cpg | 198.19 | J/mol×K | 573.57 | Joback Method |
| cpg | 209.61 | J/mol×K | 613.29 | Joback Method |

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|---|---|---|---|---|
| cpg | 220.43 | J/mol×K | 653.02 | Joback Method |
| cpg | 230.64 | J/mol×K | 692.75 | Joback Method |

# Sources

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|---|---|
| **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=C27154434&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 |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |