# Cyclooctanone, 2-methyl-

**Other names:** 2-Methylcyclooctanone
**Inchi:** InChI=1S/C9H16O/c1-8-6-4-2-3-5-7-9(8)10/h8H,2-7H2,1H3
**InchiKey:** MJFJFHJQZCMMKL-UHFFFAOYSA-N
**Formula:** C9H16O
**SMILES:** CC1CCCCCCC1=O
**Mol. weight [g/mol]:** 140.22
**CAS:** 10363-27-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -97.44 | kJ/mol | Joback Method |
| hf | -324.79 | kJ/mol | Joback Method |
| hfus | 6.21 | kJ/mol | Joback Method |
| hvap | 40.65 | kJ/mol | Joback Method |
| log10ws | -2.52 | | Crippen Method |
| logp | 2.546 | | Crippen Method |
| mcvol | 128.380 | ml/mol | McGowan Method |
| pc | 3114.04 | kPa | Joback Method |
| ripol | 1685.00 | | NIST Webbook |
| ripol | 1685.00 | | NIST Webbook |
| tb | 501.23 | K | Joback Method |
| tc | 735.45 | K | Joback Method |
| tf | 259.75 | K | Joback Method |
| vc | 0.464 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 291.74 | J/mol×K | 501.23 | Joback Method |
| cpg | 312.04 | J/mol×K | 540.27 | Joback Method |
| cpg | 331.36 | J/mol×K | 579.30 | Joback Method |
| cpg | 349.69 | J/mol×K | 618.34 | Joback Method |
| cpg | 367.00 | J/mol×K | 657.38 | Joback Method |
| cpg | 383.26 | J/mol×K | 696.41 | Joback Method |

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|---|---|---|---|---|
| cpg | 398.45 | J/mol×K | 735.45 | Joback Method |

# Sources

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|---|---|
| **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=C10363276&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |