# 2-CYCLOPENTENE-1-CARBOXYLIC ACID, 1-METHYL-

**Inchi:** InChI=1S/C7H10O2/c1-7(6(8)9)4-2-3-5-7/h2,4H,3,5H2,1H3,(H,8,9)
**InchiKey:** HGSACGMRDLYHMZ-UHFFFAOYSA-N
**Formula:** C7H10O2
**SMILES:** CC1(C(=O)O)C=CCC1
**Mol. weight [g/mol]:** 126.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 8.43 | kJ/mol | Joback Method |
| ie | 9.68 | eV | Cheméo Relay (1.0) |
| logp | 1.427 | | Crippen Method |
| mcvol | 101.770 | ml/mol | McGowan Method |
| rinpol | 1085.00 | | NIST Webbook |
| rinpol | 1073.00 | | NIST Webbook |
| rinpol | 1085.00 | | NIST Webbook |
| tb | 473.11 | K | Cheméo Relay (1.0) |
| tf | 334.00 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 232.20 | J/mol×K | 520.29 | Joback Method |
| cpg | 242.80 | J/mol×K | 554.49 | Joback Method |
| cpg | 252.63 | J/mol×K | 588.70 | Joback Method |
| cpg | 261.79 | J/mol×K | 622.90 | Joback Method |
| cpg | 270.39 | J/mol×K | 657.10 | Joback Method |
| cpg | 278.53 | J/mol×K | 691.30 | Joback Method |
| cpg | 286.30 | J/mol×K | 725.51 | Joback Method |

## Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C68317771&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |