# 1-Aminocyclopropanecarboxylic acid, methyl ester

**Other names:** 1-Aminocyclopropanecarboxylic acid, methyl ester
**Inchi:** InChI=1S/C5H9NO2/c1-8-4(7)5(6)2-3-5/h2-3,6H2,1H3
**InchiKey:** CSHMCEYIMFSLSS-UHFFFAOYSA-N
**Formula:** C5H9NO2
**SMILES:** COC(=O)C1(N)CC1
**Mol. weight [g/mol]:** 115.13

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 8.53 | kJ/mol | Joback Method |
| hvap | 51.15 | kJ/mol | Cheméo Relay (1.0) |
| logp | -0.349 | | Crippen Method |
| mcvol | 87.870 | ml/mol | McGowan Method |
| rinpol | 903.70 | | NIST Webbook |
| rinpol | 903.70 | | NIST Webbook |
| tf | 343.24 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 195.45 | J/mol×K | 469.60 | Joback Method |
| cpg | 205.62 | J/mol×K | 505.84 | Joback Method |
| cpg | 214.95 | J/mol×K | 542.08 | Joback Method |
| cpg | 223.55 | J/mol×K | 578.32 | Joback Method |
| cpg | 231.54 | J/mol×K | 614.56 | Joback Method |
| cpg | 239.03 | J/mol×K | 650.80 | Joback Method |
| cpg | 246.13 | J/mol×K | 687.04 | Joback Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

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| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C72784420&Units=SI |
| **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 |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tf:** | Normal melting (fusion) point |

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