# carbamic acid

**Inchi:** InChI=1S/C6H13NO2/c1-6(2,3)4-9-5(7)8/h4H2,1-3H3,(H2,7,8)
**InchiKey:** AFQYFVWMIRMBAE-UHFFFAOYSA-N
**Formula:** C6H13NO2
**SMILES:** CC(C)(C)COC(N)=O
**Mol. weight [g/mol]:** 131.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -164.99 | kJ/mol | Joback Method |
| hf | -386.93 | kJ/mol | Joback Method |
| hfus | 11.87 | kJ/mol | Joback Method |
| hvap | 47.45 | kJ/mol | Joback Method |
| log10ws | -0.80 | | Aqueous Solubility Prediction Method |
| logp | 1.128 | | Crippen Method |
| mcvol | 112.820 | ml/mol | McGowan Method |
| pc | 3577.07 | kPa | Joback Method |
| tb | 482.27 | K | Joback Method |
| tc | 684.80 | K | Joback Method |
| tf | 315.22 | K | Joback Method |
| vc | 0.413 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 254.23 | J/mol×K | 482.27 | Joback Method |
| cpg | 265.78 | J/mol×K | 516.03 | Joback Method |
| cpg | 276.73 | J/mol×K | 549.78 | Joback Method |
| cpg | 287.09 | J/mol×K | 583.54 | Joback Method |
| cpg | 296.88 | J/mol×K | 617.29 | Joback Method |
| cpg | 306.12 | J/mol×K | 651.05 | Joback Method |
| cpg | 314.83 | J/mol×K | 684.80 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |