# 3H-1,4-Benzodiazepin-2-one, 1,2-dihydro-5-methyl-

**Inchi:** InChI=1S/C10H10N2O/c1-7-8-4-2-3-5-9(8)12-10(13)6-11-7/h2-5H,6H2,1H3,(H,12,13)
**InchiKey:** DIDPQMKDRMWTTD-UHFFFAOYSA-N
**Formula:** C10H10N2O
**SMILES:** CC1=NCC(O)=Nc2ccccc21
**Mol. weight [g/mol]:** 174.20
**CAS:** 70656-87-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 317.76 | kJ/mol | Joback Method |
| hf | 138.48 | kJ/mol | Joback Method |
| hfus | 24.20 | kJ/mol | Joback Method |
| hvap | 72.36 | kJ/mol | Joback Method |
| ie | 7.80 | eV | NIST Webbook |
| log10ws | -1.82 | | Crippen Method |
| logp | 2.097 | | Crippen Method |
| mcvol | 134.370 | ml/mol | McGowan Method |
| pc | 4368.40 | kPa | Joback Method |
| tb | 687.67 | K | Joback Method |
| tc | 929.40 | K | Joback Method |
| tf | 487.00 | K | Joback Method |
| vc | 0.518 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 375.21 | J/mol×K | 687.67 | Joback Method |
| cpg | 388.45 | J/mol×K | 727.96 | Joback Method |
| cpg | 400.60 | J/mol×K | 768.25 | Joback Method |
| cpg | 411.66 | J/mol×K | 808.53 | Joback Method |
| cpg | 421.63 | J/mol×K | 848.82 | Joback Method |
| cpg | 430.54 | J/mol×K | 889.11 | Joback Method |
| cpg | 438.38 | J/mol×K | 929.40 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C70656870&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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 |
| **ie:** | Ionization energy |
| **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 |