# 5-Methyl-octahydroazocine

**Inchi:** InChI=1S/C8H17N/c1-8-4-2-6-9-7-3-5-8/h8-9H,2-7H2,1H3
**InchiKey:** ICNQUAIHDUOZGU-UHFFFAOYSA-N
**Formula:** C8H17N
**SMILES:** CC1CCCNCCC1
**Mol. weight [g/mol]:** 127.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 104.44 | kJ/mol | Joback Method |
| hf | -128.64 | kJ/mol | Joback Method |
| hfus | 13.70 | kJ/mol | Joback Method |
| hvap | 40.93 | kJ/mol | Joback Method |
| log10ws | -2.01 | | Crippen Method |
| logp | 1.786 | | Crippen Method |
| mcvol | 122.700 | ml/mol | McGowan Method |
| pc | 3435.91 | kPa | Joback Method |
| rinpol | 940.00 | | NIST Webbook |
| tb | 459.08 | K | Joback Method |
| tc | 685.23 | K | Joback Method |
| tf | 285.29 | K | Joback Method |
| vc | 0.438 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 257.07 | J/mol×K | 459.08 | Joback Method |
| cpg | 277.05 | J/mol×K | 496.77 | Joback Method |
| cpg | 296.06 | J/mol×K | 534.46 | Joback Method |
| cpg | 314.11 | J/mol×K | 572.16 | Joback Method |
| cpg | 331.21 | J/mol×K | 609.85 | Joback Method |
| cpg | 347.35 | J/mol×K | 647.54 | Joback Method |
| cpg | 362.53 | J/mol×K | 685.23 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R405946&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 |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |