# 5H-Dibenz[b,e]azepine, 6,11-dihydro-

**Other names:** Dibenz[b,e]azepin, 5,6(11H)dihydro-
11H-Dibenz[b,E]azepine, 5,6-dihydro-
6,11-dihydro-5H-dibenz[b,e]azepine
**Inchi:** InChI=1S/C14H13N/c1-2-7-13-10-15-14-8-4-3-6-12(14)9-11(13)5-1/h1-8,15H,9-10H2
**InchiKey:** YSHVGIKWUJCBLY-UHFFFAOYSA-N
**Formula:** C14H13N
**SMILES:** c1ccc2c(c1)CNc1ccccc1C2
**Mol. weight [g/mol]:** 195.26
**CAS:** 449-55-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 428.73 | kJ/mol | Joback Method |
| hf | 248.78 | kJ/mol | Joback Method |
| hfus | 25.97 | kJ/mol | Joback Method |
| hvap | 59.61 | kJ/mol | Joback Method |
| log10ws | -3.94 | | Crippen Method |
| logp | 3.203 | | Crippen Method |
| mcvol | 159.720 | ml/mol | McGowan Method |
| pc | 3295.37 | kPa | Joback Method |
| tb | 643.00 | K | Joback Method |
| tc | 905.54 | K | Joback Method |
| tf | 452.63 | K | Joback Method |
| vc | 0.599 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 399.28 | J/mol×K | 643.00 | Joback Method |
| cpg | 416.02 | J/mol×K | 686.76 | Joback Method |
| cpg | 431.36 | J/mol×K | 730.51 | Joback Method |
| cpg | 445.45 | J/mol×K | 774.27 | Joback Method |
| cpg | 458.39 | J/mol×K | 818.03 | Joback Method |
| cpg | 470.32 | J/mol×K | 861.78 | Joback Method |

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|---|---|---|---|---|
| cpg | 481.36 | J/mol×K | 905.54 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C449558&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |