# 3,8-Methanocyclobuta[b]naphthalene,1,2,2a,3,8,8a

**Inchi:** InChI=1S/C13H14/c1-2-4-9-8(3-1)12-7-13(9)11-6-5-10(11)12/h1-4,10-13H,5-7H2/t10-,11
**InchiKey:** SHMYIFLHMQKIPZ-MPZDIEGVSA-N
**Formula:** C13H14
**SMILES:** c1ccc2c(c1)C1CC2C2CCC12
**Mol. weight [g/mol]:** 170.25
**CAS:** 67109-90-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 360.10 | kJ/mol | Joback Method |
| hf | 123.79 | kJ/mol | Joback Method |
| hfus | 22.75 | kJ/mol | Joback Method |
| hvap | 46.56 | kJ/mol | Joback Method |
| ie | 8.60 ± 0.05 | eV | NIST Webbook |
| log10ws | -3.46 | | Crippen Method |
| logp | 3.297 | | Crippen Method |
| mcvol | 137.690 | ml/mol | McGowan Method |
| pc | 2944.08 | kPa | Joback Method |
| tb | 535.51 | K | Joback Method |
| tc | 765.41 | K | Joback Method |
| tf | 331.83 | K | Joback Method |
| vc | 0.541 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 351.57 | J/mol×K | 535.51 | Joback Method |
| cpg | 431.56 | J/mol×K | 727.09 | Joback Method |
| cpg | 418.04 | J/mol×K | 688.78 | Joback Method |
| cpg | 403.44 | J/mol×K | 650.46 | Joback Method |
| cpg | 387.60 | J/mol×K | 612.14 | Joback Method |
| cpg | 370.37 | J/mol×K | 573.83 | Joback Method |
| cpg | 444.16 | J/mol×K | 765.41 | Joback Method |
| dvisc | 0.0031647 | Pa×s | 535.51 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0028948 | Pa×s | 501.56 | Joback Method |
| dvisc | 0.0026139 | Pa×s | 467.62 | Joback Method |
| dvisc | 0.0023228 | Pa×s | 433.67 | Joback Method |
| dvisc | 0.0020232 | Pa×s | 399.72 | Joback Method |
| dvisc | 0.0017176 | Pa×s | 365.78 | Joback Method |
| dvisc | 0.0014101 | Pa×s | 331.83 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C67109904&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |