

Bicyclo[2.2.1]hept-5-ene-2-carbonitrile

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| Other names: | 5-Norbornene-2-carbonitrile 5-Cyanobicyclo[2.2.1]hept-2-ene |
| Inchi: | InChI=1S/C8H9N/c9-5-8-4-6-1-2-7(8)3-6/h1-2,6-8H,3-4H2 |
| InchiKey: | BMAXQTDMWYDIJX-UHFFFAOYSA-N |
| Formula: | C8H9N |
| SMILES: | N#CC1CC2C=CC1C2 |
| Mol. weight [g/mol]: | 119.16 |
| CAS: | 95-11-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 281.31 | kJ/mol | Joback Method |
| hf | 133.31 | kJ/mol | Joback Method |
| hfus | 14.44 | kJ/mol | Joback Method |
| hvap | 43.86 | kJ/mol | Joback Method |
| log10ws | -1.96 | | Crippen Method |
| logp | 1.722 | | Crippen Method |
| mvol | 98.940 | ml/mol | McGowan Method |
| pc | 3368.44 | kPa | Joback Method |
| tb | 496.76 | K | Joback Method |
| tc | 722.79 | K | Joback Method |
| tf | 273.79 | K | Joback Method |
| vc | 0.401 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 224.91 | J/mol×K | 496.76 | Joback Method |
| cpg | 238.38 | J/mol×K | 534.43 | Joback Method |
| cpg | 250.85 | J/mol×K | 572.10 | Joback Method |
| cpg | 262.40 | J/mol×K | 609.78 | Joback Method |
| cpg | 273.10 | J/mol×K | 647.45 | Joback Method |
| cpg | 283.03 | J/mol×K | 685.12 | Joback Method |
| cpg | 292.24 | J/mol×K | 722.79 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|---------------|------|----------------|--------------|
| tbrp | 357.20 | K | 1.30 | NIST Webbook |
| tbrp | 365.00 ± 2.00 | K | 2.70 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C95114&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

| | |
|-----------------|---|
| 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 |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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