

Spiro[8,8-dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalene]

Inchi: InChI=1S/C17H26O/c1-16(2)9-5-6-13-12-17(11-8-14(13)16)10-4-3-7-15(17)18/h3-12H2,
InchiKey: NFEUEVSLYPRIBQ-UHFFFAOYSA-N
Formula: C17H26O
SMILES: CC1(C)CCCC2=C1CCC1(CCCCC1=O)C2
Mol. weight [g/mol]: 246.39

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 86.75 | kJ/mol | Joback Method |
| hf | -264.81 | kJ/mol | Joback Method |
| hfus | 7.88 | kJ/mol | Joback Method |
| hvap | 58.08 | kJ/mol | Joback Method |
| log10ws | -5.27 | | Crippen Method |
| logp | 4.807 | | Crippen Method |
| mcvol | 215.080 | ml/mol | McGowan Method |
| pc | 2171.40 | kPa | Joback Method |
| rinpol | 1943.70 | | NIST Webbook |
| rinpol | 1958.50 | | NIST Webbook |
| rinpol | 1943.70 | | NIST Webbook |
| ripol | 2434.40 | | NIST Webbook |
| ripol | 2459.50 | | NIST Webbook |
| tb | 716.29 | K | Joback Method |
| tc | 976.75 | K | Joback Method |
| tf | 460.11 | K | Joback Method |
| vc | 0.800 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 658.76 | J/molxK | 716.29 | Joback Method |
| cpg | 683.80 | J/molxK | 759.70 | Joback Method |
| cpg | 707.91 | J/molxK | 803.11 | Joback Method |
| cpg | 731.47 | J/molxK | 846.52 | Joback Method |
| cpg | 754.86 | J/molxK | 889.93 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 778.47 | J/mol×K | 933.34 | Joback Method |
| cpg | 802.67 | J/mol×K | 976.75 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R299088&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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