

Cyclopentylethynylmethyl carbinol

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| Inchi: | InChI=1S/C9H14O/c1-3-9(2,10)8-6-4-5-7-8/h1,8,10H,4-7H2,2H3 |
| InchiKey: | POUOCSXBRGBQME-UHFFFAOYSA-N |
| Formula: | C9H14O |
| SMILES: | C#CC(C)(O)C1CCCC1 |
| Mol. weight [g/mol]: | 138.21 |
| CAS: | 100144-29-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 150.54 | kJ/mol | Joback Method |
| hf | -37.69 | kJ/mol | Joback Method |
| hfus | 12.65 | kJ/mol | Joback Method |
| hvap | 51.13 | kJ/mol | Joback Method |
| log10ws | -2.41 | | Crippen Method |
| logp | 1.561 | | Crippen Method |
| mcvol | 124.080 | ml/mol | McGowan Method |
| pc | 3704.46 | kPa | Joback Method |
| tb | 499.67 | K | Joback Method |
| tc | 706.30 | K | Joback Method |
| tf | 312.30 | K | Joback Method |
| vc | 0.451 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 288.49 | J/molxK | 499.67 | Joback Method |
| cpg | 303.20 | J/molxK | 534.11 | Joback Method |
| cpg | 316.93 | J/molxK | 568.55 | Joback Method |
| cpg | 329.73 | J/molxK | 602.99 | Joback Method |
| cpg | 341.67 | J/molxK | 637.43 | Joback Method |
| cpg | 352.80 | J/molxK | 671.86 | Joback Method |
| cpg | 363.18 | J/molxK | 706.30 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C100144294&Units=SI |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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