

1,2,4-Methenoazulene, decahydro-1,5,5,8a-tetramethyl-,

[1S-(1a',2a',3aa',4a',8aa',9R')]-
InChI=1S/C15H24/c13(2)6-5-7-4(3)9-10-12(11(9)13)15(10,14)4/h9-12H,5-8H2,1-4H
InChIKey:WCEIQUQVIOGRBF-UHFFFAOYSA-N

Formula: C15H24
SMILES: CC1(C)CCCC2(C)C3CC4C(C31)C42C
Mol. weight [g/mol]: 204.35

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 290.92 | kJ/mol | Joback Method |
| hf | -70.87 | kJ/mol | Joback Method |
| hfus | 13.56 | kJ/mol | Joback Method |
| hvap | 44.08 | kJ/mol | Joback Method |
| log10ws | -3.99 | | Crippen Method |
| logp | 4.105 | | Crippen Method |
| mcvol | 178.770 | ml/mol | McGowan Method |
| pc | 2210.37 | kPa | Joback Method |
| rinpol | 1376.20 | | NIST Webbook |
| rinpol | 1376.20 | | NIST Webbook |
| tb | 552.00 | K | Joback Method |
| tc | 775.96 | K | Joback Method |
| tf | 393.07 | K | Joback Method |
| vc | 0.703 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 503.97 | J/mol×K | 552.00 | Joback Method |
| cpg | 526.89 | J/mol×K | 589.33 | Joback Method |
| cpg | 547.94 | J/mol×K | 626.65 | Joback Method |
| cpg | 567.56 | J/mol×K | 663.98 | Joback Method |
| cpg | 586.20 | J/mol×K | 701.31 | Joback Method |
| cpg | 604.29 | J/mol×K | 738.63 | Joback Method |
| cpg | 622.26 | J/mol×K | 775.96 | 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=R518126&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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