

1H-3a,7-Methanoazulene, octahydro-3,6,8,8-tetramethyl-, [3R-(3«alpha»,3a«beta»,6«alpha»,7«beta»,8a«alpha»)-Cedrane]

Inchi: InChI=1S/C15H26/c1-10-7-8-15-9-12(10)14(3,4)13(15)6-5-11(15)2/h10-13H,5-9H2,1-4H3
InchiKey: JJTQQGNEXQKQRF-UHFFFAOYSA-N
Formula: C15H26
SMILES: CC1CCC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]: 206.37
CAS: 13567-54-9

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 199.36 | kJ/mol | Joback Method |
| hf | -177.39 | kJ/mol | Joback Method |
| hfus | 15.43 | kJ/mol | Joback Method |
| hvap | 45.84 | kJ/mol | Joback Method |
| log10ws | -4.34 | | Crippen Method |
| logp | 4.495 | | Crippen Method |
| mcvol | 189.630 | ml/mol | McGowan Method |
| pc | 2016.32 | kPa | Joback Method |
| tb | 557.83 | K | Joback Method |
| tc | 780.06 | K | Joback Method |
| tf | 340.67 | K | Joback Method |
| vc | 0.724 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 522.52 | J/molxK | 557.83 | Joback Method |
| cpg | 547.59 | J/molxK | 594.87 | Joback Method |
| cpg | 570.94 | J/molxK | 631.91 | Joback Method |
| cpg | 592.86 | J/molxK | 668.95 | Joback Method |
| cpg | 613.64 | J/molxK | 705.99 | Joback Method |
| cpg | 633.54 | J/molxK | 743.02 | Joback Method |
| cpg | 652.86 | J/molxK | 780.06 | 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=C13567549&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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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