

1,4-Methano-1H-indene, octahydro-1,7a-dimethyl-4-(1-methylethenyl)-, [1S-(1«alpha»,3a«beta»,4«alpha»,7a«beta»)]-

Other names:

Alloisocingifolene

InChI: InChI=1S/C15H24/c1-11(2)15-8-5-7-14(4)12(15)6-9-13(14,3)10-15/h12H,1,5-10H2,2-4H3

InchiKey: MTBNHGFRLZSOTC-UHFFFAOYSA-N

Formula: C15H24

SMILES: C=C(C)C12CCCC3(C)C1CCC3(C)C2

Mol. weight [g/mol]: 204.35

CAS: 87064-18-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 300.68 | kJ/mol | Joback Method |
| hf | 0.33 | kJ/mol | Joback Method |
| hfus | 6.50 | kJ/mol | Joback Method |
| hvap | 44.54 | kJ/mol | Joback Method |
| log10ws | -4.67 | | Crippen Method |
| logp | 4.559 | | Crippen Method |
| mcvol | 185.330 | ml/mol | McGowan Method |
| pc | 2280.59 | kPa | Joback Method |
| rinpol | 1409.00 | | NIST Webbook |
| rinpol | 1409.00 | | NIST Webbook |
| tb | 559.70 | K | Joback Method |
| tc | 792.42 | K | Joback Method |
| tf | 360.85 | K | Joback Method |
| vc | 0.714 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 498.32 | J/molxK | 559.70 | Joback Method |
| cpg | 521.02 | J/molxK | 598.49 | Joback Method |
| cpg | 541.91 | J/molxK | 637.27 | Joback Method |
| cpg | 561.45 | J/molxK | 676.06 | Joback Method |
| cpg | 580.10 | J/molxK | 714.85 | Joback Method |
| cpg | 598.31 | J/molxK | 753.63 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C87064184&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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

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