

1H-Indene, 2,3-dihydro-1,1,5,6-tetramethyl-

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|-----------------------------|---|
| Other names: | 2,3-Dihydro-1,1,5,6-tetramethyl-1H-indene |
| Inchi: | InChI=1S/C13H18/c1-9-7-11-5-6-13(3,4)12(11)8-10(9)2/h7-8H,5-6H2,1-4H3 |
| InchiKey: | SOVJMXNIZUPIFE-UHFFFAOYSA-N |
| Formula: | C13H18 |
| SMILES: | <chem>Cc1cc2c(cc1C)C(C)(C)CC2</chem> |
| Mol. weight [g/mol]: | 174.28 |
| CAS: | 942-43-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 197.36 | kJ/mol | Joback Method |
| hf | -21.49 | kJ/mol | Joback Method |
| hfus | 14.14 | kJ/mol | Joback Method |
| hvap | 47.56 | kJ/mol | Joback Method |
| log10ws | -4.02 | | Crippen Method |
| logp | 3.527 | | Crippen Method |
| mcvol | 159.410 | ml/mol | McGowan Method |
| pc | 2487.55 | kPa | Joback Method |
| rinpol | 1311.00 | | NIST Webbook |
| rinpol | 248.24 | | NIST Webbook |
| tb | 545.44 | K | Joback Method |
| tc | 769.28 | K | Joback Method |
| tf | 342.09 | K | Joback Method |
| vc | 0.611 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 379.74 | J/molxK | 545.44 | Joback Method |
| cpg | 397.09 | J/molxK | 582.75 | Joback Method |
| cpg | 413.31 | J/molxK | 620.05 | Joback Method |
| cpg | 428.55 | J/molxK | 657.36 | Joback Method |
| cpg | 442.97 | J/molxK | 694.67 | Joback Method |
| cpg | 456.71 | J/molxK | 731.97 | 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=C942438&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 |
| mccvol: | 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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<https://www.chemeo.com/cid/47-069-4/1H-Indene-2-3-dihydro-1-1-5-6-tetramethyl.pdf>

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