

1,2,3,4-Tetrahydro-1,6-dimethyl-4-(1-methylethyl)naphthalene

InChI: InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9-10,12-13H,6,8H2
InChIKey: PGTJIOWQJWHTJJ-UHFFFAOYSA-N

Formula: C15H22

SMILES: Cc1ccc2c(c1)C(C(C)C)CCC2C

Mol. weight [g/mol]: 202.34

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 207.07 | kJ/mol | Joback Method |
| hf | -98.32 | kJ/mol | Joback Method |
| hfus | 21.45 | kJ/mol | Joback Method |
| hvap | 51.97 | kJ/mol | Joback Method |
| log10ws | -4.81 | | Crippen Method |
| logp | 4.632 | | Crippen Method |
| mcvol | 187.590 | ml/mol | McGowan Method |
| pc | 2016.32 | kPa | Joback Method |
| rinpol | 1518.00 | | NIST Webbook |
| tb | 585.14 | K | Joback Method |
| tc | 803.63 | K | Joback Method |
| tf | 305.45 | K | Joback Method |
| vc | 0.710 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 482.92 | J/molxK | 585.14 | Joback Method |
| cpg | 575.50 | J/molxK | 767.21 | Joback Method |
| cpg | 559.26 | J/molxK | 730.80 | Joback Method |
| cpg | 541.93 | J/molxK | 694.38 | Joback Method |
| cpg | 523.46 | J/molxK | 657.97 | Joback Method |
| cpg | 503.81 | J/molxK | 621.55 | Joback Method |
| cpg | 590.72 | J/molxK | 803.63 | Joback Method |
| dvisc | 0.0003052 | Paxs | 585.14 | Joback Method |
| dvisc | 0.0003614 | Paxs | 538.52 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0004418 | Paxs | 491.91 | Joback Method |
| dvisc | 0.0005632 | Paxs | 445.30 | Joback Method |
| dvisc | 0.0007601 | Paxs | 398.68 | Joback Method |
| dvisc | 0.0011104 | Paxs | 352.07 | Joback Method |
| dvisc | 0.0018212 | Paxs | 305.45 | 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=R341674&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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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<https://www.chemeo.com/cid/30-217-7/1-2-3-4-Tetrahydro-1-6-dimethyl-4-1-methylethyl-naphthalene.pdf>

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