

1-Ethyl-2-methyl-cis-2-heptyl-cyclopropane

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|-----------------------------|---|
| Inchi: | InChI=1S/C13H26/c1-4-6-7-8-9-10-13(3)11-12(13)5-2/h12H,4-11H2,1-3H3/t12-,13+/m1/s |
| InchiKey: | HNJDEOSFIWOKFD-OLZOCXBDSA-N |
| Formula: | C13H26 |
| SMILES: | CCCCCCCC1(C)CC1CC |
| Mol. weight [g/mol]: | 182.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 106.13 | kJ/mol | Joback Method |
| hf | -243.95 | kJ/mol | Joback Method |
| hfus | 22.33 | kJ/mol | Joback Method |
| hvap | 42.98 | kJ/mol | Joback Method |
| log10ws | -4.68 | | Crippen Method |
| logp | 4.783 | | Crippen Method |
| mcvol | 183.170 | ml/mol | McGowan Method |
| pc | 1851.52 | kPa | Joback Method |
| rinpol | 1218.60 | | NIST Webbook |
| rinpol | 1218.60 | | NIST Webbook |
| tb | 499.15 | K | Joback Method |
| tc | 676.75 | K | Joback Method |
| tf | 273.87 | K | Joback Method |
| vc | 0.718 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 442.67 | J/mol×K | 499.15 | Joback Method |
| cpg | 461.68 | J/mol×K | 528.75 | Joback Method |
| cpg | 479.69 | J/mol×K | 558.35 | Joback Method |
| cpg | 496.79 | J/mol×K | 587.95 | Joback Method |
| cpg | 513.05 | J/mol×K | 617.55 | Joback Method |
| cpg | 528.56 | J/mol×K | 647.15 | Joback Method |
| cpg | 543.39 | J/mol×K | 676.75 | 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=R137074&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

Legend

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|------------------|---|
| 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 |
| h vap: | 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 |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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