

Cyclohexane, 1,1'-(1-methylethylidene)bis-

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|-----------------------------|---|
| Other names: | 2,2-Dicyclohexylpropane |
| Inchi: | InChI=1S/C15H28/c1-15(2,13-9-5-3-6-10-13)14-11-7-4-8-12-14/h13-14H,3-12H2,1-2H3 |
| InchiKey: | CCXLOQVMDTWRSP-UHFFFAOYSA-N |
| Formula: | C15H28 |
| SMILES: | CC(C)(C1CCCCC1)C1CCCCC1 |
| Mol. weight [g/mol]: | 208.38 |
| CAS: | 54934-90-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| chl | -8996.00 | kJ/mol | NIST Webbook |
| gf | 127.16 | kJ/mol | Joback Method |
| hf | -253.04 | kJ/mol | Joback Method |
| hfus | 10.86 | kJ/mol | Joback Method |
| hvap | 48.55 | kJ/mol | Joback Method |
| log10ws | -5.17 | | Crippen Method |
| logp | 5.173 | | Crippen Method |
| mvol | 200.490 | ml/mol | McGowan Method |
| pc | 2012.70 | kPa | Joback Method |
| tb | 559.40 ± 0.50 | K | NIST Webbook |
| tb | 559.40 ± 0.60 | K | NIST Webbook |
| tc | 812.06 | K | Joback Method |
| tf | 288.76 ± 1.00 | K | NIST Webbook |
| tf | 288.76 ± 0.30 | K | NIST Webbook |
| vc | 0.731 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 547.37 | J/mol×K | 578.47 | Joback Method |
| cpg | 670.68 | J/mol×K | 773.13 | Joback Method |
| cpg | 649.57 | J/mol×K | 734.20 | Joback Method |
| cpg | 626.78 | J/mol×K | 695.27 | Joback Method |
| cpg | 602.22 | J/mol×K | 656.33 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 575.78 | J/mol×K | 617.40 | Joback Method |
| cpg | 690.18 | J/mol×K | 812.06 | Joback Method |
| dvisc | 0.0001755 | Paxs | 578.47 | Joback Method |
| dvisc | 0.0002528 | Paxs | 528.06 | Joback Method |
| dvisc | 0.0003934 | Paxs | 477.64 | Joback Method |
| dvisc | 0.0006794 | Paxs | 427.23 | Joback Method |
| dvisc | 0.0013582 | Paxs | 376.82 | Joback Method |
| dvisc | 0.0033629 | Paxs | 326.40 | Joback Method |
| dvisc | 0.0115959 | Paxs | 275.99 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.39148e+01 |
| Coeff. B | -4.30247e+03 |
| Coeff. C | -9.65940e+01 |
| Temperature range (K), min. | 412.32 |
| Temperature range (K), max. | 596.69 |

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=C54934906&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|---------------|---|
| chl: | Standard liquid enthalpy of combustion |
| 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 |
| 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 |
| pvap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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