# n-Pentadecylcyclohexane

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|---|---|
| **Other names:** | Cyclohexane, pentadecyl-<br>Pentadecylcyclohexane<br>pentadecane, 1-cyclohexyl- |
| **Inchi:** | InChI=1S/C21H42/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-21-19-16-14-17-20-21/h21H,2- |
| **InchiKey:** | ZNUABQHWFGTOCO-UHFFFAOYSA-N |
| **Formula:** | C21H42 |
| **SMILES:** | CCCCCCCCCCCCCCCC1CCCCC1 |
| **Mol. weight [g/mol]:** | 294.56 |
| **CAS:** | 6006-95-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -13826.50 ± 3.20 | kJ/mol | NIST Webbook |
| gf | 150.39 | kJ/mol | Joback Method |
| hf | -439.90 ± 3.50 | kJ/mol | NIST Webbook |
| hfus | 41.98 | kJ/mol | Joback Method |
| hvap | 104.40 | kJ/mol | NIST Webbook |
| log10ws | -8.27 | | Crippen Method |
| logp | 8.048 | | Crippen Method |
| mcvol | 295.890 | ml/mol | McGowan Method |
| pc | 1089.94 | kPa | Joback Method |
| tb | 699.43 | K | Joback Method |
| tc | 877.85 | K | Joback Method |
| tf | 333.81 | K | Joback Method |
| vc | 1.145 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 899.74 | J/mol×K | 699.43 | Joback Method |
| cpg | 923.15 | J/mol×K | 729.17 | Joback Method |
| cpg | 945.40 | J/mol×K | 758.90 | Joback Method |
| cpg | 966.53 | J/mol×K | 788.64 | Joback Method |
| cpg | 986.58 | J/mol×K | 818.38 | Joback Method |

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|---|---|---|---|---|
| cpg | 1005.58 | J/mol×K | 848.11 | Joback Method |
| cpg | 1023.58 | J/mol×K | 877.85 | Joback Method |
| dvisc | 0.0012939 | Pa×s | 394.75 | Joback Method |
| dvisc | 0.0039477 | Pa×s | 333.81 | Joback Method |
| dvisc | 0.0005715 | Pa×s | 455.68 | Joback Method |
| dvisc | 0.0003061 | Pa×s | 516.62 | Joback Method |
| dvisc | 0.0001870 | Pa×s | 577.56 | Joback Method |
| dvisc | 0.0001256 | Pa×s | 638.49 | Joback Method |
| dvisc | 0.0000903 | Pa×s | 699.43 | Joback Method |
| hfust | 58.70 | kJ/mol | 298.20 | NIST Webbook |
| hfust | 58.30 | kJ/mol | 301.00 | NIST Webbook |
| hvapt | 77.20 | kJ/mol | 586.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tfp | 298.10 | K | 100.00 | Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes |
| tfp | 302.60 | K | 19300.00 | Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes |
| tfp | 307.60 | K | 40000.00 | Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes |
| tfp | 312.30 | K | 60100.00 | Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes |
| tfp | 316.80 | K | 80300.00 | Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes |
| tfp | 320.80 | K | 100100.00 | Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52537e+01 |
| Coeff. B | -5.07833e+03 |
| Coeff. C | -1.46968e+02 |
| Temperature range (K), min. | 486.29 |
| Temperature range (K), max. | 657.75 |

# Sources

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|---|---|
| **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/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes:** | https://www.doi.org/10.1021/je600575r |
| **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=C6006957&Units=SI |

# 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |

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|---|---|
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tfp:** | Melting point |
| **vc:** | Critical Volume |