# 1,1-dichlorohexane

**Other names:** Hexane, 1,1-dichloro
**Inchi:** InChI=1S/C6H12Cl2/c1-2-3-4-5-6(7)8/h6H,2-5H2,1H3
**InchiKey:** RQXXCWHCUOJQGR-UHFFFAOYSA-N
**Formula:** C6H12Cl2
**SMILES:** CCCCCC(Cl)Cl
**Mol. weight [g/mol]:** 155.06
**CAS:** 62017-16-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -26.66 | kJ/mol | Joback Method |
| hf | -203.93 | kJ/mol | Joback Method |
| hfus | 16.17 | kJ/mol | Joback Method |
| hvap | 37.33 | kJ/mol | Joback Method |
| log10ws | -3.25 | | Crippen Method |
| logp | 3.370 | | Crippen Method |
| mcvol | 119.880 | ml/mol | McGowan Method |
| pc | 2890.51 | kPa | Joback Method |
| rinpol | 989.00 | | NIST Webbook |
| rinpol | 989.00 | | NIST Webbook |
| rinpol | 989.00 | | NIST Webbook |
| ripol | 1240.00 | | NIST Webbook |
| ripol | 1240.00 | | NIST Webbook |
| tb | 411.10 | K | Joback Method |
| tc | 595.37 | K | Joback Method |
| tf | 202.22 | K | Joback Method |
| vc | 0.464 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 212.27 | J/mol×K | 411.10 | Joback Method |
| cpg | 222.72 | J/mol×K | 441.81 | Joback Method |
| cpg | 232.70 | J/mol×K | 472.52 | Joback Method |

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|---|---|---|---|---|
| cpg | 242.24 | J/mol×K | 503.23 | Joback Method |
| cpg | 251.35 | J/mol×K | 533.95 | Joback Method |
| cpg | 260.04 | J/mol×K | 564.66 | Joback Method |
| cpg | 268.32 | J/mol×K | 595.37 | Joback Method |
| dvisc | 0.0074186 | Pa×s | 202.22 | Joback Method |
| dvisc | 0.0029798 | Pa×s | 237.03 | Joback Method |
| dvisc | 0.0015119 | Pa×s | 271.85 | Joback Method |
| dvisc | 0.0008949 | Pa×s | 306.66 | Joback Method |
| dvisc | 0.0005894 | Pa×s | 341.47 | Joback Method |
| dvisc | 0.0004194 | Pa×s | 376.29 | Joback Method |
| dvisc | 0.0003162 | Pa×s | 411.10 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.49996e+01 |
| Coeff. B | -4.00228e+03 |
| Coeff. C | -6.26780e+01 |
| Temperature range (K), min. | 334.72 |
| Temperature range (K), max. | 475.79 |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R116042&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/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# 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 |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |