# Cyclododecane

**Inchi:** InChI=1S/C12H24/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-12H2
**InchiKey:** DDTBPAQBQHZRDW-UHFFFAOYSA-N
**Formula:** C12H24
**SMILES:** C1CCCCCCCCCCC1
**Mol. weight [g/mol]:** 168.32
**CAS:** 294-62-2

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chg | -7434.00 | kJ/mol | NIST Webbook |
| chs | -7700.33 | kJ/mol | NIST Webbook |
| chs | -7845.40 ± 1.30 | kJ/mol | NIST Webbook |
| gf | 9.72 | kJ/mol | Joback Method |
| hf | -253.31 | kJ/mol | Joback Method |
| hfus | 5.00 | kJ/mol | Joback Method |
| hsub | 76.20 | kJ/mol | NIST Webbook |
| hvap | 63.00 | kJ/mol | NIST Webbook |
| hvap | 62.80 | kJ/mol | NIST Webbook |
| ie | 10.04 ± 0.05 | eV | NIST Webbook |
| ie | 9.72 ± 0.03 | eV | NIST Webbook |
| log10ws | -4.74 | | Crippen Method |
| logp | 4.681 | | Crippen Method |
| mcvol | 169.080 | ml/mol | McGowan Method |
| pc | 2545.61 | kPa | Joback Method |
| rinpol | 1384.00 | | NIST Webbook |
| rinpol | 1338.30 | | NIST Webbook |
| rinpol | 1351.60 | | NIST Webbook |
| rinpol | 1372.40 | | NIST Webbook |
| rinpol | 1338.30 | | NIST Webbook |
| rinpol | 1351.60 | | NIST Webbook |
| rinpol | 1372.40 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1370.00 | | NIST Webbook |
| rinpol | 1378.00 | | NIST Webbook |
| rinpol | 1323.70 | | NIST Webbook |
| rinpol | 1326.00 | | NIST Webbook |
| rinpol | 1330.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1325.00 | | NIST Webbook |
| rinpol | 1384.00 | | NIST Webbook |
| rinpol | 1316.00 | | NIST Webbook |
| rinpol | 1326.00 | | NIST Webbook |
| ripol | 1549.30 | | NIST Webbook |
| ripol | 1510.00 | | NIST Webbook |
| ripol | 1497.20 | | NIST Webbook |
| ripol | 1516.90 | | NIST Webbook |
| ripol | 1549.30 | | NIST Webbook |
| ripol | 1497.20 | | NIST Webbook |
| ripol | 1516.90 | | NIST Webbook |
| ripol | 1521.00 | | NIST Webbook |
| ripol | 1519.00 | | NIST Webbook |
| tb | 523.80 | K | Joback Method |
| tc | 764.23 | K | Joback Method |
| tf | 316.00 ± 1.66 | K | NIST Webbook |
| tf | 332.50 ± 1.00 | K | NIST Webbook |
| tf | 333.80 ± 0.30 | K | NIST Webbook |
| vc | 0.594 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 401.44 | J/mol×K | 523.80 | Joback Method |
| cpg | 455.62 | J/mol×K | 603.94 | Joback Method |
| cpg | 544.48 | J/mol×K | 764.23 | Joback Method |
| cpg | 480.28 | J/mol×K | 644.01 | Joback Method |
| cpg | 503.31 | J/mol×K | 684.08 | Joback Method |
| cpg | 524.72 | J/mol×K | 724.15 | Joback Method |
| cpg | 429.34 | J/mol×K | 563.87 | Joback Method |
| dvisc | 0.0001110 | Pa×s | 472.42 | Joback Method |
| dvisc | 0.0002468 | Pa×s | 421.03 | Joback Method |
| dvisc | 0.0006851 | Pa×s | 369.65 | Joback Method |
| dvisc | 0.0026445 | Pa×s | 318.27 | Joback Method |
| dvisc | 0.0171716 | Pa×s | 266.88 | Joback Method |
| dvisc | 0.0000584 | Pa×s | 523.80 | Joback Method |
| dvisc | 0.2721027 | Pa×s | 215.50 | Joback Method |
| hfust | 14.80 | kJ/mol | 333.80 | NIST Webbook |
| hfust | 0.60 | kJ/mol | 199.00 | NIST Webbook |
| hfust | 14.80 | kJ/mol | 333.80 | NIST Webbook |
| hvapt | 52.60 | kJ/mol | 413.50 | NIST Webbook |

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|---|---|---|---|---|
| hvapt | 49.80 | kJ/mol | 484.50 | NIST Webbook |
| sfust | 3.02 | J/mol×K | 199.00 | NIST Webbook |
| sfust | 44.34 | J/mol×K | 333.80 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46296e+01 |
| Coeff. B | -4.26369e+03 |
| Coeff. C | -7.95600e+01 |
| Temperature range (K), min. | 376.85 |
| Temperature range (K), max. | 537.13 |

# Sources

**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

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C294622&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

# Legend

**chg:** Standard gas enthalpy of combustion

**chs:** Standard solid 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

**hsub:** Enthalpy of sublimation at standard conditions

| | |
|---|---|
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |