# 4-Methyldocosane

**Other names:** Docosane, 4-methyl
**Inchi:** InChI=1S/C23H48/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-23(3)21-5-2/h23H
**InchiKey:** ATAWCABZIRDUSP-UHFFFAOYSA-N
**Formula:** C23H48
**SMILES:** CCCCCCCCCCCCCCCCCCC(C)CCC
**Mol. weight [g/mol]:** 324.63
**CAS:** 25117-30-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 140.34 | kJ/mol | Joback Method |
| hf | -523.33 | kJ/mol | Joback Method |
| hfus | 51.80 | kJ/mol | Joback Method |
| hvap | 66.40 | kJ/mol | Joback Method |
| log10ws | -9.21 | | Crippen Method |
| logp | 9.074 | | Crippen Method |
| mcvol | 334.930 | ml/mol | McGowan Method |
| pc | 855.96 | kPa | Joback Method |
| rinpol | 2260.00 | | NIST Webbook |
| rinpol | 2258.00 | | NIST Webbook |
| rinpol | 2258.00 | | NIST Webbook |
| rinpol | 2259.00 | | NIST Webbook |
| rinpol | 2257.20 | | NIST Webbook |
| rinpol | 2254.30 | | NIST Webbook |
| rinpol | 2255.00 | | NIST Webbook |
| rinpol | 2260.00 | | NIST Webbook |
| ripol | 2256.90 | | NIST Webbook |
| tb | 725.20 | K | Joback Method |
| tc | 892.42 | K | Joback Method |
| tf | 333.97 | K | Joback Method |
| vc | 1.317 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1145.09 | J/mol×K | 892.42 | Joback Method |
| cpg | 1127.28 | J/mol×K | 864.55 | Joback Method |
| cpg | 1108.60 | J/mol×K | 836.68 | Joback Method |
| cpg | 1089.04 | J/mol×K | 808.81 | Joback Method |
| cpg | 1068.56 | J/mol×K | 780.94 | Joback Method |
| cpg | 1047.11 | J/mol×K | 753.07 | Joback Method |
| cpg | 1024.67 | J/mol×K | 725.20 | Joback Method |
| dvisc | 0.0035428 | Pa×s | 333.97 | Joback Method |
| dvisc | 0.0000611 | Pa×s | 725.20 | Joback Method |
| dvisc | 0.0000860 | Pa×s | 659.99 | Joback Method |
| dvisc | 0.0001306 | Pa×s | 594.79 | Joback Method |
| dvisc | 0.0002197 | Pa×s | 529.59 | Joback Method |
| dvisc | 0.0004278 | Pa×s | 464.38 | Joback Method |
| dvisc | 0.0010359 | Pa×s | 399.17 | Joback Method |
| hvapt | 76.30 | kJ/mol | 568.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.88591e+01 |
| Coeff. B | -9.15203e+03 |
| Coeff. C | -5.54000e-01 |
| Temperature range (K), min. | 493.35 |
| Temperature range (K), max. | 676.10 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C25117300&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

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

# 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 |
| **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 |
| **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 |