# 16,20,24,28-Tetramethyl-tetratriacontyl cyanide

**Inchi:** InChI=1S/C40H79N/c1-6-7-8-19-22-28-37(2)30-25-32-39(4)34-27-35-40(5)33-26-31-38(3

**InchiKey:** BCHKRABWCXVGKY-UHFFFAOYSA-N

**Formula:** C40H79N

**SMILES:** CCCCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N

**Mol. weight [g/mol]:** 574.06

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 409.34 | kJ/mol | Joback Method |
| hf | -725.17 | kJ/mol | Joback Method |
| hfus | 86.77 | kJ/mol | Joback Method |
| hvap | 113.56 | kJ/mol | Joback Method |
| log10ws | -15.47 | | Crippen Method |
| logp | 14.777 | | Crippen Method |
| mcvol | 575.840 | ml/mol | McGowan Method |
| pc | 391.96 | kPa | Joback Method |
| rinpol | 3945.00 | | NIST Webbook |
| tb | 1214.92 | K | Joback Method |
| tc | 1633.40 | K | Joback Method |
| tf | 545.55 | K | Joback Method |
| vc | 2.277 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 2216.47 | J/mol×K | 1214.92 | Joback Method |
| cpg | 2256.07 | J/mol×K | 1284.67 | Joback Method |
| cpg | 2292.04 | J/mol×K | 1354.41 | Joback Method |
| cpg | 2325.28 | J/mol×K | 1424.16 | Joback Method |
| cpg | 2356.74 | J/mol×K | 1493.91 | Joback Method |
| cpg | 2387.35 | J/mol×K | 1563.65 | Joback Method |
| cpg | 2418.02 | J/mol×K | 1633.40 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R202287&Units=SI |
| **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

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |