# Cyanoacetic acid, hexadecyl ester

**Inchi:** InChI=1S/C19H35NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-22-19(21)16-17-20/h2-1
**InchiKey:** VYKJKXWAMIAGRC-UHFFFAOYSA-N
**Formula:** C19H35NO2
**SMILES:** CCCCCCCCCCCCCCCCOC(=O)CC#N
**Mol. weight [g/mol]:** 309.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 8.36 | kJ/mol | Joback Method |
| hf | -515.41 | kJ/mol | Joback Method |
| hfus | 49.26 | kJ/mol | Joback Method |
| hvap | 77.52 | kJ/mol | Joback Method |
| log10ws | -6.50 | | Crippen Method |
| logp | 5.925 | | Crippen Method |
| mcvol | 287.390 | ml/mol | McGowan Method |
| pc | 1095.72 | kPa | Joback Method |
| rinpol | 2357.00 | | NIST Webbook |
| rinpol | 2357.00 | | NIST Webbook |
| tb | 812.49 | K | Joback Method |
| tc | 999.36 | K | Joback Method |
| tf | 441.04 | K | Joback Method |
| vc | 1.149 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 895.17 | J/mol×K | 812.49 | Joback Method |
| cpg | 912.11 | J/mol×K | 843.63 | Joback Method |
| cpg | 928.12 | J/mol×K | 874.78 | Joback Method |
| cpg | 943.22 | J/mol×K | 905.92 | Joback Method |
| cpg | 957.43 | J/mol×K | 937.07 | Joback Method |
| cpg | 970.78 | J/mol×K | 968.21 | Joback Method |
| cpg | 983.31 | J/mol×K | 999.36 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406233&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 |

# 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 |