# 4-Cyanobenzoic acid, hexyl ester

**Inchi:** InChI=1S/C14H17NO2/c1-2-3-4-5-10-17-14(16)13-8-6-12(11-15)7-9-13/h6-9H,2-5,10H2,
**InchiKey:** GDAPFQSPDUEQRI-UHFFFAOYSA-N
**Formula:** C14H17NO2
**SMILES:** CCCCCCOC(=O)c1ccc(C#N)cc1
**Mol. weight [g/mol]:** 231.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 69.04 | kJ/mol | Joback Method |
| hf | -187.15 | kJ/mol | Joback Method |
| hfus | 29.96 | kJ/mol | Joback Method |
| hvap | 69.33 | kJ/mol | Joback Method |
| log10ws | -4.16 | | Crippen Method |
| logp | 3.295 | | Crippen Method |
| mcvol | 193.180 | ml/mol | McGowan Method |
| pc | 2019.95 | kPa | Joback Method |
| rinpol | 1800.00 | | NIST Webbook |
| rinpol | 1800.00 | | NIST Webbook |
| tb | 729.75 | K | Joback Method |
| tc | 943.44 | K | Joback Method |
| tf | 423.63 | K | Joback Method |
| vc | 0.761 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 523.77 | J/mol×K | 729.75 | Joback Method |
| cpg | 537.08 | J/mol×K | 765.36 | Joback Method |
| cpg | 549.52 | J/mol×K | 800.98 | Joback Method |
| cpg | 561.10 | J/mol×K | 836.59 | Joback Method |
| cpg | 571.87 | J/mol×K | 872.21 | Joback Method |
| cpg | 581.82 | J/mol×K | 907.82 | Joback Method |
| cpg | 591.00 | J/mol×K | 943.44 | 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=U299831&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 |