# 4-Cyanobenzoic acid, pentyl ester

**Inchi:** InChI=1S/C13H15NO2/c1-2-3-4-9-16-13(15)12-7-5-11(10-14)6-8-12/h5-8H,2-4,9H2,1H3
**InchiKey:** PSHNNCVKUDBIDE-UHFFFAOYSA-N
**Formula:** C13H15NO2
**SMILES:** CCCCCOC(=O)c1ccc(C#N)cc1
**Mol. weight [g/mol]:** 217.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 60.62 | kJ/mol | Joback Method |
| hf | -166.51 | kJ/mol | Joback Method |
| hfus | 27.37 | kJ/mol | Joback Method |
| hvap | 67.10 | kJ/mol | Joback Method |
| log10ws | -3.74 | | Crippen Method |
| logp | 2.905 | | Crippen Method |
| mcvol | 179.090 | ml/mol | McGowan Method |
| pc | 2206.22 | kPa | Joback Method |
| rinpol | 1700.00 | | NIST Webbook |
| rinpol | 1700.00 | | NIST Webbook |
| tb | 706.87 | K | Joback Method |
| tc | 923.68 | K | Joback Method |
| tf | 412.36 | K | Joback Method |
| vc | 0.706 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 471.48 | J/mol×K | 706.87 | Joback Method |
| cpg | 484.30 | J/mol×K | 743.00 | Joback Method |
| cpg | 496.28 | J/mol×K | 779.14 | Joback Method |
| cpg | 507.44 | J/mol×K | 815.27 | Joback Method |
| cpg | 517.79 | J/mol×K | 851.41 | Joback Method |
| cpg | 527.38 | J/mol×K | 887.54 | Joback Method |
| cpg | 536.20 | J/mol×K | 923.68 | 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=U299830&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 |