# 4-Cyanobenzoic acid, 4-hexadecyl ester

**Inchi:** InChI=1S/C24H37NO2/c1-3-5-6-7-8-9-10-11-12-13-15-23(14-4-2)27-24(26)22-18-16-21(
**InchiKey:** KEOGVJFULGMUAY-UHFFFAOYSA-N
**Formula:** C24H37NO2
**SMILES:** CCCCCCCCCCCCCC(CCC)OC(=O)c1ccc(C#N)cc1
**Mol. weight [g/mol]:** 371.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 150.80 | kJ/mol | Joback Method |
| hf | -398.83 | kJ/mol | Joback Method |
| hfus | 52.34 | kJ/mol | Joback Method |
| hvap | 91.20 | kJ/mol | Joback Method |
| log10ws | -8.46 | | Crippen Method |
| logp | 7.195 | | Crippen Method |
| mcvol | 334.080 | ml/mol | McGowan Method |
| pc | 990.75 | kPa | Joback Method |
| rinpol | 2541.00 | | NIST Webbook |
| tb | 958.11 | K | Joback Method |
| tc | 1174.00 | K | Joback Method |
| tf | 521.33 | K | Joback Method |
| vc | 1.315 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1101.58 | J/mol×K | 958.11 | Joback Method |
| cpg | 1117.92 | J/mol×K | 994.09 | Joback Method |
| cpg | 1133.02 | J/mol×K | 1030.07 | Joback Method |
| cpg | 1146.94 | J/mol×K | 1066.05 | Joback Method |
| cpg | 1159.74 | J/mol×K | 1102.03 | Joback Method |
| cpg | 1171.46 | J/mol×K | 1138.02 | Joback Method |
| cpg | 1182.18 | J/mol×K | 1174.00 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U292454&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 |