# 4-Cyanobenzoic acid, hexadecyl ester

**Inchi:** InChI=1S/C24H37NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-27-24(26)23-18-16-22(
**InchiKey:** WXBONVHCLKVXBG-UHFFFAOYSA-N
**Formula:** C24H37NO2
**SMILES:** CCCCCCCCCCCCCCCCOC(=O)c1ccc(C#N)cc1
**Mol. weight [g/mol]:** 371.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 153.24 | kJ/mol | Joback Method |
| hf | -393.55 | kJ/mol | Joback Method |
| hfus | 55.86 | kJ/mol | Joback Method |
| hvap | 91.59 | kJ/mol | Joback Method |
| log10ws | -8.35 | | Crippen Method |
| logp | 7.196 | | Crippen Method |
| mcvol | 334.080 | ml/mol | McGowan Method |
| pc | 985.78 | kPa | Joback Method |
| rinpol | 2848.00 | | NIST Webbook |
| tb | 958.55 | K | Joback Method |
| tc | 1174.06 | K | Joback Method |
| tf | 536.33 | K | Joback Method |
| vc | 1.321 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1101.17 | J/mol×K | 958.55 | Joback Method |
| cpg | 1117.53 | J/mol×K | 994.47 | Joback Method |
| cpg | 1132.68 | J/mol×K | 1030.39 | Joback Method |
| cpg | 1146.65 | J/mol×K | 1066.30 | Joback Method |
| cpg | 1159.52 | J/mol×K | 1102.22 | Joback Method |
| cpg | 1171.33 | J/mol×K | 1138.14 | Joback Method |
| cpg | 1182.15 | J/mol×K | 1174.06 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U299840&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 |