# 4-Cyanobenzoic acid, undec-10-enyl ester

**Inchi:** InChI=1S/C19H25NO2/c1-2-3-4-5-6-7-8-9-10-15-22-19(21)18-13-11-17(16-20)12-14-18/h
**InchiKey:** RSIRLJLMIYIZFR-UHFFFAOYSA-N
**Formula:** C19H25NO2
**SMILES:** C=CCCCCCCCCCOC(=O)c1ccc(C#N)cc1
**Mol. weight [g/mol]:** 299.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 198.98 | kJ/mol | Joback Method |
| hf | -164.92 | kJ/mol | Joback Method |
| hfus | 41.63 | kJ/mol | Joback Method |
| hvap | 79.79 | kJ/mol | Joback Method |
| log10ws | -6.11 | | Crippen Method |
| logp | 5.022 | | Crippen Method |
| mcvol | 259.330 | ml/mol | McGowan Method |
| pc | 1410.13 | kPa | Joback Method |
| rinpol | 2322.00 | | NIST Webbook |
| rinpol | 2322.00 | | NIST Webbook |
| tb | 840.83 | K | Joback Method |
| tc | 1048.65 | K | Joback Method |
| tf | 478.22 | K | Joback Method |
| vc | 1.022 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 774.67 | J/mol×K | 840.83 | Joback Method |
| cpg | 789.17 | J/mol×K | 875.47 | Joback Method |
| cpg | 802.68 | J/mol×K | 910.10 | Joback Method |
| cpg | 815.26 | J/mol×K | 944.74 | Joback Method |
| cpg | 826.94 | J/mol×K | 979.37 | Joback Method |
| cpg | 837.75 | J/mol×K | 1014.01 | Joback Method |
| cpg | 847.75 | J/mol×K | 1048.65 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U299835&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |