# 2-Chlorobenzoic acid, 4-cyanophenyl ester

**Inchi:** InChI=1S/C14H8ClNO2/c15-13-4-2-1-3-12(13)14(17)18-11-7-5-10(9-16)6-8-11/h1-8H
**InchiKey:** FBJQDKRQROMXNN-UHFFFAOYSA-N
**Formula:** C14H8ClNO2
**SMILES:** N#Cc1ccc(OC(=O)c2ccccc2Cl)cc1
**Mol. weight [g/mol]:** 257.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 159.89 | kJ/mol | Joback Method |
| hf | 22.17 | kJ/mol | Joback Method |
| hfus | 27.81 | kJ/mol | Joback Method |
| hvap | 76.65 | kJ/mol | Joback Method |
| log10ws | -4.60 | | Crippen Method |
| logp | 3.431 | | Crippen Method |
| mcvol | 181.660 | ml/mol | McGowan Method |
| pc | 2640.67 | kPa | Joback Method |
| rinpol | 2117.00 | | NIST Webbook |
| tb | 798.84 | K | Joback Method |
| tc | 1055.44 | K | Joback Method |
| tf | 492.49 | K | Joback Method |
| vc | 0.703 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 451.68 | J/mol×K | 798.84 | Joback Method |
| cpg | 461.84 | J/mol×K | 841.61 | Joback Method |
| cpg | 470.96 | J/mol×K | 884.37 | Joback Method |
| cpg | 479.08 | J/mol×K | 927.14 | Joback Method |
| cpg | 486.24 | J/mol×K | 969.91 | Joback Method |
| cpg | 492.50 | J/mol×K | 1012.67 | Joback Method |
| cpg | 497.90 | J/mol×K | 1055.44 | Joback Method |

# Sources

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|---|---|
| **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=U307818&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |