# 3-Chloro-2-fluorobenzoic acid, undecyl ester

**Inchi:** InChI=1S/C18H26ClFO2/c1-2-3-4-5-6-7-8-9-10-14-22-18(21)15-12-11-13-16(19)17(15)2
**InchiKey:** NVFSTLBFRMMBBJ-UHFFFAOYSA-N
**Formula:** C18H26ClFO2
**SMILES:** CCCCCCCCCCCOC(=O)c1cccc(Cl)c1F
**Mol. weight [g/mol]:** 328.85

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -246.83 | kJ/mol | Joback Method |
| hf | -657.91 | kJ/mol | Joback Method |
| hfus | 45.70 | kJ/mol | Joback Method |
| hvap | 71.99 | kJ/mol | Joback Method |
| log10ws | -6.92 | | Crippen Method |
| logp | 6.167 | | Crippen Method |
| mcvol | 262.170 | ml/mol | McGowan Method |
| pc | 1391.25 | kPa | Joback Method |
| rinpol | 2312.00 | | NIST Webbook |
| rinpol | 2312.00 | | NIST Webbook |
| tb | 760.87 | K | Joback Method |
| tc | 952.94 | K | Joback Method |
| tf | 446.75 | K | Joback Method |
| vc | 1.026 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 748.50 | J/mol×K | 760.87 | Joback Method |
| cpg | 764.43 | J/mol×K | 792.88 | Joback Method |
| cpg | 779.43 | J/mol×K | 824.89 | Joback Method |
| cpg | 793.53 | J/mol×K | 856.90 | Joback Method |
| cpg | 806.75 | J/mol×K | 888.92 | Joback Method |
| cpg | 819.13 | J/mol×K | 920.93 | Joback Method |
| cpg | 830.68 | J/mol×K | 952.94 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U338888&Units=SI |

# 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 |

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