# 3-Chloro2-fluorobenzoic acid, 3-tetradecyl ester

**Inchi:** InChI=1S/C21H32ClFO2/c1-3-5-6-7-8-9-10-11-12-14-17(4-2)25-21(24)18-15-13-16-19(22
**InchiKey:** NSGNMUMREZGUKQ-UHFFFAOYSA-N
**Formula:** C21H32ClFO2
**SMILES:** CCCCCCCCCCCC(CC)OC(=O)c1cccc(Cl)c1F
**Mol. weight [g/mol]:** 370.93

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -224.01 | kJ/mol | Joback Method |
| hf | -725.11 | kJ/mol | Joback Method |
| hfus | 49.95 | kJ/mol | Joback Method |
| hvap | 78.28 | kJ/mol | Joback Method |
| log10ws | -8.28 | | Crippen Method |
| logp | 7.335 | | Crippen Method |
| mcvol | 304.440 | ml/mol | McGowan Method |
| pc | 1140.57 | kPa | Joback Method |
| rinpol | 2499.00 | | NIST Webbook |
| rinpol | 2499.00 | | NIST Webbook |
| tb | 829.07 | K | Joback Method |
| tc | 1024.31 | K | Joback Method |
| tf | 465.56 | K | Joback Method |
| vc | 1.188 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 923.79 | J/mol×K | 829.07 | Joback Method |
| cpg | 940.76 | J/mol×K | 861.61 | Joback Method |
| cpg | 956.68 | J/mol×K | 894.15 | Joback Method |
| cpg | 971.57 | J/mol×K | 926.69 | Joback Method |
| cpg | 985.47 | J/mol×K | 959.23 | Joback Method |
| cpg | 998.41 | J/mol×K | 991.77 | Joback Method |
| cpg | 1010.42 | J/mol×K | 1024.31 | Joback Method |

# Sources

| | |
|---|---|
| **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=U338646&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 |