# 3-Chloro2-fluorobenzoic acid, 6-pentadecyl ester

**Inchi:** InChI=1S/C22H34ClFO2/c1-3-5-7-8-9-10-12-15-18(14-11-6-4-2)26-22(25)19-16-13-17-20

**InchiKey:** XRFKUCZZWKPQTF-UHFFFAOYSA-N

**Formula:** C22H34ClFO2

**SMILES:** CCCCCCCCCC(CCCCC)OC(=O)c1cccc(Cl)c1F

**Mol. weight [g/mol]:** 384.96

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -215.59 | kJ/mol | Joback Method |
| hf | -745.75 | kJ/mol | Joback Method |
| hfus | 52.54 | kJ/mol | Joback Method |
| hvap | 80.50 | kJ/mol | Joback Method |
| log10ws | -8.70 | | Crippen Method |
| logp | 7.726 | | Crippen Method |
| mcvol | 318.530 | ml/mol | McGowan Method |
| pc | 1070.06 | kPa | Joback Method |
| rinpol | 2546.00 | | NIST Webbook |
| rinpol | 2546.00 | | NIST Webbook |
| tb | 851.95 | K | Joback Method |
| tc | 1048.82 | K | Joback Method |
| tf | 476.83 | K | Joback Method |
| vc | 1.244 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 983.73 | J/mol×K | 851.95 | Joback Method |
| cpg | 1000.99 | J/mol×K | 884.76 | Joback Method |
| cpg | 1017.15 | J/mol×K | 917.57 | Joback Method |
| cpg | 1032.24 | J/mol×K | 950.39 | Joback Method |
| cpg | 1046.31 | J/mol×K | 983.20 | Joback Method |
| cpg | 1059.38 | J/mol×K | 1016.01 | Joback Method |
| cpg | 1071.50 | J/mol×K | 1048.82 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U338653&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 |