# Hexanoic acid, 3,5,5-trimethyl-, 2-chloro-6-fluorophenyl ester

**Inchi:** InChI=1S/C15H20ClFO2/c1-10(9-15(2,3)4)8-13(18)19-14-11(16)6-5-7-12(14)17/h5-7,10H

**InchiKey:** XPLONZOJIRMXHQ-UHFFFAOYSA-N

**Formula:** C15H20ClFO2

**SMILES:** CC(CC(=O)Oc1c(F)cccc1Cl)CC(C)(C)C

**Mol. weight [g/mol]:** 286.77

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -271.69 | kJ/mol | Joback Method |
| hf | -610.02 | kJ/mol | Joback Method |
| hfus | 27.00 | kJ/mol | Joback Method |
| hvap | 63.62 | kJ/mol | Joback Method |
| log10ws | -5.25 | | Crippen Method |
| logp | 4.847 | | Crippen Method |
| mcvol | 219.900 | ml/mol | McGowan Method |
| pc | 1786.37 | kPa | Joback Method |
| rinpol | 1743.00 | | NIST Webbook |
| rinpol | 1743.00 | | NIST Webbook |
| tb | 688.56 | K | Joback Method |
| tc | 896.76 | K | Joback Method |
| tf | 400.36 | K | Joback Method |
| vc | 0.842 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 586.11 | J/mol×K | 688.56 | Joback Method |
| cpg | 601.65 | J/mol×K | 723.26 | Joback Method |
| cpg | 616.20 | J/mol×K | 757.96 | Joback Method |
| cpg | 629.79 | J/mol×K | 792.66 | Joback Method |
| cpg | 642.47 | J/mol×K | 827.36 | Joback Method |
| cpg | 654.29 | J/mol×K | 862.06 | Joback Method |
| cpg | 665.27 | J/mol×K | 896.76 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406824&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 |