# 3-Fluoro-5-trifluoromethylbenzoic acid, 2,4-dichloro-6-formylphenyl ester

**Inchi:** InChI=1S/C15H6Cl2F4O3/c16-10-2-8(6-22)13(12(17)5-10)24-14(23)7-1-9(15(19,20)21)4
**InchiKey:** CIQBMLCHTUIDJO-UHFFFAOYSA-N
**Formula:** C15H6Cl2F4O3
**SMILES:** O=Cc1cc(Cl)cc(Cl)c1OC(=O)c1cc(F)cc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 381.11

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -881.61 | kJ/mol | Joback Method |
| hf | -1092.27 | kJ/mol | Joback Method |
| hfus | 39.12 | kJ/mol | Joback Method |
| hvap | 76.93 | kJ/mol | Joback Method |
| log10ws | -6.61 | | Crippen Method |
| logp | 5.183 | | Crippen Method |
| mcvol | 215.260 | ml/mol | McGowan Method |
| pc | 2092.66 | kPa | Joback Method |
| rinpol | 2020.00 | | NIST Webbook |
| rinpol | 2020.00 | | NIST Webbook |
| tb | 814.52 | K | Joback Method |
| tc | 1036.79 | K | Joback Method |
| tf | 553.03 | K | Joback Method |
| vc | 0.860 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 550.01 | J/mol×K | 814.52 | Joback Method |
| cpg | 558.68 | J/mol×K | 851.56 | Joback Method |
| cpg | 566.53 | J/mol×K | 888.61 | Joback Method |
| cpg | 573.58 | J/mol×K | 925.65 | Joback Method |
| cpg | 579.89 | J/mol×K | 962.70 | Joback Method |
| cpg | 585.49 | J/mol×K | 999.74 | Joback Method |
| cpg | 590.44 | J/mol×K | 1036.79 | 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=U357345&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 |