# 3-Fluoro-5-trifluoromethylbenzoic acid, 4-methoxyphenyl ester

**Inchi:** InChI=1S/C15H10F4O3/c1-21-12-2-4-13(5-3-12)22-14(20)9-6-10(15(17,18)19)8-11(16)7

**InchiKey:** WGTVOYHDLOSARH-UHFFFAOYSA-N

**Formula:** C15H10F4O3

**SMILES:** COc1ccc(OC(=O)c2cc(F)cc(C(F)(F)F)c2)cc1

**Mol. weight [g/mol]:** 314.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -843.97 | kJ/mol | Joback Method |
| hf | -1084.49 | kJ/mol | Joback Method |
| hfus | 30.40 | kJ/mol | Joback Method |
| hvap | 62.52 | kJ/mol | Joback Method |
| log10ws | -5.11 | | Crippen Method |
| logp | 4.072 | | Crippen Method |
| mcvol | 195.080 | ml/mol | McGowan Method |
| pc | 2117.78 | kPa | Joback Method |
| rinpol | 1811.00 | | NIST Webbook |
| tb | 703.46 | K | Joback Method |
| tc | 913.82 | K | Joback Method |
| tf | 448.38 | K | Joback Method |
| vc | 0.762 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 523.99 | J/mol×K | 703.46 | Joback Method |
| cpg | 536.60 | J/mol×K | 738.52 | Joback Method |
| cpg | 548.25 | J/mol×K | 773.58 | Joback Method |
| cpg | 558.99 | J/mol×K | 808.64 | Joback Method |
| cpg | 568.85 | J/mol×K | 843.70 | Joback Method |
| cpg | 577.85 | J/mol×K | 878.76 | Joback Method |
| cpg | 586.02 | J/mol×K | 913.82 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357960&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

| | |
|---|---|
| **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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