# 2,6-Difluoro-3-methylbenzoic acid, 4-methoxyphenyl ester

**Inchi:** InChI=1S/C15H12F2O3/c1-9-3-8-12(16)13(14(9)17)15(18)20-11-6-4-10(19-2)5-7-11/h3-8

**InchiKey:** UNVDFUZGQSCMBI-UHFFFAOYSA-N

**Formula:** C15H12F2O3

**SMILES:** COc1ccc(OC(=O)c2c(F)ccc(C)c2F)cc1

**Mol. weight [g/mol]:** 278.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -466.82 | kJ/mol | Joback Method |
| hf | -694.99 | kJ/mol | Joback Method |
| hfus | 31.27 | kJ/mol | Joback Method |
| hvap | 66.12 | kJ/mol | Joback Method |
| log10ws | -4.82 | | Crippen Method |
| logp | 3.501 | | Crippen Method |
| mcvol | 191.540 | ml/mol | McGowan Method |
| pc | 2231.30 | kPa | Joback Method |
| rinpol | 2064.00 | | NIST Webbook |
| tb | 713.13 | K | Joback Method |
| tc | 931.03 | K | Joback Method |
| tf | 457.30 | K | Joback Method |
| vc | 0.738 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 504.17 | J/mol×K | 713.13 | Joback Method |
| cpg | 517.49 | J/mol×K | 749.45 | Joback Method |
| cpg | 529.87 | J/mol×K | 785.76 | Joback Method |
| cpg | 541.33 | J/mol×K | 822.08 | Joback Method |
| cpg | 551.86 | J/mol×K | 858.40 | Joback Method |
| cpg | 561.47 | J/mol×K | 894.72 | Joback Method |
| cpg | 570.16 | J/mol×K | 931.03 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357684&Units=SI |

# 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 |