# 2,3,4-Trifluorobenzoic acid, 4-methoxyphenyl ester

**Inchi:** InChI=1S/C14H9F3O3/c1-19-8-2-4-9(5-3-8)20-14(18)10-6-7-11(15)13(17)12(10)16/h2-7H

**InchiKey:** BUDRKSKGWADFOT-UHFFFAOYSA-N

**Formula:** C14H9F3O3

**SMILES:** COc1ccc(OC(=O)c2ccc(F)c(F)c2F)cc1

**Mol. weight [g/mol]:** 282.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -670.05 | kJ/mol | Joback Method |
| hf | -870.46 | kJ/mol | Joback Method |
| hfus | 31.76 | kJ/mol | Joback Method |
| hvap | 63.07 | kJ/mol | Joback Method |
| log10ws | -4.67 | | Crippen Method |
| logp | 3.332 | | Crippen Method |
| mcvol | 179.220 | ml/mol | McGowan Method |
| pc | 2342.82 | kPa | Joback Method |
| rinpol | 1846.00 | | NIST Webbook |
| rinpol | 1846.00 | | NIST Webbook |
| tb | 689.52 | K | Joback Method |
| tc | 901.81 | K | Joback Method |
| tf | 446.62 | K | Joback Method |
| vc | 0.700 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 460.63 | J/mol×K | 689.52 | Joback Method |
| cpg | 472.83 | J/mol×K | 724.90 | Joback Method |
| cpg | 484.20 | J/mol×K | 760.28 | Joback Method |
| cpg | 494.75 | J/mol×K | 795.67 | Joback Method |
| cpg | 504.48 | J/mol×K | 831.05 | Joback Method |
| cpg | 513.39 | J/mol×K | 866.43 | Joback Method |
| cpg | 521.47 | J/mol×K | 901.81 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308033&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 |

# 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 |