# 3-Methoxy-2,4,5-trifluorobenzoic acid, 2,2,2-trichloroethyl ester

**Inchi:** InChI=1S/C10H6Cl3F3O3/c1-18-8-6(15)4(2-5(14)7(8)16)9(17)19-3-10(11,12)13/h2H,3H2

**InchiKey:** ZQBRAJZNGINPAK-UHFFFAOYSA-N

**Formula:** C10H6Cl3F3O3

**SMILES:** COc1c(F)c(F)cc(C(=O)OCC(Cl)(Cl)Cl)c1F

**Mol. weight [g/mol]:** 337.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -849.09 | kJ/mol | Joback Method |
| hf | -1080.40 | kJ/mol | Joback Method |
| hfus | 32.53 | kJ/mol | Joback Method |
| hvap | 63.75 | kJ/mol | Joback Method |
| log10ws | -4.81 | | Crippen Method |
| logp | 3.640 | | Crippen Method |
| mcvol | 183.340 | ml/mol | McGowan Method |
| pc | 2256.81 | kPa | Joback Method |
| rinpol | 1739.00 | | NIST Webbook |
| rinpol | 1739.00 | | NIST Webbook |
| tb | 680.38 | K | Joback Method |
| tc | 888.91 | K | Joback Method |
| tf | 467.30 | K | Joback Method |
| vc | 0.720 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.14 | J/mol×K | 680.38 | Joback Method |
| cpg | 428.03 | J/mol×K | 715.13 | Joback Method |
| cpg | 436.30 | J/mol×K | 749.89 | Joback Method |
| cpg | 443.95 | J/mol×K | 784.64 | Joback Method |
| cpg | 450.99 | J/mol×K | 819.40 | Joback Method |
| cpg | 457.43 | J/mol×K | 854.15 | Joback Method |
| cpg | 463.27 | J/mol×K | 888.91 | Joback Method |

# Sources

| | |
|---|---|
| **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=U360572&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |