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

**Inchi:** InChI=1S/C22H33F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-28-22(26)17-16-18(23)20(2

**InchiKey:** ANKSIQFSTWOYQI-UHFFFAOYSA-N

**Formula:** C22H33F3O3

**SMILES:** CCCCCCCCCCCCCCOC(=O)c1cc(F)c(F)c(OC)c1F

**Mol. weight [g/mol]:** 402.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -715.10 | kJ/mol | Joback Method |
| hf | -1272.11 | kJ/mol | Joback Method |
| hfus | 58.44 | kJ/mol | Joback Method |
| hvap | 78.61 | kJ/mol | Joback Method |
| log10ws | -8.27 | | Crippen Method |
| logp | 6.970 | | Crippen Method |
| mcvol | 315.700 | ml/mol | McGowan Method |
| pc | 998.28 | kPa | Joback Method |
| rinpol | 2558.00 | | NIST Webbook |
| rinpol | 2558.00 | | NIST Webbook |
| tb | 845.88 | K | Joback Method |
| tc | 1036.33 | K | Joback Method |
| tf | 510.36 | K | Joback Method |
| vc | 1.256 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 997.69 | J/mol×K | 845.88 | Joback Method |
| cpg | 1014.86 | J/mol×K | 877.62 | Joback Method |
| cpg | 1030.93 | J/mol×K | 909.36 | Joback Method |
| cpg | 1045.91 | J/mol×K | 941.10 | Joback Method |
| cpg | 1059.82 | J/mol×K | 972.84 | Joback Method |
| cpg | 1072.66 | J/mol×K | 1004.58 | Joback Method |
| cpg | 1084.46 | J/mol×K | 1036.33 | 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=U338771&Units=SI |

# 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 |