# 2,4,5-Trifluoro-3-methoxybenzoic acid, 5-pentadecyl ester

**Inchi:** InChI=1S/C23H35F3O3/c1-4-6-8-9-10-11-12-13-15-17(14-7-5-2)29-23(27)18-16-19(24)2
**InchiKey:** FGHWXONJVBRQRC-UHFFFAOYSA-N
**Formula:** C23H35F3O3
**SMILES:** CCCCCCCCCCC(CCCC)OC(=O)c1cc(F)c(F)c(OC)c1F
**Mol. weight [g/mol]:** 416.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -709.12 | kJ/mol | Joback Method |
| hf | -1298.03 | kJ/mol | Joback Method |
| hfus | 57.50 | kJ/mol | Joback Method |
| hvap | 80.44 | kJ/mol | Joback Method |
| log10ws | -8.80 | | Crippen Method |
| logp | 7.359 | | Crippen Method |
| mcvol | 329.790 | ml/mol | McGowan Method |
| pc | 945.00 | kPa | Joback Method |
| rinpol | 2489.00 | | NIST Webbook |
| rinpol | 2489.00 | | NIST Webbook |
| tb | 868.32 | K | Joback Method |
| tc | 1063.27 | K | Joback Method |
| tf | 506.63 | K | Joback Method |
| vc | 1.306 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1059.02 | J/mol×K | 868.32 | Joback Method |
| cpg | 1076.63 | J/mol×K | 900.81 | Joback Method |
| cpg | 1093.03 | J/mol×K | 933.30 | Joback Method |
| cpg | 1108.24 | J/mol×K | 965.79 | Joback Method |
| cpg | 1122.29 | J/mol×K | 998.28 | Joback Method |
| cpg | 1135.19 | J/mol×K | 1030.78 | Joback Method |
| cpg | 1146.96 | J/mol×K | 1063.27 | Joback Method |

# Sources

| | |
|---|---|
| **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=U338468&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |