# 2-Fluoro-3-trifluoromethylbenzoic acid, eicosyl ester

**Inchi:** InChI=1S/C28H44F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-34-27(33

**InchiKey:** XUEAFLOQFPVLSA-UHFFFAOYSA-N

**Formula:** C28H44F4O2

**SMILES:** CCCCCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(F)(F)F)c1F

**Mol. weight [g/mol]:** 488.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -732.29 | kJ/mol | Joback Method |
| hf | -1445.65 | kJ/mol | Joback Method |
| hfus | 69.23 | kJ/mol | Joback Method |
| hvap | 86.11 | kJ/mol | Joback Method |
| log10ws | -11.10 | | Crippen Method |
| logp | 10.043 | | Crippen Method |
| mcvol | 396.140 | ml/mol | McGowan Method |
| pc | 722.63 | kPa | Joback Method |
| rinpol | 2979.00 | | NIST Webbook |
| rinpol | 2979.00 | | NIST Webbook |
| tb | 946.82 | K | Joback Method |
| tc | 1165.03 | K | Joback Method |
| tf | 533.72 | K | Joback Method |
| vc | 1.581 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1347.17 | J/mol×K | 946.82 | Joback Method |
| cpg | 1367.59 | J/mol×K | 983.19 | Joback Method |
| cpg | 1386.59 | J/mol×K | 1019.56 | Joback Method |
| cpg | 1404.26 | J/mol×K | 1055.93 | Joback Method |
| cpg | 1420.71 | J/mol×K | 1092.30 | Joback Method |
| cpg | 1436.02 | J/mol×K | 1128.66 | Joback Method |
| cpg | 1450.30 | J/mol×K | 1165.03 | 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=U338735&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 |