# 4-Fluoro-2-trifluoromethylbenzoic acid, tetradecyl ester

**Inchi:** InChI=1S/C22H32F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-28-21(27)19-15-14-18(23)17

**InchiKey:** KUVWDPMBGFYORJ-UHFFFAOYSA-N

**Formula:** C22H32F4O2

**SMILES:** CCCCCCCCCCCCCCOC(=O)c1ccc(F)cc1C(F)(F)F

**Mol. weight [g/mol]:** 404.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -782.81 | kJ/mol | Joback Method |
| hf | -1321.81 | kJ/mol | Joback Method |
| hfus | 53.69 | kJ/mol | Joback Method |
| hvap | 72.76 | kJ/mol | Joback Method |
| log10ws | -8.59 | | Crippen Method |
| logp | 7.702 | | Crippen Method |
| mcvol | 311.600 | ml/mol | McGowan Method |
| pc | 1011.66 | kPa | Joback Method |
| rinpol | 2315.00 | | NIST Webbook |
| rinpol | 2315.00 | | NIST Webbook |
| tb | 809.54 | K | Joback Method |
| tc | 994.06 | K | Joback Method |
| tf | 466.10 | K | Joback Method |
| vc | 1.244 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 975.71 | J/mol×K | 809.54 | Joback Method |
| cpg | 992.89 | J/mol×K | 840.29 | Joback Method |
| cpg | 1009.07 | J/mol×K | 871.05 | Joback Method |
| cpg | 1024.29 | J/mol×K | 901.80 | Joback Method |
| cpg | 1038.60 | J/mol×K | 932.55 | Joback Method |
| cpg | 1052.04 | J/mol×K | 963.31 | Joback Method |
| cpg | 1064.65 | J/mol×K | 994.06 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U338831&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |