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

**Inchi:** InChI=1S/C24H36F4O2/c1-3-5-6-7-8-9-10-11-12-13-14-16-19(4-2)30-23(29)20-17-15-18
**InchiKey:** QHQWVHABXBKBRU-UHFFFAOYSA-N
**Formula:** C24H36F4O2
**SMILES:** CCCCCCCCCCCCCC(CC)OC(=O)c1cccc(C(F)(F)F)c1F
**Mol. weight [g/mol]:** 432.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -768.41 | kJ/mol | Joback Method |
| hf | -1368.37 | kJ/mol | Joback Method |
| hfus | 55.35 | kJ/mol | Joback Method |
| hvap | 76.82 | kJ/mol | Joback Method |
| log10ws | -9.54 | | Crippen Method |
| logp | 8.481 | | Crippen Method |
| mcvol | 339.780 | ml/mol | McGowan Method |
| pc | 902.89 | kPa | Joback Method |
| rinpol | 2446.00 | | NIST Webbook |
| rinpol | 2446.00 | | NIST Webbook |
| tb | 854.86 | K | Joback Method |
| tc | 1047.04 | K | Joback Method |
| tf | 473.64 | K | Joback Method |
| vc | 1.351 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1097.37 | J/mol×K | 854.86 | Joback Method |
| cpg | 1115.45 | J/mol×K | 886.89 | Joback Method |
| cpg | 1132.40 | J/mol×K | 918.92 | Joback Method |
| cpg | 1148.30 | J/mol×K | 950.95 | Joback Method |
| cpg | 1163.19 | J/mol×K | 982.98 | Joback Method |
| cpg | 1177.13 | J/mol×K | 1015.01 | Joback Method |
| cpg | 1190.17 | J/mol×K | 1047.04 | 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=U338528&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 |