# 3-Fluoro-5-trifluoromethylbenzoic acid, neopentyl ester

**Inchi:** InChI=1S/C13H14F4O2/c1-12(2,3)7-19-11(18)8-4-9(13(15,16)17)6-10(14)5-8/h4-6H,7H2

**InchiKey:** SGHDTNDWCXOFSQ-UHFFFAOYSA-N

**Formula:** C13H14F4O2

**SMILES:** CC(C)(C)COC(=O)c1cc(F)cc(C(F)(F)F)c1

**Mol. weight [g/mol]:** 278.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -855.75 | kJ/mol | Joback Method |
| hf | -1144.80 | kJ/mol | Joback Method |
| hfus | 22.97 | kJ/mol | Joback Method |
| hvap | 51.43 | kJ/mol | Joback Method |
| log10ws | -4.58 | | Crippen Method |
| logp | 4.047 | | Crippen Method |
| mcvol | 184.790 | ml/mol | McGowan Method |
| pc | 1956.14 | kPa | Joback Method |
| rinpol | 1248.00 | | NIST Webbook |
| rinpol | 1248.00 | | NIST Webbook |
| tb | 600.39 | K | Joback Method |
| tc | 791.41 | K | Joback Method |
| tf | 367.09 | K | Joback Method |
| vc | 0.730 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 481.60 | J/mol×K | 600.39 | Joback Method |
| cpg | 495.65 | J/mol×K | 632.23 | Joback Method |
| cpg | 508.79 | J/mol×K | 664.06 | Joback Method |
| cpg | 521.09 | J/mol×K | 695.90 | Joback Method |
| cpg | 532.59 | J/mol×K | 727.74 | Joback Method |
| cpg | 543.32 | J/mol×K | 759.58 | Joback Method |
| cpg | 553.33 | J/mol×K | 791.41 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357951&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 |