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

**Inchi:** InChI=1S/C13H15F3O3/c1-13(2,3)6-19-12(17)7-5-8(14)10(16)11(18-4)9(7)15/h5H,6H2,1

**InchiKey:** NPFGROSBKBLGQG-UHFFFAOYSA-N

**Formula:** C13H15F3O3

**SMILES:** COc1c(F)c(F)cc(C(=O)OCC(C)(C)C)c1F

**Mol. weight [g/mol]:** 276.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -788.04 | kJ/mol | Joback Method |
| hf | -1095.10 | kJ/mol | Joback Method |
| hfus | 27.71 | kJ/mol | Joback Method |
| hvap | 57.28 | kJ/mol | Joback Method |
| log10ws | -4.26 | | Crippen Method |
| logp | 3.315 | | Crippen Method |
| mcvol | 188.890 | ml/mol | McGowan Method |
| pc | 1920.30 | kPa | Joback Method |
| rinpol | 1533.00 | | NIST Webbook |
| tb | 636.73 | K | Joback Method |
| tc | 826.71 | K | Joback Method |
| tf | 411.35 | K | Joback Method |
| vc | 0.741 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 495.08 | J/mol×K | 636.73 | Joback Method |
| cpg | 508.45 | J/mol×K | 668.39 | Joback Method |
| cpg | 521.12 | J/mol×K | 700.06 | Joback Method |
| cpg | 533.11 | J/mol×K | 731.72 | Joback Method |
| cpg | 544.41 | J/mol×K | 763.39 | Joback Method |
| cpg | 555.03 | J/mol×K | 795.05 | Joback Method |
| cpg | 564.99 | J/mol×K | 826.71 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357607&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

| | |
|---|---|
| **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 |