# 6-Fluoro-2-trifluoromethylbenzoic acid, nonyl ester

**Inchi:** InChI=1S/C17H22F4O2/c1-2-3-4-5-6-7-8-12-23-16(22)15-13(17(19,20)21)10-9-11-14(15

**InchiKey:** CRNYPPIXOSSGIP-UHFFFAOYSA-N

**Formula:** C17H22F4O2

**SMILES:** CCCCCCCCCOC(=O)c1c(F)cccc1C(F)(F)F

**Mol. weight [g/mol]:** 334.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -824.91 | kJ/mol | Joback Method |
| hf | -1218.61 | kJ/mol | Joback Method |
| hfus | 40.74 | kJ/mol | Joback Method |
| hvap | 61.63 | kJ/mol | Joback Method |
| log10ws | -6.50 | | Crippen Method |
| logp | 5.752 | | Crippen Method |
| mcvol | 241.150 | ml/mol | McGowan Method |
| pc | 1409.07 | kPa | Joback Method |
| rinpol | 1847.00 | | NIST Webbook |
| rinpol | 1847.00 | | NIST Webbook |
| tb | 695.14 | K | Joback Method |
| tc | 873.15 | K | Joback Method |
| tf | 409.75 | K | Joback Method |
| vc | 0.965 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 688.03 | J/mol×K | 695.14 | Joback Method |
| cpg | 703.30 | J/mol×K | 724.81 | Joback Method |
| cpg | 717.74 | J/mol×K | 754.48 | Joback Method |
| cpg | 731.37 | J/mol×K | 784.15 | Joback Method |
| cpg | 744.21 | J/mol×K | 813.81 | Joback Method |
| cpg | 756.32 | J/mol×K | 843.48 | Joback Method |
| cpg | 767.70 | J/mol×K | 873.15 | Joback Method |

# Sources

| | |
|---|---|
| **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=U338983&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |