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

**Inchi:** InChI=1S/C11H10F4O2/c1-2-3-17-10(16)7-4-8(11(13,14)15)6-9(12)5-7/h4-6H,2-3H2,1H3

**InchiKey:** UHMOYGBVUYEYOA-UHFFFAOYSA-N

**Formula:** C11H10F4O2

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

**Mol. weight [g/mol]:** 250.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -875.43 | kJ/mol | Joback Method |
| hf | -1094.77 | kJ/mol | Joback Method |
| hfus | 25.20 | kJ/mol | Joback Method |
| hvap | 48.27 | kJ/mol | Joback Method |
| log10ws | -3.99 | | Crippen Method |
| logp | 3.411 | | Crippen Method |
| mcvol | 156.610 | ml/mol | McGowan Method |
| pc | 2293.71 | kPa | Joback Method |
| rinpol | 1186.00 | | NIST Webbook |
| rinpol | 1186.00 | | NIST Webbook |
| tb | 557.86 | K | Joback Method |
| tc | 743.16 | K | Joback Method |
| tf | 342.13 | K | Joback Method |
| vc | 0.628 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 382.19 | J/mol×K | 557.86 | Joback Method |
| cpg | 394.31 | J/mol×K | 588.74 | Joback Method |
| cpg | 405.75 | J/mol×K | 619.63 | Joback Method |
| cpg | 416.53 | J/mol×K | 650.51 | Joback Method |
| cpg | 426.68 | J/mol×K | 681.40 | Joback Method |
| cpg | 436.21 | J/mol×K | 712.28 | Joback Method |
| cpg | 445.15 | J/mol×K | 743.16 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U338893&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 |

# 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 |