# 3-Fluoro-4-trifluoromethylbenzoic acid, 4-benzyloxyphenyl ester

**Inchi:** InChI=1S/C21H14F4O3/c22-19-12-15(6-11-18(19)21(23,24)25)20(26)28-17-9-7-16(8-10-

**InchiKey:** BPFSQMGOPHHUMR-UHFFFAOYSA-N

**Formula:** C21H14F4O3

**SMILES:** O=C(Oc1ccc(OCc2ccccc2)cc1)c1ccc(C(F)(F)F)c(F)c1

**Mol. weight [g/mol]:** 390.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -681.04 | kJ/mol | Joback Method |
| hf | -971.80 | kJ/mol | Joback Method |
| hfus | 39.98 | kJ/mol | Joback Method |
| hvap | 78.16 | kJ/mol | Joback Method |
| log10ws | -7.22 | | Crippen Method |
| logp | 5.643 | | Crippen Method |
| mcvol | 255.860 | ml/mol | McGowan Method |
| pc | 1710.36 | kPa | Joback Method |
| rinpol | 2618.00 | | NIST Webbook |
| rinpol | 2618.00 | | NIST Webbook |
| tb | 867.42 | K | Joback Method |
| tc | 1094.88 | K | Joback Method |
| tf | 542.42 | K | Joback Method |
| vc | 0.991 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 755.82 | J/mol×K | 867.42 | Joback Method |
| cpg | 768.15 | J/mol×K | 905.33 | Joback Method |
| cpg | 779.27 | J/mol×K | 943.24 | Joback Method |
| cpg | 789.25 | J/mol×K | 981.15 | Joback Method |
| cpg | 798.16 | J/mol×K | 1019.06 | Joback Method |
| cpg | 806.08 | J/mol×K | 1056.97 | Joback Method |
| cpg | 813.07 | J/mol×K | 1094.88 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357948&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 |