# 2,5-Di(trifluoromethyl)benzoic acid, 3-fluorophenyl ester

**Inchi:** InChI=1S/C15H7F7O2/c16-9-2-1-3-10(7-9)24-13(23)11-6-8(14(17,18)19)4-5-12(11)15(20

**InchiKey:** LWBRNIAJKIFWCD-UHFFFAOYSA-N

**Formula:** C15H7F7O2

**SMILES:** O=C(Oc1cccc(F)c1)c1cc(C(F)(F)F)ccc1C(F)(F)F

**Mol. weight [g/mol]:** 352.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1320.56 | kJ/mol | Joback Method |
| hf | -1549.35 | kJ/mol | Joback Method |
| hfus | 31.04 | kJ/mol | Joback Method |
| hvap | 56.37 | kJ/mol | Joback Method |
| log10ws | -6.10 | | Crippen Method |
| logp | 5.082 | | Crippen Method |
| mcvol | 194.520 | ml/mol | McGowan Method |
| pc | 1937.24 | kPa | Joback Method |
| rinpol | 1528.00 | | NIST Webbook |
| rinpol | 1528.00 | | NIST Webbook |
| tb | 675.62 | K | Joback Method |
| tc | 873.27 | K | Joback Method |
| tf | 430.34 | K | Joback Method |
| vc | 0.787 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 525.89 | J/mol×K | 675.62 | Joback Method |
| cpg | 537.54 | J/mol×K | 708.56 | Joback Method |
| cpg | 548.27 | J/mol×K | 741.50 | Joback Method |
| cpg | 558.13 | J/mol×K | 774.44 | Joback Method |
| cpg | 567.19 | J/mol×K | 807.39 | Joback Method |
| cpg | 575.50 | J/mol×K | 840.33 | Joback Method |
| cpg | 583.12 | J/mol×K | 873.27 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357366&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 |