

# 6-Fluoro-3-trifluoromethylbenzoic acid, 3-fluorophenyl ester

**Other names:** 6-Fluoro-3-trifluorobenzoic acid, 3-fluorophenyl ester

**Inchi:** InChI=1S/C14H7F5O2/c15-9-2-1-3-10(7-9)21-13(20)11-6-8(14(17,18)19)4-5-12(11)16/h1

**InchiKey:** FBUXMQXMFIVGEF-UHFFFAOYSA-N

**Formula:** C14H7F5O2

**SMILES:** O=C(Oc1cccc(F)c1)c1cc(C(F)(F)F)ccc1F

**Mol. weight [g/mol]:** 302.20

## Physical Properties

Property code	Value	Unit	Source
gf	-942.20	kJ/mol	Joback Method
hf	-1127.74	kJ/mol	Joback Method
hfus	29.70	kJ/mol	Joback Method
hvap	57.07	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.203		Crippen Method
mcvol	176.890	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1596.00		NIST Webbook
rinpol	1596.00		NIST Webbook
tb	657.43	K	Joback Method
tc	864.10	K	Joback Method
tf	415.47	K	Joback Method
vc	0.707	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.51	J/mol×K	657.43	Joback Method
cpg	468.38	J/mol×K	691.87	Joback Method
cpg	479.35	J/mol×K	726.32	Joback Method
cpg	489.48	J/mol×K	760.76	Joback Method
cpg	498.79	J/mol×K	795.21	Joback Method
cpg	507.35	J/mol×K	829.65	Joback Method
cpg	515.17	J/mol×K	864.10	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U343783&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343783&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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