

2-Fluoro-3-(trifluoromethyl)phenol, tert-butyl dimethylsilyl ether

Other names:	2-Fluoro-3-(trifluoromethyl)phenol, tbdms derivative
Inchi:	InChI=1S/C13H18F4OSi/c1-12(2,3)19(4,5)18-10-8-6-7-9(11(10)14)13(15,16)17/h6-8H,1-
InchiKey:	FAFWUTVIHQCVBA-UHFFFAOYSA-N
Formula:	C13H18F4OSi
SMILES:	CC(C)(C)[Si](C)(C)Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	294.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	5.229		Crippen Method
rinpol	1289.20		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/29-334-9/2-Fluoro-3-trifluoromethyl-phenol-tert-butyl-dimethylsilyl-ether.pdf>

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