

2-Fluorobenzoic acid, tert-butyldimethylsilyl ester

Other names:	tert-Butyldimethylsilyl 2-fluorobenzoate
Inchi:	InChI=1S/C13H19FO2Si/c1-13(2,3)17(4,5)16-12(15)10-8-6-7-9-11(10)14/h6-9H,1-5H3
InchiKey:	WQUPZSPFDKBRQY-UHFFFAOYSA-N
Formula:	C13H19FO2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1F
Mol. weight [g/mol]:	254.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	3.988		Crippen Method
rinpol	1522.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/34-036-4/2-Fluorobenzoic-acid-tert-butyldimethylsilyl-ester.pdf>

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