tert-Butyldimethylsilyl 4-(trifluoromethyl)benzoate

Inchi: InChI=1S/C14H19F3O2Si/c1-13(2,3)20(4,5)19-12(18)10-6-8-11(9-7-10)14(15,16)17/h6-9

InchiKey: BXOAIFGVRSDJRE-UHFFFAOYSA-N

Formula: C14H19F3O2Si

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	4.867		Crippen Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373177&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/40-172-6/tert-Butyldimethylsilyl-4-trifluoromethyl-benzoate.pdf

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