Pholedrine N-TFA-O-TMS

Inchi:	InChI=1S/C15H22F3NO2Si/c1-11(19(2)14(20)15(16,17)18)10-12-6-8-13(9-7-12)21-22(3,
InchiKey:	BXTHWTVTDNVFJY-UHFFFAOYSA-N
Formula:	C15H22F3NO2Si
SMILES:	CC(Cc1ccc(O[Si](C)(C)C)cc1)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]:	333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	3.852		Crippen Method
rinpol	1734.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R83685&Units=SI

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/18-368-4/Pholedrine-N-TFA-O-TMS.pdf

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