

Flufenamic acid, tert-butyldimethylsilyl ester

Other names:	Flufenamic acid, TBDMS Flufenamic acid, tbdms derivative
Inchi:	InChI=1S/C20H24F3NO2Si/c1-19(2,3)27(4,5)26-18(25)16-11-6-7-12-17(16)24-15-10-8-9
InchiKey:	QIRMOLPCESLBND-UHFFFAOYSA-N
Formula:	C20H24F3NO2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1cccc1Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	395.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	6.611		Crippen Method
rinpol	2232.20		NIST Webbook
rinpol	2258.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333178&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/65-283-6/Flufenamic-acid-tert-butyldimethylsilyl-ester.pdf>

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