N-Trifluoroacetyl-O,O'-bis(trimethylsilyl)-l-dopa, trimethylsilyl ester

Other names: 3,4-Dihydroxyphenylalanine, N-TFA-O-TMS

Inchi: InChI=1S/C20H34F3NO5Si3/c1-30(2,3)27-16-11-10-14(13-17(16)28-31(4,5)6)12-15(18(2

InchiKey: OGIZXHXABNSGRO-UHFFFAOYSA-N

Formula: C20H34F3NO5Si3

SMILES: C[Si](C)(C)OC(=O)C(Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)NC(=O)C(F)(F)F

Mol. weight [g/mol]: 509.74

Physical Properties

Property code	Value	Unit	Source
log10ws	0.55		Crippen Method
logp	5.082		Crippen Method
rinpol	2057.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U72266&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices