N-Methyl-3,4-dihydroxyphenylalanine, N-TFA-O-TMS

Inchi: InChI=1S/C21H36F3NO5Si3/c1-25(20(27)21(22,23)24)16(19(26)30-33(8,9)10)13-15-11-

InchiKey: YHZNNDRWAXPVGP-UHFFFAOYSA-N

Formula: C21H36F3NO5Si3

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

Mol. weight [g/mol]: 523.77

Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	5.424		Crippen Method
rinpol	2165.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R139189&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