

3,4-Dihydroxy-dl-phenylalanine, N,O,O'-tris(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl
N,O,O'-tris(tert-butyldimethylsilyl)-3,4-dihydroxy-dl-phenylalanine, 3-tyrrol[tert-butyl(dimethyl)silyl]oxymorphotyrosinate
3-Hydroxy-dl-tyrosine, 4tbdm's derivative

Inchi:	InChI=1S/C33H67NO4Si4/c1-30(2,3)39(13,14)34-26(29(35)38-42(19,20)33(10,11)12)23-
InchiKey:	RQNRUYXQVVJYOC-UHFFFAOYSA-N
Formula:	C33H67NO4Si4
SMILES:	CC(C)(C)[Si](C)(C)NC(Cc1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1)C(=O)O[S
Mol. weight [g/mol]:	654.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	10.509		Crippen Method
rinpol	3035.40		NIST Webbook
rinpol	3035.40		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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