L-Tryptophan, N,1-bis(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names: Try, TBDMS, L-tryptophan, 3tbdms derivative

Inchi: InChI=1S/C29H54N2O2Si3/c1-27(2,3)34(10,11)30-24(26(32)33-36(14,15)29(7,8)9)20-22

InchiKey: JCQLAQJLIDUWOW-DEOSSOPVSA-N

Formula: C29H54N2O2Si3

SMILES: CC(C)(C)[Si](C)(C)NC(Cc1cn([Si](C)(C)C(C)(C)C)c2ccccc12)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 547.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	8.549		Crippen Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U143132&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