tert-Butyldimethylsilyl 2-[(tert-butyldimethylsilyl)amino]-3-(4-[(tert-butyld

Other names: 2-Amino-3-(3-chloro-4-hydroxy-phenyl)propanoic acid, N,O,O'-tris(tert-butyldimethylsilyl)-
tert-Butyldimethylsilyl 2-[(tert-butyldimethylsilyl)amino]-3-{4-[(tert-butyldimethylsilyl)oxy]-3-chlorophenyl}propanc

Inchi: InChI=1S/C27H52ClNO3Si3/c1-25(2,3)33(10,11)29-22(24(30)32-35(14,15)27(7,8)9)19-2

InchiKey: PSYIWVRQSLWOAQ-UHFFFAOYSA-N

Formula: C27H52ClNO3Si3

SMILES: CC(C)(C)[Si](C)(C)NC(Cc1ccc(O[Si](C)(C)C(C)(C)C)c(Cl)c1)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 558.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	8.778		Crippen Method
rinpol	2808.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U378757&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