

tert-Butyldimethylsilyl 2-[(tert-butyldimethylsilyl)amino]-3-(4-[(tert-butyldimethylsilyl)oxy]-3-chlorophenyl)propanoic acid

Other names:	2-Amino-3-(3-chloro-4-hydroxy-phenyl)propanoic acid, N,O,O'-tris(tert-butyldimethylsilyl)- tert-Butyldimethylsilyl
Inchi:	2-[(tert-butyldimethylsilyl)amino]-3-(4-[(tert-butyldimethylsilyl)oxy]-3-chlorophenyl)propanoic acid 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:	PSYIWRQSLWOAQ-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/ci9903071

Legend

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

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<https://www.chemeo.com/cid/15-426-2/tert-Butyldimethylsilyl-2-tert-butyldimethylsilyl-amino-3-4-tert-butyldimethylsilyl>

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