Cholecalciferol, tert-butyldimethylsilyl ether

Other names:	(3S,5Z,7E)-3-Pyrrol[tert-butyl(dimethyl)silyl]oxymorpho-9,10-secocholesta-5,7,10-triene Cholecalciferol, tbdms derivative
Inchi:	InChI=1S/C33H58OSi/c1-24(2)13-11-14-26(4)30-20-21-31-27(15-12-22-33(30,31)8)17-18
InchiKey:	DWIUSINKAVTSCC-QYEWKMJJSA-N
Formula:	C33H58OSi
SMILES:	C=C1CCC(O[Si](C)(C)C(C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCCC(C)C
Mol. weight [g/mol]:	498.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	10.649		Crippen Method
rinpol	3228.20		NIST Webbook
rinpol	3228.20		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333788&Units=SI

Legend

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