Cholecalciferol, trimethylsilyl ether

Other names:	(3S,5Z,7E)-3-Methoxy-9,10-secocholesta-5,7,10-triene
	Cholecalciferol, tms derivative
Inchi:	InChI=1S/C30H52OSi/c1-22(2)11-9-12-24(4)28-18-19-29-25(13-10-20-30(28,29)5)15-16-
InchiKey:	GWVMYANKBNXDQN-RYQLWAFASA-N
Formula:	C30H52OSi
SMILES:	C=C1CCC(O[Si](C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCCC(C)C
Mol. weight [g/mol]:	456.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.67		Crippen Method
logp	9.478		Crippen Method
rinpol	3104.10		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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