Methyl (25RS)-3«beta»-hydroxy-5-cholesten-26-oate, trimethylsilyl ether

Other names:	3«beta»-Hydroxy-5-cholestenoate, MeTMS Methyl 3-hydroxycholest-5-en-26-oate, tms derivative
Inchi:	InChI=1S/C31H54O3Si/c1-21(10-9-11-22(2)29(32)33-5)26-14-15-27-25-13-12-23-20-24(
InchiKey:	DNXGNXYNSBCWGX-QBUYVTDMSA-N
Formula:	C31H54O3Si
SMILES:	COC(=O)C(C)CCCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	502.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	8.401		Crippen Method
rinpol	3425.00		NIST Webbook
rinpol	3425.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U99777&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

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