

3«beta»,7a-Dihydroxy-5-cholestenoate, MeTMS

Other names:	3-«beta»,7-«alpha»-Dihydroxy-5-cholestenoic acid, methyl ester, TMS
Inchi:	InChI=1S/C34H62O4Si2/c1-23(13-12-14-24(2)32(35)36-5)27-15-16-28-31-29(18-20-34(2
InchiKey:	XMQRPHQEIMCXFD-NJJFLDHASA-N
Formula:	C34H62O4Si2
SMILES:	COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]:	591.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	9.231		Crippen Method
rinpol	3411.00		NIST Webbook
rinpol	3415.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R264423&Units=SI

Legend

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

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