Hyocholic acid, trimethyl ether-methyl ester

Other names:	3-«alpha»,6-«alpha»,7-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS 5-«beta»-Cholanoic acid, 3-«alpha»,6-«alpha»,7-«alpha»-trihydroxy, methyl ester, TMS 3«alpha»,6«alpha»,7«alpha»-Trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether
Inchi:	InChI=1S/C34H66O5Si3/c1-23(14-17-29(35)36-4)25-15-16-26-30-27(19-21-33(25,26)2)3
InchiKey:	MPBUWUAYSDIDGN-LSZIAPHPSA-N
Formula:	C34H66O5Si3
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(
Mol. weight [g/mol]:	639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3336.00		NIST Webbook
rinpol	3361.00		NIST Webbook
rinpol	3336.00		NIST Webbook
rinpol	3304.00		NIST Webbook
rinpol	3304.00		NIST Webbook
rinpol	3336.00		NIST Webbook
rinpol	3304.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182584&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