5-«alpha»-Cholanoic acid, 3-«alpha»-6-«alpha»,7-«alpha»,12-«alpha»-tetrahy methyl ester, TMS

Inchi:	InChI=1S/C37H74O6Si4/c1-25(17-20-32(38)39-4)27-18-19-28-33-29(24-31(37(27,28)3)4
InchiKey:	CAHBNWKLPVHQBG-HEVXDBMNSA-N
Formula:	C37H74O6Si4
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]:	727.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3226.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393823&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

Latest version available from:

https://www.chemeo.com/cid/56-959-6/5-alpha-Cholanoic-acid-3-alpha-6-alpha-7-alpha-12-alpha-tetrahydroxy-methy

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