allo-Cholanic acid, 3«beta»,7«beta»,12«alpha»-trihydroxy, Me-TMS

Other names:	3«beta»,7«beta»,12«alpha»-Trihydroxy-5«alpha»-cholanic acid, methyl ester, TMS
Inchi:	InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3
InchiKey:	DQKFOBXAKZGIPX-DGWXSNGGSA-N
Formula:	C34H66O5Si3
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si]
Mol. weight [g/mol]:	639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3340.00		NIST Webbook
rinpol	3340.00		NIST Webbook
rinpol	3340.00		NIST Webbook
ripol	3713.00		NIST Webbook
ripol	3713.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R533630&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
ripol:	Polar retention indices

Latest version available from:

https://www.chemeo.com/cid/66-691-2/allo-Cholanic-acid-3-beta-7-beta-12-alpha-trihydroxy-Me-TMS.pdf

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