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

Other names:	3«alpha»,7«alpha»,12«alpha»-Trihydroxy-5«beta»-cholanic acid, methyl ester, TMS 5«beta»-Cholan-24-oic acid, 3«alpha»,7«alpha»,12«alpha»-tris(trimethylsiloxy)-, methyl ester Methyl 3,7,12-tris[(trimethylsilyl)oxy]cholan-24-oate, (3«alpha»,5«beta»,7«alpha»,12«alpha»)- 3«alpha»,7«alpha»,12«alpha»-Trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether 3-«alpha»,7-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS 5-«beta»-Cholanoic acid, 3-«alpha»-7-«alpha»12-«alpha»-trihydroxy, methyl ester, TMS Cholic acid, methyl ester, TMS Cholic acid, trimethylsilyl ether-methyl ester 3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-cholestanoic acid, trimethylsilyl ether-methyl ester Methyl cholate, 3tms derivative
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-VBGMGSDVSA-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	3228.00		NIST Webbook
rinpol	3227.00		NIST Webbook
rinpol	3228.00		NIST Webbook
rinpol	3261.00		NIST Webbook
rinpol	3212.00		NIST Webbook
rinpol	3228.00		NIST Webbook
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook
ripol	3455.00		NIST Webbook
ripol	3455.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6818435&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