

Methyl 3-«beta»,7-«alpha»,12-«alpha»-trihydroxy-5-«beta»-cholanoate-TMS

Other names:	3-«beta»,7-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS
Inchi:	5-«beta»-Cholanoic acid, 3-«beta»-7-«alpha»,12-«alpha»-trihydroxy, methyl ester, TMS
InchiKey:	DQKFOBXAKZGIPX-XXOUCPERSA-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](C)(C)C)C
Mol. weight [g/mol]:	639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3210.00		NIST Webbook
rinpol	3186.00		NIST Webbook
rinpol	3186.00		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=R393269&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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