

3-«beta»-Hydroxy-5-«beta»-cholanoic acid, MeTMS

Other names:	5-«beta»-Cholanoic acid, 3-«beta»-hydroxy, methyl ester, TMS
Inchi:	InChI=1S/C28H50O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6
InchiKey:	MMCLGKIAEUXBCF-WFDHFQHDSA-N
Formula:	C28H50O3Si
SMILES:	COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	462.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	7.455		Crippen Method
rinpol	3087.00		NIST Webbook
rinpol	3087.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R271624&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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