

allo-Cholanic acid, 7«alpha»-hydroxy, Me-TMS

Other names:	7«alpha»-Hydroxy-5«alpha»-cholanic acid, methyl ester, TMS
Inchi:	InChI=1S/C28H50O3Si/c1-19(11-14-25(29)30-4)21-12-13-22-26-23(15-17-28(21,22)3)27
InchiKey:	MVTBGPOIYGFTLR-CWSXKACCSA-N
Formula:	C28H50O3Si
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CCCCC4(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	2992.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R533754&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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