

Cholanic acid, 12«beta»-hydroxy, Me-TMS

Other names:	12«beta»-Hydroxy-5«beta»-cholanic acid, methyl ester, TMS
Inchi:	InChI=1S/C28H50O3Si/c1-19(11-16-26(29)30-4)22-14-15-23-21-13-12-20-10-8-9-17-27(
InchiKey:	GVHHSUABUMNRNR-MXGARSGJSA-N
Formula:	C28H50O3Si
SMILES:	COC(=O)CCC(C)C1CCC2C3CCC4CCCC4(C)C3CC(O[Si](C)(C)C)C12C
Mol. weight [g/mol]:	462.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	7.455		Crippen Method
rinpol	2981.00		NIST Webbook
ripol	3426.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R533858&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/98-243-4/Cholanic-acid-12-beta-hydroxy-Me-TMS.pdf>

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