

3«beta»,7«alpha»-Dihydroxy-5«beta»-cholanoic acid, MeTMS

Other names:	Methyl 3-«beta»,7-«alpha»-dihydroxy-5-«beta»-cholanoate, TMS
Inchi:	InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3
InchiKey:	FUVKOFYYHKWFJK-QVGSVIFDSA-N
Formula:	C31H58O4Si2
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	550.96
CAS:	81445-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
rinpol	3155.00		NIST Webbook
ripol	3536.00		NIST Webbook
ripol	3536.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81445730&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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