3«beta»-Hydroxy-7«beta»-methoxycholanic acid, methyl ester, TMS

Inchi: InChI=1S/C29H52O4Si/c1-19(9-12-26(30)32-5)22-10-11-23-27-24(14-16-29(22,23)3)28(

InchiKey: JBDNEAGIZQUFGR-FOSJPWCMSA-N

Formula: C29H52O4Si

SMILES: COC(=O)CCC(C)C1CCC2C3C(OC)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 492.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	7.080		Crippen Method
rinpol	3319.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R535314&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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