

3«alpha»-Hydroxy-«DELTA»6-5«beta»-cholanoic acid, MeTMS

Other names: «DELTA»

InChI: InChI=1S/C28H48O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6

InchiKey: BIPZZLZEQQMIIO-FNUFWSQISA-N

Formula: C28H48O3Si

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

Mol. weight [g/mol]: 460.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Crippen Method
logp	7.231		Crippen Method
rinpol	3136.00		NIST Webbook
rinpol	3157.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R182242&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Legend

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

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