16«alpha»-Hydroxyetiocholanolone(I), MO TMS

Inchi: InChI=1S/C26H49NO3Si2/c1-25-14-12-19(29-31(4,5)6)16-18(25)10-11-20-21(25)13-15-2

InchiKey: TVJNIUFLVUUMNG-BDQYVTRZSA-N

Formula: C26H49NO3Si2

SMILES: CON=C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 479.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	7.082		Crippen Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R250365&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