15«beta»,17«alpha»-Dihydroxypregnenolone, MO-TMS

Inchi: InChI=1S/C31H59NO4Si3/c1-22(32-33-4)31(36-39(11,12)13)21-27(35-38(8,9)10)28-25-1

InchiKey: HGNJIMJEZYWJLX-ZNFNMRCWSA-N

Formula: C31H59NO4Si3

SMILES: CON=C(C)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3

Mol. weight [g/mol]: 594.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.612		Crippen Method
rinpol	2938.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537038&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices