3«alpha»,11«beta»-dihydroxy-5«alpha»-androstan
MO-TMS

Inchi: InChI=1S/C28H55NO3Si3/c1-27-17-16-21(30-33(3,4)5)18-20(27)12-13-22-23-14-15-25(2

InchiKey: TVBYBJXCGVRLFJ-NXOPZDHZSA-N

Formula: C28H55NO3Si3

SMILES: CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2=NO[Si](C)(C)C

Mol. weight [g/mol]: 538.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	8.287		Crippen Method
rinpol	2681.00		NIST Webbook
rinpol	2681.00		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=R488258&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices