3-«beta»,18-Dihydroxy-5-androsten-17-one, MO TMS

Inchi: InChI=1S/C26H47NO3Si2/c1-25-15-14-23-21(22(25)11-12-24(25)27-28-2)10-9-19-17-20

InchiKey: FYYNDCHEIILVCB-NNYBWSOPSA-N

Formula: C26H47NO3Si2

SMILES: CON=C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(CO[Si](C)(C)C)C3CCC12C

Mol. weight [g/mol]: 477.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	7.003		Crippen Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R386028&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