3«beta»,7«alpha»-Dihydroxy-5«alpha»-androstan-17-one TMS

InChI: InChI=1S/C28H54O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)19-24(30-33(6,7)8)26-22-12-13-25(31-34(9,10)11)28(22,2)17-15-23(26)27/h19,21-26H,12-18H2,1-11H3/t21-,22-,23-,24+,25-,26-,27+,28-/m0/s1

InChIKey: VMAJAJNKRDOOQG-SKCCZNDUSA-N

Formula: C28H54O3Si3

SMILES: CC12CCC3C(C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C

Mol. weight [g/mol]: 522.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	8.424		Crippen Method
rinpol	2685.00		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=R306993&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices