5«alpha»-Androstane-3«beta»,6«alpha»,17«beta»-triol, TMS

InChI: InChI=1S/C28H56O3Si3/c1-27-16-14-20(29-32(3,4)5)18-24(27)25(30-33(6,7)8)19-21-22-12-13-26(2,31-34(9,10)11)23(22)15-17-28(21,27)C1CCC2O[Si](C)(C)C

InChIKey: KVQPAVGFDTUVFY-MFIVHVGQSA-N

Formula: C28H56O3Si3

SMILES: CC12CCC3C(CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC43C)C1CCC2O[Si](C)(C)C

Mol. weight [g/mol]: 525.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	8.299		Crippen Method
rinpol	2854.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R307149&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