5«beta»-Androstan-3«alpha»,11«beta»-diol-17-on
TMS

InChI: InChI=1S/C28H54O3Si3/c1-27-17-16-21(29-32(3,4)5)18-20(27)12-13-22-23-14-15-25(31

InchiKey: HTALMMXGRYNYNV-YTCVGTBISA-N

Formula: C28H54O3Si3

SMILES: CC12CC(O[Si](C)(C)C)C3C(CCC4CC(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	2696.00		NIST Webbook
rinpol	2672.00		NIST Webbook
rinpol	2696.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R321883&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