3«alpha»,15«alpha»-dihydroxy-5«beta»-androstan-17-one, TMS

Inchi: InChI=1S/C28H54O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)12-13-22-23(27)15-17-28

InchiKey: VFJHDKUHDGAWQC-QZFPZXFTSA-N

Formula: C28H54O3Si3

SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1C(O[Si](C)(C)C)C=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	2621.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2621.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R488169&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