3B,16A,17B-Trihydroxyandrost-5-ene, tris-TMS

Other names: Androst-5-ene-3«beta»,16«alpha»,17«beta»-triol, 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: HVNNEDKUOOQWAG-OXKJMOMGSA-N
Formula: C28H54O3Si3
SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]: 522.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	8.219		Crippen Method
rinpol	2889.00		NIST Webbook
rinpol	2858.00		NIST Webbook
rinpol	2889.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R108759&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