3«alpha»,16«beta»,17«alpha»-Trihydroxy-5«beta»-androstane, tris-TMS

Other names: 3A,16B,17A-Trihydroxy-5B-androstane, TMS

Inchi: InChI=1S/C28H56O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)12-13-22-23(27)15-17-28

InchiKey: RQCSPBXXGJRUKU-KBNVHCSPSA-N

Formula: C28H56O3Si3

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2O[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	2747.00		NIST Webbook
rinpol	2648.00		NIST Webbook
rinpol	2747.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R16648&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