3«alpha»,16«alpha»-dihydroxy-5«beta»-androstan-17-one-MO-TMS, (syn,anti)

Inchi: InChI=1S/C28H55NO3Si3/c1-27-16-14-21(30-33(3,4)5)18-20(27)12-13-22-23(27)15-17-28(6)24(22)19-25(26(28)31-32(7)8)29-34(9,10)11/h20-26H,12-19H2,1-11H3/b29-25-/t20-,21-,22-,23-,24-,26-,27+,28+/m0/s1

InchiKey: GZYUNKFWUXTIDF-OHCZDJKISA-N

Formula: C28H55NO3Si3

SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CC(O[Si](C)(C)C)C2=NO[Si](C)(C)C

Mol. weight [g/mol]: 538.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	8.287		Crippen Method
rinpol	2590.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2590.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R488129&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/13-805-3/3-alpha-16-alpha-dihydroxy-5-beta-androstan-17-one-MO-TMS-syn-anti.pdf
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