Androst-5-en-17-one, 3,16-bis[(trimethylsilyl)oxy]-, O-(trimethylsilyl)oxime, (3«beta»,16«beta»)-

Other names: 3«beta»,16«beta»-dihydroxy-5-androsten-17-one, MO-TMS

Inchi: InChI=1S/C28H53NO3Si3/c1-27-16-14-21(30-33(3,4)5)18-20(27)12-13-22-23(27)15-17-2

InchiKey: IPLOJYZPQLPSQP-PCNOWQCUSA-N

Formula: C28H53NO3Si3

SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(=NO[Si](C)(C)C)C(O[Si](C)(C)C)CC1

Mol. weight [g/mol]: 535.98

CAS: 69833-81-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.56		Crippen Method
logp	8.207		Crippen Method
rinpol	2800.00		NIST Webbook
rinpol	2763.00		NIST Webbook
rinpol	2773.00		NIST Webbook
rinpol	2762.00		NIST Webbook
rinpol	2800.00		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=C69833814&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: