5«alpha»-Androstan-3«alpha»-ol-17-one, TBDMS

Inchi: InChI=1S/C31H58O2Si2/c1-28(2,3)34(9,10)32-23-17-19-30(7)22(21-23)13-14-24-25-15-1

InchiKey: CLHFTFZHTPFECO-GZVREXEZSA-N

Formula: C31H58O2Si2

SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 518.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.66		Crippen Method
logp	9.935		Crippen Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R526068&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