3B-Hydroxy-5B-androstan-17-one, enol, bis-TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-

InchiKey: WRVSWIFKEWFLRU-GFXKHVTPSA-N

Formula: C25H46O2Si2

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

Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	7.594		Crippen Method
rinpol	2529.00		NIST Webbook
rinpol	2531.00		NIST Webbook
rinpol	2519.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R108784&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