3«beta»-Hydroxy-5«alpha»-androstane-6,17-dione TMS

InChI: InChI=1S/C25H44O3Si2/c1-24-13-11-17(27-29(3,4)5)15-21(24)22(26)16-18-19-9-10-23(

InchiKey: ROUPNNKSTWCYDL-GMPWYMRSSA-N

Formula: C25H44O3Si2

SMILES: CC12CCC3C(CC(=O)C4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C

Mol. weight [g/mol]: 448.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	6.774		Crippen Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R307010&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