Androst-5,9(11)-diene-3-«beta»,17-«beta»-diol, TMS

Inchi: InChI=1S/C25H44O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-

InchiKey: GUZYQHLPCCWDQG-SUQRNSRXSA-N

Formula: C25H44O2Si2

SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2=CCC2(C)C(O[Si](C)(C)C)CCC12

Mol. weight [g/mol]: 432.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	7.309		Crippen Method
rinpol	2618.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2618.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R385387&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