5-Androsten-3-«alpha»,17-«beta»-diol, 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: YXSPGYZGGCSNLG-ALCOCYKUSA-N
Formula: C25H46O2Si2
SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	7.389		Crippen Method
rinpol	2538.00		NIST Webbook
rinpol	2561.00		NIST Webbook
rinpol	2538.00		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=R385263&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices