5A-Androstan-3-on-17B-ol, TMS

Inchi: InChI=1S/C22H38O2Si/c1-21-12-10-16(23)14-15(21)6-7-17-18-8-9-20(24-25(3,4)5)22(18

InchiKey: YNHGEJGZDSFBFR-TVOSAUFZSA-N

Formula: C22H38O2Si

SMILES: CC12CCC(=O)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

Mol. weight [g/mol]: 362.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	5.818		Crippen Method
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R485551&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