3A-Hydroxy-5A-androst-16-ene, TMS

Other names: 5-«alpha»,16-Androsten-3-«alpha»-ol, TMS
Inchi: InChI=1S/C22H38OSi/c1-21-12-6-7-19(21)18-9-8-16-15-17(23-24(3,4)5)10-14-22(16,2)2
InchiKey: HUNGYZOAGOETMS-TVUKYMPLSA-N
Formula: C22H38OSi
SMILES: CC12C=CCC1C1CCC3CC(O[Si](C)(C)C)CCC3(C)C1CC2
Mol. weight [g/mol]: 346.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	6.415		Crippen Method
rinpol	2186.00		NIST Webbook
rinpol	2170.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R108719&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