5-«alpha»-Androstan-3-«alpha»-ol, TMS

Inchi: InChI=1S/C22H40OSi/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: XQQDDEIBTCOQHD-TVUKYMPLSA-N
Formula: C22H40OSi
SMILES: CC12CCCC1C1CCC3CC(O[Si](C)(C)C)CCC3(C)C1CC2
Mol. weight [g/mol]: 348.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	6.639		Crippen Method
rinpol	2210.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R149696&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