16-oxoandrostenediol, MO TMS

Inchi: InChI=1S/C23H39NO2Si/c1-22-11-10-20-19(21(22)14-17(15-22)24-25-3)8-7-16-13-18(26
InchiKey: NRPJRKXOGHWDLY-YIUKKTQASA-N
Formula: C23H39NO2Si
SMILES: CON=C1CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC2(C)C1
Mol. weight [g/mol]: 389.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	6.172		Crippen Method
rinpol	2851.00		NIST Webbook
rinpol	2902.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R250385&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