17-epi-Mestanolone, 17-TMS

Inchi: InChI=1S/C23H40O2Si/c1-21-12-9-17(24)15-16(21)7-8-18-19(21)10-13-22(2)20(18)11-1
InchiKey: DVEUJDWURSKKQN-OBRWFMAWSA-N
Formula: C23H40O2Si
SMILES: CC12CCC(=O)CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]: 376.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	6.208		Crippen Method
rinpol	2700.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R257782&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