17-Epimetandienone (Androst-1,4-dien-17B-methyl-17A-ol-3-one), TMS

Inchi: InChI=1S/C23H36O2Si/c1-21-12-9-17(24)15-16(21)7-8-18-19(21)10-13-22(2)20(18)11-1

InchiKey: GVUXJYDHSUSHTG-VRBBIHERSA-N

Formula: C23H36O2Si

SMILES: CC12C=CC(=O)C=C1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]: 372.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.06		Crippen Method
logp	5.905		Crippen Method
rinpol	2668.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R585389&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices