17-epi-Bolasterone, 17-TMS

Inchi: InChI=1S/C24H40O2Si/c1-16-14-17-15-18(25)8-11-22(17,2)19-9-12-23(3)20(21(16)19)1
InchiKey: YODBBXQVBBUISJ-LJJFCTPYSA-N
Formula: C24H40O2Si
SMILES: CC1CC2=CC(=O)CCC2(C)C2CCC3(C)C(CCC3(C)O[Si](C)(C)C)C12
Mol. weight [g/mol]: 388.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	6.375		Crippen Method
rinpol	2731.00		NIST Webbook
rinpol	2731.00		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=R257693&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices