17«beta»-Hydroxy-5«alpha»-androstane-3,6-dione, TMS

Other names: 17«BETA»-hydroxy-5«alpha»-androstane-3,6-dione, tms derivative
Inchi: InChI=1S/C22H36O3Si/c1-21-10-8-14(23)12-18(21)19(24)13-15-16-6-7-20(25-26(3,4)5)2
InchiKey: DPRDHSNOPIJZCX-JEJUZZDKSA-N
Formula: C22H36O3Si
SMILES: CC12CCC3C(CC(=O)C4CC(=O)CCC43C)C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]: 376.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	4.997		Crippen Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U69382&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