Androst-1,4-dien-2z-hydroxymethyl-17«alpha»-me TMS

InChI: InChI=1S/C33H61ClO4Si4/c1-31-20-23(22-35-39(4,5)6)30(37-41(10,11)12)29(34)26(31)
InchiKey: ZWXLHKJPWDCPNC-QMEUVGHYSA-N
Formula: C33H61ClO4Si4
SMILES: CC12C=C(CO[Si](C)(C)C)C(O[Si](C)(C)C)=C(Cl)C1=CCC1C2C(O[Si](C)(C)C)CC2(C)C1
Mol. weight [g/mol]: 669.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	10.299		Crippen Method
rinpol	3096.00		NIST Webbook
rinpol	3027.00		NIST Webbook
rinpol	3096.00		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=R322019&Units=SI

Legend

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