Androst-1,4-dien-17«alpha»-methyl-4-chloro-17«b
TMS

Inchi: InChI=1S/C26H43ClO2Si2/c1-24-15-14-22(28-30(4,5)6)23(27)21(24)11-10-18-19(24)12-
InchiKey: GBKVYVYEVCEEMU-KEGRRINUSA-N
Formula: C26H43ClO2Si2
SMILES: CC12C=CC(O[Si](C)(C)C)=C(Cl)C1=CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]: 479.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	8.247		Crippen Method
rinpol	2977.00		NIST Webbook
rinpol	2990.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R322004&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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