5«alpha»-Androstan-3«beta»-ol-17-one, VDMS

Inchi: InChI=1S/C27H46O2Si2/c1-9-30(5,6)28-21-15-17-26(3)20(19-21)11-12-22-23-13-14-25(
InchiKey: PTJWVHSUJDZMHD-ISTZPGECSA-N
Formula: C27H46O2Si2
SMILES: C=C[Si](C)(C)OC1=CCC2C3CCC4CC(O[Si](C)(C)C=C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 458.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	7.785		Crippen Method
rinpol	2637.00		NIST Webbook
rinpol	2637.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529354&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