5«alpha»-Androstan-3«beta»16«beta»-diol, VDMS

Inchi: InChI=1S/C27H48O2Si2/c1-9-30(5,6)28-21-13-16-27(4)20(17-21)11-12-23-24(27)14-15-
InchiKey: ZEWADCUHEJMTLP-XYVHJWKUSA-N
Formula: C27H48O2Si2
SMILES: C=C[Si](C)(C)OC1CCC2(C)C(CCC3C4CC(O[Si](C)(C)C=C)CC4(C)CCC32)C1
Mol. weight [g/mol]: 460.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	7.660		Crippen Method
rinpol	2800.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529334&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