5«alpha»-Androstan-3«alpha»-ol-17-one, allyl-DMS

Inchi: InChI=1S/C29H50O2Si2/c1-9-19-32(5,6)30-23-15-17-28(3)22(21-23)11-12-24-25-13-14-

InchiKey: VRULWPUWUNLLTM-MDAWDBSJSA-N

Formula: C29H50O2Si2

SMILES: C=CC[Si](C)(C)OC1=CCC2C3CCC4CC(O[Si](C)(C)CC=C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 486.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	8.707		Crippen Method
rinpol	2650.00		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=R526053&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices