

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/ci9903071>
Crippen Method: https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/23-417-3/5-alpha-Androstan-3-alpha-ol-17-one-allyl-DMS.pdf>

Generated by Cheméo on 2024-04-30 06:28:27.400661979 +0000 UTC m=+16747756.321239290.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.