

5«beta»-Androstan-3«beta»-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-SFWVBKFNSA-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	2656.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R526197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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.chemeo.com/cid/70-841-0/5-beta-Androstan-3-beta-ol-17-one-allyl-DMS.pdf>

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