

5«alpha»-Pregnan-3«beta»,20«alpha»-diol, allyl-DMS

Inchi:	InChI=1S/C30H54O2Si2/c1-9-19-33(5,6)31-22(3)28-15-16-29-27-13-11-23-21-24(32-34)
InchiKey:	OIQFAVVJRZEEBZ-YRGPVTPUSA-N
Formula:	C30H54O2Si2
SMILES:	C=CC[Si](C)(C)OC1CCC2C(CCC3C2CCC2(C)C(C(C)O[Si](C)(C)CC=C)CCC3)C1
Mol. weight [g/mol]:	502.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	8.828		Crippen Method
rinpol	3287.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R526117&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/49-975-6/5-alpha-Pregnan-3-beta-20-alpha-diol-allyl-DMS.pdf>

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