

Silane, [[(3«beta»,20S)-pregn-5-ene-3,20,21-triyl]tris(oxy)]

Other names:	5-Pregnene-3«beta»,20«beta»,21-triol, tris-TMS
Inchi:	InChI=1S/C30H58O3Si3/c1-29-18-16-23(32-35(6,7)8)20-22(29)12-13-24-25-14-15-27(30)31
InchiKey:	RBSXFFWTNZTHKA-FPPZZAMFSA-N
Formula:	C30H58O3Si3
SMILES:	CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC1
Mol. weight [g/mol]:	551.04
CAS:	57305-40-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	8.857		Crippen Method
rinpol	3110.00		NIST Webbook
rinpol	3110.00		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=C57305405&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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