

3,16,20-Tris[(trimethylsilyl)oxy]-5.alpha-pregnane (3«beta»,16«alpha»,20«alpha»)-

Other names:	Silane, (5«alpha»-pregnane-3«beta»,16«alpha»,20«alpha»-trioxy)tris(trimethyl-3,16,20-Tris[(trimethylsilyl)oxy]pregnane, (5«alpha»,3«beta»,16«alpha»,20«alpha»)-5-«alpha»-Pregnan-3-«beta»,16-«alpha»,20-«alpha»-triol, tris-TMS 5«alpha»-Pregnane-3«beta»,16«alpha»,20«alpha»-triol, (3TMS) 5«alpha»-Pregnane-3«beta»,16«alpha»,20«alpha»--triol, MO TMS 5-«alpha»-Pregnan-3-«beta»,16-«alpha»,20-«alpha»-triol, MeTMS
Inchi:	InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)28-27(33-36(10,11)12)20-26-24-14-13-22-19
InchiKey:	GKSDWCMXICLASA-UHFFFAOYSA-N
Formula:	C30H60O3Si3
SMILES:	CC(O[Si](C)(C)C)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	553.05
CAS:	33287-36-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.935		Crippen Method
rinpol	3022.00		NIST Webbook
rinpol	3060.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33287364&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

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