

5-«alpha»-Pregnan-3-«beta»,20-«alpha»,21-triol, TMS

Other names:	5-«alpha»-Pregnan-3-«beta»,20-«alpha»,21-triol, MeTMS
Inchi:	InChI=1S/C30H60O3Si3/c1-29-18-16-23(32-35(6,7)8)20-22(29)12-13-24-25-14-15-27(30)31
InchiKey:	PCDMVFRHMJMCFX-ZXTTUGLOSA-N
Formula:	C30H60O3Si3
SMILES:	CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	8.937		Crippen Method
rinpol	3091.00		NIST Webbook
rinpol	3091.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393383&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.chemeo.com/cid/41-865-6/5-alpha-Pregnan-3-beta-20-alpha-21-triol-TMS.pdf>

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