

5-Pregnen-3-«beta»,11-«beta»,20-«beta»-triol, TMS

Inchi:	InChI=1S/C30H58O3Si3/c1-21(31-34(4,5)6)25-15-16-26-24-14-13-22-19-23(32-35(7,8)9)
InchiKey:	CDNCGBYGIFCFSC-WNOFEJARSA-N
Formula:	C30H58O3Si3
SMILES:	CC(O[Si](C)(C)C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12
Mol. weight [g/mol]:	551.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	8.856		Crippen Method
rinpol	3050.00		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=R487166&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/18-468-3/5-Pregnen-3-beta-11-beta-20-beta-triol-TMS.pdf>

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