

5-«beta»-Pregnan-11-«beta»,20-«alpha»-diol, TMS

Inchi:	InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)22-15-16-23-21-14-13-20-12-10-11-17-26(20)
InchiKey:	JDGPTGUSLGSINV-IQSROUIGSA-N
Formula:	C27H52O2Si2
SMILES:	CC(O[Si](C)(C)C)C1CCC2C3CCC4CCCCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]:	464.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	8.105		Crippen Method
rinpol	2698.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486752&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/59-566-9/5-beta-Pregnan-11-beta-20-alpha-diol-TMS.pdf>

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