5-Pregnane-11-one-3«alpha»,20«alpha»-diol, MO-TMS

Inchi:	InChI=1S/C28H53NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(32-34(8,9)
InchiKey:	YXNCMXWVSHUSLE-CGLUMZSKSA-N
Formula:	C28H53NO3Si2
SMILES:	CON=C1CC2(C)C(C(C)O[Si](C)(C)C)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3(C)C12
Mol. weight [g/mol]:	507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2893.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R527294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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