5-«alpha»-Pregnan-3-«beta»,15 or 16-diol-20-one, MeTMS

Inchi:	InChI=1S/C27H50O3Si2/c1-18(28)25-24(30-32(7,8)9)17-23-21-11-10-19-16-20(29-31(4,5
InchiKey:	WEEZFJRNCVQVEU-XOBUQTBLSA-N
Formula:	C27H50O3Si2
SMILES:	CC(=O)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	478.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	7.284		Crippen Method
rinpol	2856.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393358&Units=SI

Legend

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

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