

5«beta»-Pregnane-3«alpha»,6«alpha»-diol-20-one

Other names:	5«beta»-Pregnan-20-one, 3«alpha»,6«alpha»-bis(trimethylsiloxy)-Pregnan-20-one, 3,6-bis[(trimethylsilyl)oxy]-, (3«alpha»,5«beta»,6«alpha»)-3,6-Bis[(trimethylsilyl)oxy]pregnan-20-one-, (3«alpha»,5«beta»,6«alpha»)-5-«beta»-Pregnan-3-«alpha»,6-«alpha»-diol-20-one, MeTMS
Inchi:	InChI=1S/C27H50O3Si2/c1-18(28)21-10-11-22-20-17-25(30-32(7,8)9)24-16-19(29-31(4,5)6)3
InchiKey:	FHYVDDGQKARSHA-BGAYJKQGSA-N
Formula:	C27H50O3Si2
SMILES:	CC(=O)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	478.86
CAS:	33287-43-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	7.284		Crippen Method

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=C33287433&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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