

5«beta»-Pregnane-3«alpha»,17«alpha»-diol-20-one

Other names:	Pregnan-3,17-diol-20-one, TMS
Inchi:	InChI=1S/C27H50O3Si2/c1-19(28)27(30-32(7,8)9)17-14-24-22-11-10-20-18-21(29-31(4,5)6)3
InchiKey:	VKPBHMNDXUQKPO-CLJHMYPUA-N
Formula:	C ₂₇ H ₅₀ O ₃ Si ₂
SMILES:	CC(=O)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	478.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	7.429		Crippen Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U69419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/91-412-3/5-beta-Pregnane-3-alpha-17-alpha-diol-20-one-di-TMS.pdf>

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