

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

Inchi:	InChI=1S/C28H53NO3Si2/c1-20(29-30-4)28(32-34(8,9)10)18-15-25-23-12-11-21-19-22(3)
InchiKey:	WPPGDMRLWMCELS-RPEJMBDLA-N
Formula:	C28H53NO3Si2
SMILES:	CON=C(C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	7.862		Crippen Method
rinpol	2725.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490701&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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