

5«alpha»-Pregnane-3«beta», 16«alpha»-diol-20-one, MO TMS

Other names:	16«alpha»-Hydroxypregnanolone, MO TMS
Inchi:	InChI=1S/C28H53NO3Si2/c1-19(29-30-4)26-25(32-34(8,9)10)18-24-22-12-11-20-17-21(3)
InchiKey:	RQHCBMPEWAEMBW-SXWNTBQOSA-N
Formula:	C28H53NO3Si2
SMILES:	CON=C(C)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2961.00		NIST Webbook
rinpol	2972.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R250370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/66-209-7/5-alpha-Pregnane-3-beta-16-alpha-diol-20-one-MO-TMS.pdf>

Generated by Cheméo on 2024-04-28 13:48:53.403373507 +0000 UTC m=+16601382.323950820.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.