

4-Pregnen-3-«beta»,11-«beta»-diol-20-one, MO-TMS

Inchi:	InChI=1S/C28H51NO3Si2/c1-19(29-30-4)23-13-14-24-22-12-11-20-17-21(31-33(5,6)7)15
InchiKey:	SUMPKNGBSGVILZ-QOMLESJASA-N
Formula:	C28H51NO3Si2
SMILES:	CON=C(C)C1CCC2C3CCC4=CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]:	505.88

Physical Properties

Property code	Value	Unit	Source
logp	7.638		Crippen Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486252&Units=SI

Legend

logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/113-797-2/4-Pregnen-3-beta-11-beta-diol-20-one-MO-TMS.pdf>

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