

5-«alpha»-Pregnan-3-«beta»,21-diol-20-one, MeTMS

Inchi:	InChI=1S/C27H50O3Si2/c1-26-15-13-20(30-32(6,7)8)17-19(26)9-10-21-22-11-12-24(25)(
InchiKey:	LHAVSYHEPNCPLB-VYTFNHSISA-N
Formula:	C27H50O3Si2
SMILES:	CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(C(=O)CO[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	478.86

Physical Properties

Property code	Value	Unit	Source
logp	7.286		Crippen Method
rinpol	3023.00		NIST Webbook
rinpol	3023.00		NIST Webbook
rinpol	3023.00		NIST Webbook
tf	405.18	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393407&Units=SI

Legend

logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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<https://www.cheméo.com/cid/124-022-9/5-alpha-Pregnan-3-beta-21-diol-20-one-MeTMS.pdf>

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