

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

Inchi:	InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)
InchiKey:	PSZRAFDARWUCMW-TYUACMPWSA-N
Formula:	C27H52O2Si2
SMILES:	CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	464.87

Physical Properties

Property code	Value	Unit	Source
logp	8.105		Crippen Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tf	374.21	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393501&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/69-704-4/5-beta-Pregnan-3-beta-20-alpha-diol-MeTMS.pdf>

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