

5-«beta»-Pregnan-3-«beta»,20-«beta»-diol, TMS

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	2732.00		NIST Webbook
rinpol	2754.00		NIST Webbook
rinpol	2753.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2753.00		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=R385238&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.cheméo.com/cid/69-703-5/5-beta-Pregnan-3-beta-20-beta-diol-TMS.pdf>

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