

5-«alpha»-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-LWSJOAPHSA-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	2820.00		NIST Webbook
rinpol	2839.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tf	374.21	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R385030&Units=SI
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):	

Legend

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

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