

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

Other names:	5«beta»-Pregnane-3«alpha»,20«alpha»-diol, diTMSi
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-GQLJITBLSA-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
log10ws	-3.51		Crippen Method
logp	8.105		Crippen Method
rinpol	2783.00		NIST Webbook
rinpol	2817.00		NIST Webbook
rinpol	2777.00		NIST Webbook
rinpol	2794.00		NIST Webbook
rinpol	2797.00		NIST Webbook
rinpol	2768.00		NIST Webbook
rinpol	2802.00		NIST Webbook
rinpol	2783.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R144364&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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