

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

Other names:	5«alpha»-Pregnane-3«beta»,20«alpha»-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-XOSNHBCNSA-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	2823.00		NIST Webbook
rinpol	2847.00		NIST Webbook
rinpol	2836.00		NIST Webbook
rinpol	2854.00		NIST Webbook
rinpol	2886.00		NIST Webbook
rinpol	2848.00		NIST Webbook
rinpol	2847.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R265966&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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