

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

Other names:	5«alpha»-Pregnane-3«alpha»,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-RVQJNZAQSA-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	2764.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2754.00		NIST Webbook
rinpol	2770.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2786.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2754.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R265931&Units=SI

Legend

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

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