

5-«alpha»-Pregnane-20-«alpha»,21-diol, bis-TMS

Inchi:	InChI=1S/C27H52O2Si2/c1-26-17-10-9-11-20(26)12-13-21-22-14-15-24(27(22,2)18-16-2
InchiKey:	IQDPJDLDPJDYHF-XFJVSCRESA-N
Formula:	C27H52O2Si2
SMILES:	CC12CCCCC1CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	464.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	8.107		Crippen Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149869&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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<https://www.chemeo.com/cid/10-816-4/5-alpha-Pregnane-20-alpha-21-diol-bis-TMS.pdf>

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