

5-Pregnane-11-one-3«alpha»,20«alpha»-diol, EO-TMS

Inchi:	InChI=1S/C29H55NO3Si2/c1-11-31-30-26-19-29(4)24(20(2)32-34(5,6)7)14-15-25(29)23-
InchiKey:	KPEYZBRSMGUJJ-SDTXVYFQSA-N
Formula:	C29H55NO3Si2
SMILES:	CCON=C1CC2(C)C(C(C)O[Si](C)(C)C)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3(C)C12
Mol. weight [g/mol]:	521.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	8.108		Crippen Method
rinpol	2887.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R527289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/57-612-9/5-Pregnane-11-one-3-alpha-20-alpha-diol-EO-TMS.pdf>

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