

3A,17A,21-Trihydroxy-5B-pregnan-20-one, MO TMS

Inchi:	InChI=1S/C31H61NO4Si3/c1-29-18-15-24(35-38(7,8)9)21-23(29)13-14-25-26(29)16-19-3
InchiKey:	ZDGFYSBILJZZFV-ALDOAKTFSA-N
Formula:	C31H61NO4Si3
SMILES:	CON=C(CO[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]:	596.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	8.693		Crippen Method
rinpol	2880.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486049&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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