22-Hydroxy-4-cholesten-3-one, TMS

Inchi:	InChI=1S/C30H52O2Si/c1-20(2)9-14-28(32-33(6,7)8)21(3)25-12-13-26-24-11-10-22-19-2
InchiKey:	MNQCLSQWCTWEBG-GKIJCXLUSA-N
Formula:	C30H52O2Si
SMILES:	CC(C)CCC(O[Si](C)(C)C)C(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	472.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	8.427		Crippen Method
rinpol	3325.00		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=R11670&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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