6-Ketocholestanol, TMS

Inchi:	InChI=1S/C33H62O2Si2/c1-23(2)13-12-14-24(3)27-15-16-28-26-22-31(35-37(9,10)11)30
InchiKey:	HJXPRSHKFOPRQH-ZAQJYQHZSA-N
Formula:	C33H62O2Si2
SMILES:	CC(C)CCCC(C)C1CCC2C3CC(O[Si](C)(C)C)=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	547.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.02		Crippen Method
logp	10.427		Crippen Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		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=R262274&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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