Prednisone, tetra-TMS

Inchi:	InChI=1S/C33H58O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38
InchiKey:	VYLAUAYARLRLOZ-VMPMDZIUSA-N
Formula:	C33H58O5Si4
SMILES:	CC12C=CC(O[Si](C)(C)C)=CC1=CCC1C2=C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)
Mol. weight [g/mol]:	647.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	9.181		Crippen Method
rinpol	3153.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R558119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/42-975-3/Prednisone-tetra-TMS.pdf

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