Prednisone, MO TMS

Inchi:	InChI=1S/C36H69N3O5Si5/c1-34-22-20-28(37-42-47(9,10)11)24-27(34)18-19-29-30-21-
InchiKey:	YMWWDIXGLZZAAH-SMZJNTQJSA-N
Formula:	C36H69N3O5Si5
SMILES:	CC12C=CC(=NO[Si](C)(C)C)C=C1CCC1C2C(=NO[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)
Mol. weight [g/mol]:	764.38

Physical Properties

Property code	Value	Unit	Source
log10ws	0.76		Crippen Method
logp	10.399		Crippen Method
rinpol	3192.00		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=R66184&Units=SI

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/15-057-2/Prednisone-MO-TMS.pdf

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