

Prednisolone, MO TMS

Other names:	Prednisolone (1-dehydrocortisol), MO-TMS
Inchi:	InChI=1S/C36H70N2O5Si5/c1-34-22-20-28(37-42-47(12,13)14)24-27(34)18-19-29-30-21
InchiKey:	REIKNJJJDMOPBV-HUGFTRFBSA-N
Formula:	C36H70N2O5Si5
SMILES:	CC12C=CC(=NO[Si](C)(C)C)C=C1CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)
Mol. weight [g/mol]:	751.38

Physical Properties

Property code	Value	Unit	Source
log10ws	0.81		Crippen Method
logp	10.412		Crippen Method
rinpol	3280.00		NIST Webbook
rinpol	3269.00		NIST Webbook
rinpol	3280.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R66170&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/56-466-3/Prednisolone-MO-TMS.pdf>

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