Prednisolone, bis-MO-tris-TMS

Inchi:	InChI=1S/C32H58N2O5Si3/c1-30-18-16-24(33-35-3)20-23(30)14-15-25-26-17-19-32(39-
InchiKey:	BZDGXDIJTGFBMR-SPYODXAFSA-N
Formula:	C32H58N2O5Si3
SMILES:	CON=C1C=CC2(C)C(=C1)CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C(CC
Mol. weight [g/mol]:	635.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	8.002		Crippen Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R558075&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/29-058-6/Prednisolone-bis-MO-tris-TMS.pdf
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