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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R66184&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