6,7-dehydro-11-keto-methylprednisolone, diMO-diTMS (2)

Inchi: InChI=1S/C30H48N2O5Si2/c1-20-16-22-23-13-15-30(37-39(9,10)11,26(32-35-5)19-36-3
InchiKey: DGTIXRGNNMOEFD-BGLVPXFKSA-N
Formula: C30H48N2O5Si2
SMILES: CON=C1CC2(C)C(CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)C2C=C(C)C3=CC(=O)C
Mol. weight [g/mol]: 572.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	6.517		Crippen Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		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=R252054&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices