6,7-dehydro-methylprednisolone, diMO-triTMS (2)

Inchi: InChI=1S/C33H58N2O5Si3/c1-23-19-25-26-16-18-33(40-43(12,13)14,29(35-37-5)22-38-
InchiKey: JYIRPBUJCSIZJM-HQKYZGFESA-N
Formula: C33H58N2O5Si3
SMILES: CON=C1C=CC2(C)C(=C1)C(C)=CC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C
Mol. weight [g/mol]: 647.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	8.168		Crippen Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		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=R252118&Units=SI

Legend

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