6-«beta»-Hydrohyprednisolone, MO TMS

Inchi: InChI=1S/C39H78N2O6Si6/c1-37-23-21-29(40-46-52(15,16)17)25-32(37)33(43-49(6,7)8)
InchiKey: TWASIRPNOCCOTG-QXCLRXNISA-N
Formula: C39H78N2O6Si6
SMILES: CC12C=CC(=NO[Si](C)(C)C)C=C1C(O[Si](C)(C)C)CC1C2C(O[Si](C)(C)C)CC2(C)C1CC
Mol. weight [g/mol]: 839.56

Physical Properties

Property code	Value	Unit	Source
log10ws	2.30		Crippen Method
logp	11.242		Crippen Method
rinpol	3300.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R66152&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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