Prednisone, bis-MO-bis-TMS, syn

Inchi: InChI=1S/C29H48N2O5Si2/c1-27-15-13-21(30-33-3)17-20(27)11-12-22-23-14-16-29(36-
InchiKey: CFFYDAOQAVFLSY-BCOJFYKYSA-N
Formula: C29H48N2O5Si2
SMILES: CON=C1C=CC2(C)C(=C1)CCC1C2C(=NOC)CC2(C)C1CCC2(O[Si](C)(C)C)C(=O)CO[Si
Mol. weight [g/mol]: 560.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	6.351		Crippen Method
rinpol	2893.00		NIST Webbook
rinpol	2893.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R558104&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