Dexamethasone, MO TMS

Inchi: InChI=1S/C33H59FN2O5Si3/c1-23-19-27-26-16-15-24-20-25(35-37-4)17-18-30(24,2)32(
InchiKey: LQJAJGCNYDJNPW-QFCDCLMFSA-N
Formula: C33H59FN2O5Si3
SMILES: CON=C1C=CC2(C)C(=C1)CCC1C3CC(C)C(O[Si](C)(C)C)(C(CO[Si](C)(C)C)=NOC)C3(C
Mol. weight [g/mol]: 667.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	8.340		Crippen Method
rinpol	3376.00		NIST Webbook
rinpol	3376.00		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=R44085&Units=SI

Legend

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