Tetrahydrocortisone, MO-tris-TMS

Inchi: InChI=1S/C32H62N2O5Si3/c1-30-18-16-24(38-41(8,9)10)20-23(30)14-15-25-26-17-19-3
InchiKey: GRUGCVVBQPMXKS-HGUZWOMISA-N
Formula: C32H62N2O5Si3
SMILES: CON=C1CC2(C)C(CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)C2CCC3CC(O[Si](C)(C)C)(C)
Mol. weight [g/mol]: 639.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	8.306		Crippen Method
rinpol	2666.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R558139&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