11-Desoxycortisol, bis-MO-bis-TMS

Inchi: InChI=1S/C29H50N2O4Si2/c1-27-16-13-22(30-32-3)19-21(27)11-12-23-24(27)14-17-28(
InchiKey: AVOMLMPIWXTDIX-PZCHXQGASA-N
Formula: C29H50N2O4Si2
SMILES: CON=C1C=CC2(C)C(=C1)CCC1C2CCC2(C)C1CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)=N
Mol. weight [g/mol]: 546.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	7.172		Crippen Method
rinpol	2792.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2792.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R557874&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