11-Deoxycortisol, bis(trimethylsilyl) ether, bis(O-methyloxime)

Other names: 11-deoxycortisol, MO-TMS
Inchi: InChI=1S/C29H52N2O4Si2/c1-27-16-13-22(30-32-3)19-21(27)11-12-23-24(27)14-17-28(
InchiKey: MUPBZKSHPSGNPV-UHFFFAOYSA-N
Formula: C29H52N2O4Si2
SMILES: CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)C2(C)C
Mol. weight [g/mol]: 548.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	7.396		Crippen Method
rinpol	3070.00		NIST Webbook
rinpol	3124.00		NIST Webbook
rinpol	3070.00		NIST Webbook
rinpol	3124.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U394488&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.