

Prednisolone, bis-MO-tris-TMS

Inchi: InChI=1S/C32H58N2O5Si3/c1-30-18-16-24(33-35-3)20-23(30)14-15-25-26-17-19-32(39-41-40)/1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: BZDGXDIJTGFMBR-SPYODXAFSA-N
Formula: C32H58N2O5Si3
SMILES: CON=C1C=CC2(C)C(=C1)CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)C1
Mol. weight [g/mol]: 635.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	8.002		Crippen Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R558075&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/29-058-6/Prednisolone-bis-MO-tris-TMS.pdf>

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