

4,5-Dihydroprednisone, MO TMS

Inchi: InChI=1S/C36H71N3O5Si5/c1-34-22-20-28(37-42-47(9,10)11)24-27(34)18-19-29-30-21-
InchiKey: VYDMMUZXMDXTSH-OCHZSEBLSA-N
Formula: C36H71N3O5Si5
SMILES: CC12C=CC(=NO[Si](C)(C)C)CC1CCC1C2C(=NO[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C
Mol. weight [g/mol]: 766.39

Physical Properties

Property code	Value	Unit	Source
log10ws	0.86		Crippen Method
logp	10.479		Crippen Method
rinpol	3092.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R66148&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/26-945-4/4-5-Dihydroprednisone-MO-TMS.pdf>

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