

4,5-Dihydroprednisolone, MO TMS

Inchi: InChI=1S/C36H72N2O5Si5/c1-34-22-20-28(37-42-47(12,13)14)24-27(34)18-19-29-30-21
InchiKey: AZEBTRKHZNRXRY-KUEDVXJSSA-N
Formula: C36H72N2O5Si5
SMILES: CC12C=CC(=NO[Si](C)(C)C)CC1CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C
Mol. weight [g/mol]: 753.39

Physical Properties

Property code	Value	Unit	Source
log10ws	0.90		Crippen Method
logp	10.492		Crippen Method
rinpol	3130.00		NIST Webbook
rinpol	3130.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R66134&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/113-895-3/4-5-Dihydroprednisolone-MO-TMS.pdf>

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