20-hydroxy-methylprednisolone, MO-tetraTMS (2)

Inchi: InChI=1S/C35H67NO5Si4/c1-25-21-27-28-18-20-35(41-45(14,15)16,31(40-44(11,12)13)2

InchiKey: METMJCRIDWEDOX-GQTIQGSJSA-N

Formula: C35H67NO5Si4

SMILES: CON=C1C=CC2(C)C(=C1)C(C)CC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C(

Mol. weight [g/mol]: 694.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.44		Crippen Method
logp	9.465		Crippen Method
rinpol	3318.00		NIST Webbook
rinpol	3318.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R252014&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/123-980-7/20-hydroxy-methylprednisolone-MO-tetraTMS-2.pdf

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