

6,7-Dehydro-20-hydroxy-methylprednisolone, MO-tetraTMS (4)

Inchi: InChI=1S/C35H65NO5Si4/c1-25-21-27-28-18-20-35(41-45(14,15)16,31(40-44(11,12)13)29-30)/p1
InchiKey: UEBSTVXONQGEBZ-FXLJMYBASA-N
Formula: C35H65NO5Si4
SMILES: CON=C1C=CC2(C)C(=C1)C(C)=CC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 692.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	9.386		Crippen Method
rinpol	3342.00		NIST Webbook
rinpol	3342.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R252094&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/119-062-1/6-7-Dehydro-20-hydroxy-methylprednisolone-MO-tetraTMS-4.pdf>

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