

Prednisolone, tetra-TMS

Inchi: InChI=1S/C33H60O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38)
InchiKey: AWFNVAAHFNIRPH-VWAFQAQGSA-N
Formula: C33H60O5Si4
SMILES: CC12C=CC(O[Si](C)(C)C)=CC1=CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C
Mol. weight [g/mol]: 649.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.12		Crippen Method
logp	8.911		Crippen Method
rinpol	3295.00		NIST Webbook
rinpol	3295.00		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=R558080&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/113-593-8/Prednisolone-tetra-TMS.pdf>

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