

Prednisone, tetra-TMS

Inchi: InChI=1S/C33H58O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38)
InchiKey: VYLAUAYARLRLOZ-VMPMDZIUSA-N
Formula: C33H58O5Si4
SMILES: CC12C=CC(O[Si](C)(C)C)=CC1=CCC1C2=C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)
Mol. weight [g/mol]: 647.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	9.181		Crippen Method
rinpol	3153.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R558119&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/42-975-3/Prednisone-tetra-TMS.pdf>

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