

Dehydroxy-20-hydroxy-methylprednisolone, MO-triTMS (1)

Inchi: InChI=1S/C32H59NO4Si3/c1-22-19-25-26-16-18-32(37-40(12,13)14,23(2)35-38(6,7)8)31
InchiKey: YMQJXXHRCKFDER-LAJSSNOOSA-N
Formula: C32H59NO4Si3
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]: 606.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	8.634		Crippen Method
rinpol	3276.00		NIST Webbook
rinpol	3276.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R252123&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/117-655-5/Dehydroxy-20-hydroxy-methylprednisolone-MO-triTMS-1.pdf>

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