

6«alpha»-Methylprednisolone, tetra-TMS

Inchi: InChI=1S/C34H62O5Si4/c1-24-20-26-27-17-19-34(39-43(13,14)15,30(35)23-36-40(4,5)6
InchiKey: FEUBEJZGKUBSGR-JVJUJFTESA-N
Formula: C34H62O5Si4
SMILES: CC1=C2C=C(O[Si](C)(C)C)C=CC2(C)C2C(O[Si](C)(C)C)CC3(C)C(CCC3(O[Si](C)(C)C)C
Mol. weight [g/mol]: 663.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	9.301		Crippen Method
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R557903&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/97-166-1/6-alpha-Methylprednisolone-tetra-TMS.pdf>

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