

Betamethasone tetra-TMS

Inchi: InChI=1S/C34H61FO5Si4/c1-24-20-28-27-17-16-25-21-26(38-42(7,8)9)18-19-31(25,2)33
InchiKey: AAGPTIWGPYUODA-AVOBCZQGSA-N
Formula: C34H61FO5Si4
SMILES: CC1CC2C3CC=C4C=C(O[Si](C)(C)C)C=CC4(C)C3(F)C(O[Si](C)(C)C)CC2(C)C1(O[Si](C)(C)C)C(F)(C)C
Mol. weight [g/mol]: 681.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.50		Crippen Method
logp	9.249		Crippen Method
rinpol	3251.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R284972&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/51-362-3/Betamethasone-tetra-TMS.pdf>

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