

Dexamethasone tetra-TMS

Inchi: InChI=1S/C31H53FO5Si3/c1-21-17-25-24-14-13-22-18-23(33)15-16-28(22,2)30(24,32)2
InchiKey: LXHCVAWDDVUPNO-VLNHXOEZSA-N
Formula: C₃₁H₅₃FO₅Si₃
SMILES: CC1CC2C3CCC4=CC(=O)C=CC4(C)C3(F)C(O[Si](C)(C)C)CC2(C)C1(O[Si](C)(C)C)C(=O)C
Mol. weight [g/mol]: 609.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Crippen Method
logp	7.473		Crippen Method
rinpol	3251.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R285019&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/20-693-0/Dexamethasone-tetra-TMS.pdf>

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