

Desoxycorticosterone, tris-TMS

Inchi: InChI=1S/C30H54O3Si3/c1-29-18-16-23(32-35(6,7)8)20-22(29)12-13-24-25-14-15-27(30)
InchiKey: OPIUUUJUXQRPIC-RXDBUSOLSA-N
Formula: C30H54O3Si3
SMILES: CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2CCC2(C)C(C(=CO[Si](C)(C)C)O[Si](C)(C)C)CC
Mol. weight [g/mol]: 547.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	9.455		Crippen Method
rinpol	3172.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R558040&Units=SI>

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/97-182-3/Desoxycorticosterone-tris-TMS.pdf>

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