

11-Deoxycortisol enol-TMS

Other names:	11-Desoxycortisol, tris-TMS
Inchi:	InChI=1S/C30H54O4Si3/c1-28-17-14-23(33-36(6,7)8)20-22(28)12-13-24-25(28)15-18-29
InchiKey:	TVDQQQUUDKYUDQX-HUXCJGEFSA-N
Formula:	C30H54O4Si3
SMILES:	CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2CCC2(C)C1CCC2(O[Si](C)(C)C)C(=O)CO[Si](C)(C)C
Mol. weight [g/mol]:	563.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	8.305		Crippen Method
rinpol	3162.00		NIST Webbook
rinpol	3178.00		NIST Webbook
rinpol	3162.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R384057&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/121-087-1/11-Deoxycortisol-enol-TMS.pdf>

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