Deoxycorticosterone enol-TMS

Inchi:	InChI=1S/C27H46O3Si2/c1-26-15-13-20(30-32(6,7)8)17-19(26)9-10-21-22-11-12-24(25(
InchiKey:	HETVOBUPLWDXBU-VHXHPCHCSA-N
Formula:	C27H46O3Si2
SMILES:	CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2CCC2(C)C(C(=O)CO[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	474.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	7.331		Crippen Method
rinpol	3089.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R384097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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.chemeo.com/cid/45-574-5/Deoxycorticosterone-enol-TMS.pdf

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