

Tetrahydrocortisol, TMS

Other names:	Tetrahydrocortisol, tetrakis-TMS Tetrahydrocortisol tetra-TMS
Inchi:	InChI=1S/C33H66O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38)
InchiKey:	FHFQXMWINWAKEZ-UHFFFAOYSA-N
Formula:	C33H66O5Si4
SMILES:	CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C(=O)C1
Mol. weight [g/mol]:	655.22

Physical Properties

Property code	Value	Unit	Source
log10ws	0.07		Crippen Method
logp	9.090		Crippen Method
rinpol	3118.00		NIST Webbook
rinpol	3131.00		NIST Webbook
rinpol	3127.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U144325&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/32-734-1/Tetrahydrocortisol-TMS.pdf>

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