Cortisol tetra-TMS

Inchi: InChI=1S/C33H62O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38
InchiKey: HYSKEWMPQZGXIQ-ISGILSMGSA-N
Formula: C33H62O5Si4
SMILES: CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)
Mol. weight [g/mol]: 651.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.27		Crippen Method
logp	9.135		Crippen Method
rinpol	3314.00		NIST Webbook

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=R284987&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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