

Tetrahydrocortosterone, TMSO-TMS # 2

Inchi: InChI=1S/C33H67NO4Si4/c1-32-20-19-25(36-40(6,7)8)21-24(32)15-16-26-27-17-18-28(2
InchiKey: PPNLCQXZSCQULC-QUTOVEOWSA-N
Formula: C33H67NO4Si4
SMILES: CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2C(CO[Si](C)(C)C)
Mol. weight [g/mol]: 654.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.45		Crippen Method
logp	9.754		Crippen Method
rinpol	3088.00		NIST Webbook
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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=R527625&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/70-203-8/Tetrahydrocortosterone-TMSO-TMS-2.pdf>

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