

allo-Tetrahydrocortosterone, EO-TMS # 1

Inchi: InChI=1S/C32H63NO4Si3/c1-13-34-33-28(22-35-38(4,5)6)27-17-16-26-25-15-14-23-20-21
InchiKey: PZZJZTGGSDVDCQ-NXLWCHMLSA-N
Formula: C32H63NO4Si3
SMILES: CCON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 610.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	8.939		Crippen Method
rinpol	3058.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527452&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/70-615-1/allo-Tetrahydrocortosterone-EO-TMS-1.pdf>

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