

A-Tetrahydrocortisol, TMS

Inchi: InChI=1S/C36H74O5Si5/c1-34-22-20-28(38-43(6,7)8)24-27(34)18-19-29-30-21-23-36(41)
InchiKey: CPQXZBROIXYNLU-FJHGZWAUSA-N
Formula: C36H74O5Si5
SMILES: CC12CCC(O[Si](C)(C)C)=CC1CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C
Mol. weight [g/mol]: 727.40

Physical Properties

Property code	Value	Unit	Source
log10ws	0.60		Crippen Method
logp	10.866		Crippen Method
rinpol	3151.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R35933&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.cheméo.com/cid/66-194-4/A-Tetrahydrocortisol-TMS.pdf>

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