

6«beta»-Hydroxycortisol, tetra-TMS

Inchi: InChI=1S/C33H62O6Si4/c1-31-17-15-23(34)19-26(31)27(37-41(6,7)8)20-24-25-16-18-33
InchiKey: MYCYLBNCIUWUND-JYFOKUQJSA-N
Formula: C33H62O6Si4
SMILES: CC12CCC(=O)C=C1C(O[Si](C)(C)C)CC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C
Mol. weight [g/mol]: 667.18

Physical Properties

Property code	Value	Unit	Source
log10ws	0.69		Crippen Method
logp	8.189		Crippen Method
rinpol	3419.00		NIST Webbook
rinpol	3419.00		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=R557938&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/24-164-3/6-beta-Hydroxycortisol-tetra-TMS.pdf>

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