

6«beta»-Hydroxycortisol, bis-MO-tetra-TMS, syn

Inchi: InChI=1S/C35H68N2O6Si4/c1-33-19-17-25(36-38-3)21-28(33)29(41-45(8,9)10)22-26-27
InchiKey: XYRURNQWZVXHNN-FVGXWCSESA-N
Formula: C35H68N2O6Si4
SMILES: CON=C1C=C2C(O[Si](C)(C)C)CC3C(C(O[Si](C)(C)C)CC4(C)C3CCC4(O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 725.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.07		Crippen Method
logp	9.056		Crippen Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook

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=R557923&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/68-047-5/6-beta-Hydroxycortisol-bis-MO-tetra-TMS-syn.pdf>

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