Hydrocortisone (cortisol), MO-TMS

Inchi: InChI=1S/C32H60N2O5Si3/c1-30-18-16-24(33-35-3)20-23(30)14-15-25-26-17-19-32(39-
InchiKey: PRZGIUIKCGRVGY-MOWCZZONSA-N
Formula: C32H60N2O5Si3
SMILES: CON=C1C=C2CCC3C(C(O[Si](C)(C)C)CC4(C)C3CCC4(O[Si](C)(C)C)C(CO[Si](C)(C)C)=
Mol. weight [g/mol]: 637.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.56		Crippen Method
logp	8.226		Crippen Method
rinpol	3290.00		NIST Webbook
rinpol	3290.00		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=R512811&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/22-213-0/Hydrocortisone-cortisol-MO-TMS.pdf
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