Cortisone, MO-TMS

Inchi: InChI=1S/C30H53N3O5Si2/c1-28-16-14-22(31-34-3)18-21(28)12-13-23-24-15-17-30(38-
InchiKey: DBQJJNSWAVLDND-VKNNHANSSA-N
Formula: C30H53N3O5Si2
SMILES: CON=C1C=C2CCC3C(C(=NOC)CC4(C)C3CCC4(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)
Mol. weight [g/mol]: 591.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	7.008		Crippen Method
rinpol	3223.00		NIST Webbook
rinpol	3279.00		NIST Webbook
rinpol	3248.00		NIST Webbook
rinpol	3279.00		NIST Webbook
rinpol	3248.00		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=R318926&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.