

Cortisone enol-TMS

Inchi: InChI=1S/C30H52O5Si3/c1-28-16-14-22(34-37(6,7)8)18-21(28)12-13-23-24-15-17-30(35)
InchiKey: FLOZJHDKJDRAEJ-VKNNHANSSA-N
Formula: C30H52O5Si3
SMILES: CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2C(=O)CC2(C)C1CCC2(O[Si](C)(C)C)C(=O)CO[Si](C)(C)C
Mol. weight [g/mol]: 576.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Crippen Method
logp	7.484		Crippen Method
rinpol	3276.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384082&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/41-830-4/Cortisone-enol-TMS.pdf>

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