

«beta»-Cortolone, tetrakis-TMS

Inchi: InChI=1S/C33H66O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38)
InchiKey: LTOJWDHWCDVAFF-CZCGPAPPSA-N
Formula: C33H66O5Si4
SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(=O)CC2(C)C1CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)C12
Mol. weight [g/mol]: 655.22

Physical Properties

Property code	Value	Unit	Source
log10ws	0.07		Crippen Method
logp	9.090		Crippen Method
rinpol	3246.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R16513&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/55-607-7/beta-Cortolone-tetrakis-TMS.pdf>

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