

A-Cortolone, MO TMS

Inchi: InChI=1S/C34H69NO5Si4/c1-32-20-18-26(38-42(7,8)9)22-25(32)16-17-27-28-19-21-34(4)
InchiKey: XELWYCNVFGIFEQ-UPLCRBOCSA-N
Formula: C34H69NO5Si4
SMILES: CON=C1CC2(C)C(CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C)C2CCC3CC(O[Si](C)(C)C)C3
Mol. weight [g/mol]: 684.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.31		Crippen Method
logp	9.523		Crippen Method
rinpol	3071.00		NIST Webbook
rinpol	3040.00		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=R104371&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/48-340-1/A-Cortolone-MO-TMS.pdf>

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