

B-Cortolone MO TMS

Other names: «beta»-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-PLHDFEIJSA-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]
Mol. weight [g/mol]: 684.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.31		Crippen Method
logp	9.523		Crippen Method
rinpol	3096.00		NIST Webbook
rinpol	3102.00		NIST Webbook
rinpol	3070.00		NIST Webbook
rinpol	3079.00		NIST Webbook
rinpol	3095.00		NIST Webbook
rinpol	3095.00		NIST Webbook
rinpol	3080.00		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=R92773&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/49-447-2/B-Cortolone-MO-TMS.pdf>

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