

Betaxolol, TBDMS

Inchi: InChI=1S/C24H43NO3Si/c1-19(2)25-16-23(28-29(6,7)24(3,4)5)18-27-22-12-10-20(11-13)
InchiKey: LOASLLDCGXJCJHM-UHFFFAOYSA-N
Formula: C24H43NO3Si
SMILES: CC(C)NCC(COc1ccc(CCOCC2CC2)cc1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 421.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	5.423		Crippen Method
rinpol	2600.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435160&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/119-224-1/Betaxolol-TBDMS.pdf>

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