

Betaxolol, N-ethoxycarbonylated, TMS

Inchi:	InChI=1S/C24H41NO5Si/c1-7-28-24(26)25(19(2)3)16-23(30-31(4,5)6)18-29-22-12-10-20
InchiKey:	MWKFMDDLKAINHT-UHFFFAOYSA-N
Formula:	C24H41NO5Si
SMILES:	CCOC(=O)N(CC(COc1ccc(CCOCC2CC2)cc1)O[Si])(C)(C)C(C)C
Mol. weight [g/mol]:	451.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	5.121		Crippen Method
rinpol	2723.50		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435155&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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