

# Betaxolol, PFB-TMS

<b>Inchi:</b>	InChI=1S/C28H36F5NO4Si/c1-17(2)34(28(35)22-23(29)25(31)27(33)26(32)24(22)30)14-
<b>InchiKey:</b>	ABYBJKXWOAFKLA-UHFFFAOYSA-N
<b>Formula:</b>	C28H36F5NO4Si
<b>SMILES:</b>	CC(C)N(CC(COc1ccc(CCOCC2CC2)cc1)O[Si](C)(C)C)C(=O)c1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	573.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.13		Crippen Method
logp	6.501		Crippen Method
rinpol	2968.00		NIST Webbook
rinpol	2968.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R175021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R175021&amp;Units=SI</a>

## Legend

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

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