

# Metoprolol, TBDMS

<b>Inchi:</b>	InChI=1S/C21H39NO3Si/c1-17(2)22-15-20(25-26(7,8)21(3,4)5)16-24-19-11-9-18(10-12-
<b>InchiKey:</b>	KYDUFKHOCGTGDV-UHFFFAOYSA-N
<b>Formula:</b>	C21H39NO3Si
<b>SMILES:</b>	COCCc1ccc(OCC(CNC(C)C)O[Si](C)(C)C(C)(C)C)cc1
<b>Mol. weight [g/mol]:</b>	381.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	4.643		Crippen Method
rinpol	2297.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R435224&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R435224&amp;Units=SI</a>
<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>

## 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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<https://www.chemeo.com/cid/66-662-4/Metoprolol-TBDMS.pdf>

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