

Timolol TMS derivative

Other names:	Timolol O-TMS Timolol TMS
Inchi:	InChI=1S/C16H32N4O3SSi/c1-16(2,3)17-11-13(23-25(4,5)6)12-22-15-14(18-24-19-15)2
InchiKey:	OZLQNKYRHDADJG-UHFFFAOYSA-N
Formula:	C16H32N4O3SSi
SMILES:	CC(C)(C)NCC(COC1nsc1N1CCOCC1)O[Si](C)(C)C
Mol. weight [g/mol]:	388.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.93		Crippen Method
logp	2.362		Crippen Method

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=U137148&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/113-629-8/Timolol-TMS-derivative.pdf>

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