Timolol, TBDMS

Inchi: InChI=1S/C18H36N4O3SSi/c1-14(2)19-12-15(25-27(6,7)18(3,4)5)13-24-17-16(20-26-21-
InchiKey: DCGFAXJUYDXAJO-UHFFFAOYSA-N
Formula: C18H36N4O3SSi
SMILES: CC(C)NCC(COc1nsnc1N1CCOCC1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 416.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	3.142		Crippen Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R435388&Units=SI

Legend

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