

Timolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C18H34N4O5SSi/c1-7-25-18(23)22(14(2)3)12-15(27-29(4,5)6)13-26-17-16(19)
InchiKey: BNAHVGOCKCBGDF-UHFFFAOYSA-N
Formula: C18H34N4O5SSi
SMILES: CCOC(=O)N(CC(COc1nsc1N1CCOCC1)O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 446.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	2.841		Crippen Method
rinpol	2644.40		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435373&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/113-540-6/Timolol-N-ethoxycarbonylated-TMS.pdf>

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