

Sotalol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C18H32N2O5SSi/c1-8-24-18(21)20(14(2)3)13-17(25-27(5,6)7)15-9-11-16(12-1
InchiKey: AAMVPZMGYSCIEG-UHFFFAOYSA-N
Formula: C18H32N2O5SSi
SMILES: CCOC(=O)N(CC(O[Si](C)(C)C)c1ccc(NS(C)(=O)=O)cc1)C(C)C
Mol. weight [g/mol]: 416.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	3.818		Crippen Method
rinpol	2588.60		NIST Webbook
rinpol	2588.60		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=R435353&Units=SI>

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/19-210-7/Sotalol-N-ethoxycarbonylated-TMS.pdf>

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