

Sotalol, TBDMS

Inchi: InChI=1S/C18H34N2O3SSi/c1-14(2)19-13-17(23-25(7,8)18(3,4)5)15-9-11-16(12-10-15)2
InchiKey: CQNLFZQLLOSKIV-UHFFFAOYSA-N
Formula: C18H34N2O3SSi
SMILES: CC(C)NCC(O[Si](C)(C)C(C)(C)C)c1ccc(NS(C)(=O)=O)cc1
Mol. weight [g/mol]: 386.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	4.119		Crippen Method
rinpol	2726.40		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435368&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/41-676-6/Sotalol-TBDMS.pdf>

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