

Acebutolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C24H40N2O6Si/c1-9-11-23(28)25-19-12-13-22(21(14-19)18(5)27)31-16-20(32)
InchiKey: HDMJMPISKBKFMW-UHFFFAOYSA-N
Formula: C24H40N2O6Si
SMILES: CCCC(=O)Nc1ccc(OCC(CN(C(=O)OCC)C(C)C)O[Si](C)(C)C)c(C(C)=O)c1
Mol. weight [g/mol]: 480.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	5.094		Crippen Method
rinpol	2877.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435115&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/63-486-3/Acebutolol-N-ethoxycarbonylated-TMS.pdf>

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