

Alprenolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C21H35NO4Si/c1-8-12-18-13-10-11-14-20(18)25-16-19(26-27(5,6)7)15-22(17)
InchiKey: MVXAIJNKQGROAC-UHFFFAOYSA-N
Formula: C21H35NO4Si
SMILES: C=CCc1ccccc1OCC(CN(C(=O)OCC)C(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 393.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	4.881		Crippen Method
rinpol	2192.50		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435120&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/59-593-9/Alprenolol-N-ethoxycarbonylated-TMS.pdf>

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