

Oxprenolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C21H35NO5Si/c1-8-14-25-19-12-10-11-13-20(19)26-16-18(27-28(5,6)7)15-22
InchiKey: QVZSZCOMZAZZGW-UHFFFAOYSA-N
Formula: C21H35NO5Si
SMILES: C=CCOc1ccccc1OCC(CN(C(=O)OCC)C(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 409.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	4.717		Crippen Method
rinpol	2276.10		NIST Webbook
rinpol	2276.10		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435239&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/80-290-1/Oxprenolol-N-ethoxycarbonylated-TMS.pdf>

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