

Metoprolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C21H37NO5Si/c1-8-25-21(23)22(17(2)3)15-20(27-28(5,6)7)16-26-19-11-9-18(4)
InchiKey: HOWFNYGNEUKGBU-UHFFFAOYSA-N
Formula: C21H37NO5Si
SMILES: CCOC(=O)N(CC(COc1ccc(CCOC)cc1)O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 411.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	4.341		Crippen Method
rinpol	2418.50		NIST Webbook
rinpol	2418.50		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=R435219&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/117-833-7/Metoprolol-N-ethoxycarbonylated-TMS.pdf>

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