

Propranolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C22H33NO4Si/c1-7-25-22(24)23(17(2)3)15-19(27-28(4,5)6)16-26-21-14-10-12
InchiKey: GRNLDYIXJBLJJU-UHFFFAOYSA-N
Formula: C22H33NO4Si
SMILES: CCOC(=O)N(CC(COc1cccc2ccccc12)O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 403.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	5.306		Crippen Method
rinpol	2519.30		NIST Webbook
rinpol	2519.30		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=R435333&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/68-749-6/Propranolol-N-ethoxycarbonylated-TMS.pdf>

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