

Pronethalol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C21H31NO3Si/c1-7-24-21(23)22(16(2)3)15-20(25-26(4,5)6)19-13-12-17-10-8-9
InchiKey: UYDYTIDJVJOWGK-UHFFFAOYSA-N
Formula: C21H31NO3Si
SMILES: CCOC(=O)N(CC(O[Si](C)(C)C)c1ccc2ccccc2c1)C(C)C
Mol. weight [g/mol]: 373.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	5.599		Crippen Method
rinsol	2266.20		NIST Webbook
rinsol	2266.20		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=R435313&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/61-278-6/Pronethalol-N-ethoxycarbonylated-TMS.pdf>

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