

Pronethalol, TBDMS

Inchi: InChI=1S/C21H33NOSi/c1-16(2)22-15-20(23-24(6,7)21(3,4)5)19-13-12-17-10-8-9-11-18
InchiKey: JFOOIRWBBIJMOV-UHFFFAOYSA-N
Formula: C21H33NOSi
SMILES: CC(C)NCC(O[Si](C)(C)C(C)(C)C)c1ccc2ccccc2c1
Mol. weight [g/mol]: 343.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	5.901		Crippen Method
rinpol	2156.70		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435328&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/96-187-9/Pronethalol-TBDMS.pdf>

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