4-(3-Phenoxypropyl)pyridine

Inchi: InChI=1S/C14H15NO/c1-2-6-14(7-3-1)16-12-4-5-13-8-10-15-11-9-13/h1-3,6-11H,4-5,12H
InchiKey: TYMHXGLDRUMFJW-UHFFFAOYSA-N
Formula: C14H15NO
SMILES: c1ccc(OCCCc2ccncc2)cc1
Mol. weight [g/mol]: 213.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	3.093		Crippen Method
mcvol	176.450	ml/mol	McGowan Method
rinpol	1887.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R545490&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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