2-(6-Phenoxyhexyl)pyridine

Inchi: InChI=1S/C17H21NO/c1(4-10-16-11-7-8-14-18-16)2-9-15-19-17-12-5-3-6-13-17/h3,5-8,1
InchiKey: VWRAVIGRENBNNG-UHFFFAOYSA-N
Formula: C17H21NO
SMILES: c1ccc(OCCCCCCc2ccccn2)cc1
Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	4.263		Crippen Method
mcvol	218.720	ml/mol	McGowan Method
rinpol	2104.00		NIST Webbook
rinpol	2104.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R545430&Units=SI
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

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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