

4-[3-(4-Methylphenoxy)propyl]pyridine

Inchi:	InChI=1S/C15H17NO/c1-13-4-6-15(7-5-13)17-12-2-3-14-8-10-16-11-9-14/h4-11H,2-3,12
InchiKey:	SQINSSGTURBK KY-UHFFFAOYSA-N
Formula:	C15H17NO
SMILES:	Cc1ccc(OCCCc2ccncc2)cc1
Mol. weight [g/mol]:	227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	3.402		Crippen Method
mcvol	190.540	ml/mol	McGowan Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R545485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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