

2-[3-(4-Methylphenoxy)propyl]pyridine

Inchi: InChI=1S/C15H17NO/c1-13-7-9-15(10-8-13)17-12-4-6-14-5-2-3-11-16-14/h2-3,5,7-11H,4
InchiKey: MCWOZAOLMZWQMV-UHFFFAOYSA-N
Formula: C15H17NO
SMILES: Cc1ccc(OCCCc2ccccc2)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	1905.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R545396&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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<https://www.chemeo.com/cid/47-101-7/2-3-4-Methylphenoxy-propyl-pyridine.pdf>

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