

1-[2-(4-Methoxyphenyl)ethyl]pyridinium

Inchi:	InChI=1S/C14H16NO/c1-16-14-7-5-13(6-8-14)9-12-15-10-3-2-4-11-15/h2-8,10-11H,9,12
InchiKey:	WTDUWYFKAPRORY-UHFFFAOYSA-N
Formula:	C14H16NO
SMILES:	COc1ccc(CC[n+]2ccccc2)cc1
Mol. weight [g/mol]:	214.28
CAS:	118177-96-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	2.225		Crippen Method
mcvol	178.600	ml/mol	McGowan Method

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=C118177961&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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