1-[2-(4-Methyl phenyl)ethyl]pyridinium

Inchi:	InChI=1S/C14H16N/c1-13-5-7-14(8-6-13)9-12-15-10-3-2-4-11-15/h2-8,10-11H,9,12H2,1
InchiKey:	VSGVHARORBOYKO-UHFFFAOYSA-N
Formula:	C14H16N
SMILES:	Cc1ccc(CC[n+]2ccccc2)cc1
Mol. weight [g/mol]:	198.28
CAS:	118177-93-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	2.525		Crippen Method
mcvol	172.730	ml/mol	McGowan Method

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=C118177938&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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