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

Inchi:	InChI=1S/C13H13N2O2/c16-15(17)13-6-4-12(5-7-13)8-11-14-9-2-1-3-10-14/h1-7,9-10H,
InchiKey:	AOZIQWMPOFXLEG-UHFFFAOYSA-N
Formula:	C13H13N2O2
SMILES:	O=[N+]([O-])c1ccc(CC[n+]2ccccc2)cc1
Mol. weight [g/mol]:	229.25
CAS:	118177-67-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	2.125		Crippen Method
mcvol	176.060	ml/mol	McGowan Method

Sources

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=C118177676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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