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,8

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: 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=C118177676&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume