1-[(4-Nitrophenyl)methyl]pyridinium

Inchi: InChI=1S/C12H11N2O2/c15-14(16)12-6-4-11(5-7-12)10-13-8-2-1-3-9-13/h1-9H,10H2/q+
InchiKey: NQZWJOKNWNCQJK-UHFFFAOYSA-N
Formula: C12H11N2O2
SMILES: O=[N+]([O-])c1ccc(C[n+]2ccccc2)cc1
Mol. weight [g/mol]: 215.23
CAS: 24837-70-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	1.931		Crippen Method
mcvol	161.970	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24837705&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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