

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:	NQZWJOKNWNQCQJK-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

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<https://www.chemeo.com/cid/14-163-5/1-4-Nitrophenyl-methyl-pyridinium.pdf>

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