

2-Pyrrolidinemethanol, 1-(4-nitrophenyl)-

Other names:	1-(4-nitrophenyl)-2-pyrrolidinemethanol
Inchi:	InChI=1S/C11H14N2O3/c14-8-11-2-1-7-12(11)9-3-5-10(6-4-9)13(15)16/h3-6,11,14H,1-2
InchiKey:	HCVBBVTZZJFVLA-UHFFFAOYSA-N
Formula:	C11H14N2O3
SMILES:	O=[N+]([O-])c1ccc(N2CCCC2CO)cc1
Mol. weight [g/mol]:	222.24
CAS:	105173-13-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.556		Crippen Method
mcvol	164.500	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105173135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/121-512-8/2-Pyrrolidinemethanol-1-4-nitrophenyl.pdf>

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