

# 1-(4-Nitrophenyl)piperazine

<b>Other names:</b>	Piperazine, 1-(4-nitrophenyl)- N-p-Nitrophenylpiperazine
<b>Inchi:</b>	InChI=1S/C10H13N3O2/c14-13(15)10-3-1-9(2-4-10)12-7-5-11-6-8-12/h1-4,11H,5-8H2
<b>InchiKey:</b>	VWOJSRICKSKDKAW-UHFFFAOYSA-N
<b>Formula:</b>	C10H13N3O2
<b>SMILES:</b>	O=[N+]([O-])c1ccc(N2CCNCC2)cc1
<b>Mol. weight [g/mol]:</b>	207.23
<b>CAS:</b>	6269-89-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.004		Crippen Method
mvol	154.520	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6269892&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6269892&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume

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