

# Imidazole, 5-(o-aminophenylthio)-1-methyl-4-nitro-

<b>Inchi:</b>	InChI=1S/C10H10N4O2S/c1-13-6-12-9(14(15)16)10(13)17-8-5-3-2-4-7(8)11/h2-6H,11H2
<b>InchiKey:</b>	QYHRABNYVGQVDZ-UHFFFAOYSA-N
<b>Formula:</b>	C10H10N4O2S
<b>SMILES:</b>	Cn1cnc([N+](=O)[O-])c1Sc1cccc1N
<b>Mol. weight [g/mol]:</b>	250.28
<b>CAS:</b>	53900-32-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	2.062		Crippen Method
mcvol	172.250	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=C53900326&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53900326&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>mcvol:</b>	McGowan's characteristic volume

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