

# Isoxazole, 3-methyl-5-phenyl-

<b>Other names:</b>	3-Methyl-5-phenylisoxazole
<b>Inchi:</b>	InChI=1S/C10H9NO/c1-8-7-10(12-11-8)9-5-3-2-4-6-9/h2-7H,1H3
<b>InchiKey:</b>	FBYQIYSAUFWXQK-UHFFFAOYSA-N
<b>Formula:</b>	C10H9NO
<b>SMILES:</b>	Cc1cc(-c2ccccc2)on1
<b>Mol. weight [g/mol]:</b>	159.18
<b>CAS:</b>	1008-75-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.05		Crippen Method
logp	2.650		Crippen Method
mcvol	124.390	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=C1008759&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1008759&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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