

# 2-Methoxy-5-(4-nitrophenyl)-1,3,4-oxadiazole

<b>Inchi:</b>	InChI=1S/C9H7N3O4/c1-15-9-11-10-8(16-9)6-2-4-7(5-3-6)12(13)14/h2-5H,1H3
<b>InchiKey:</b>	YKGDYDUGVHEJSG-UHFFFAOYSA-N
<b>Formula:</b>	C9H7N3O4
<b>SMILES:</b>	COc1nnc(-c2ccc([N+](=O)[O-])cc2)o1
<b>Mol. weight [g/mol]:</b>	221.17
<b>CAS:</b>	102925-87-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.11		Crippen Method
logp	1.653		Crippen Method
mcvol	143.570	ml/mol	McGowan Method

## Sources

<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>
<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=C102925871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C102925871&amp;Units=SI</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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