

# Acrylonitrile, 2-furan-

<b>Inchi:</b>	InChI=1S/C7H5NO/c8-4-1-2-7-3-5-9-6-7/h1-3,5-6H/b2-1+
<b>InchiKey:</b>	IZJSWYCZEOTWRI-OWOJBTEDSA-N
<b>Formula:</b>	C7H5NO
<b>SMILES:</b>	N#CC=Cc1ccoc1
<b>Mol. weight [g/mol]:</b>	119.12
<b>CAS:</b>	87995-19-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.31		Crippen Method
logp	1.816		Crippen Method
mcvol	92.980	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=C87995195&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C87995195&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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<https://www.chemeo.com/cid/27-625-8/Acrylonitrile-2-furan.pdf>

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