

# 1,3,5-Triazine-2,4(1H,3H)-dione

<b>Other names:</b>	5-Azauracil s-Triazine-2,4(1H,3H)-dione Allantoxaidin Allantoxaidine Oxaidin
<b>Inchi:</b>	InChI=1S/C3H3N3O2/c7-2-4-1-5-3(8)6-2/h1H,(H2,4,5,6,7,8)
<b>InchiKey:</b>	GEWRKGDZYIFNP-UHFFFAOYSA-N
<b>Formula:</b>	C3H3N3O2
<b>SMILES:</b>	O=c1nc[nH]c(=O)[nH]1
<b>Mol. weight [g/mol]:</b>	113.07
<b>CAS:</b>	71-33-0

## Physical Properties

Property code	Value	Unit	Source
ie	10.10	eV	NIST Webbook
ie	10.59	eV	NIST Webbook
log10ws	1.48		Crippen Method
logp	-2.506		Crippen Method
mcvol	71.050	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=C71330&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C71330&amp;Units=SI</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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