1,3,5-TRIAZINE-2,4(1H,3H)-DIONE

Other names:	5-Azauracil
	s-Triazine-2,4(1H,3H)-dione
	Allantoxaidin
	Allantoxaidine
	Oxaidin
Inchi:	InChI=1S/C3H3N3O2/c7-2-4-1-5-3(8)6-2/h1H,(H2,4,5,6,7,8)
InchiKey:	GEWRKGDRYZIFNP-UHFFFAOYSA-N
Formula:	C3H3N3O2
SMILES:	O=c1nc[nH]c(=O)[nH]1
Mol. weight [g/mol]:	113.08

Physical Properties

Property code	Value	Unit	Source
ie	10.10	eV	NIST Webbook
ie	10.59	eV	NIST Webbook
logp	-2.506		Crippen Method
mcvol	71.050	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71330&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume