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

Other names:	1,2,4-triazine-3,5-diol
	2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione
	4(6)-Azauracil
	6-azauracil
	AZU
	Azauracil
	IPO 3834
	NSC 3425
	USAF CB-30
	as-Triazine-3,5(2H,4H)-dione
	as-Triazine-3,5-diol
Inchi:	InChI=1S/C3H3N3O2/c7-2-1-4-6-3(8)5-2/h1H,(H2,5,6,7,8)
InchiKey:	SSPYSWLZOPCOLO-UHFFFAOYSA-N
Formula:	C3H3N3O2
SMILES:	O=c1cn[nH]c(=O)[nH]1
Mol. weight [g/mol]:	113.07
CAS:	461-89-2

Physical Properties

Property code	Value	Unit	Source
ie	10.00	eV	NIST Webbook
ie	10.20 ± 0.10	eV	NIST Webbook
ie	10.18	eV	NIST Webbook
log10ws	1.48		Crippen Method
logp	-2.506		Crippen Method
mcvol	71.050	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hvapt	118.10	kJ/mol	298.15	Experimental and computational thermochemical studies of 6-azauracil derivatives

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical studies of 6-azauracil derivatives:	https://www.doi.org/10.1016/j.jct.2015.12.020
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C461892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume