Violuric acid

Other names:	2,4,5,6(1H,3H)-Pyrimidinetetrone, 5-oxime
	Alloxan 5-oxime
	5-(Hydroxyimino)barbituric acid
	5-Isonitrosobarbituric acid
Inchi:	InChI=1S/C4H3N3O4/c8-2-1(7-11)3(9)6-4(10)5-2/h11H,(H2,5,6,8,9,10)
InchiKey:	JMUJZTASUDOAGC-UHFFFAOYSA-N
Formula:	C4H3N3O4
SMILES:	O=C1NC(=O)C(=NO)C(=O)N1
Mol. weight [g/mol]:	157.08
CAS:	87-39-8

Physical Properties

Property code	Value	Unit	Source
hf	-499.91	kJ/mol	Joback Method
hvap	72.31	kJ/mol	Joback Method
log10ws	1.11		Crippen Method
logp	-1.817		Crippen Method
mcvol	92.580	ml/mol	McGowan Method
pc	6451.51	kPa	Joback Method
tb	787.04	K	Joback Method
tc	1048.62	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87398&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature