2,4(1H,3H)-Pyrimidinedione, 5-nitro-

Other names:	5-Nitrouracil
	2,4-Dihydroxy-5-nitropyrimidine
	Uracil, 5-nitro-
Inchi:	InChI=1S/C4H3N3O4/c8-3-2(7(10)11)1-5-4(9)6-3/h1H,(H2,5,6,8,9)
InchiKey:	TUARVSWVPPVUGS-UHFFFAOYSA-N
Formula:	C4H3N3O4
SMILES:	O=c1[nH]cc([N+](=O)[O-])c(=O)[nH]1
Mol. weight [g/mol]:	157.08
CAS:	611-08-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.59		Crippen Method
logp	-1.992		Crippen Method
mcvol	92.580	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume