

Acetamide, n-(6-chloro-5-nitro-4-oxo-3,4-dihydro-pyrimidin-2-

Inchi:	InChI=1S/C6H5ClN4O4/c1-2(12)8-6-9-4(7)3(11(14)15)5(13)10-6/h1H3,(H2,8,9,10,12,13)
InchiKey:	YBOCORODVPIHME-UHFFFAOYSA-N
Formula:	C6H5ClN4O4
SMILES:	CC(=O)Nc1nc(Cl)c([N+](=O)[O-])c(=O)[nH]1
Mol. weight [g/mol]:	232.58
CAS:	51471-45-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	-0.192		Crippen Method
mcvol	138.680	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51471455&Units=SI

Legend

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

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