

4(3H)-pyrimidinone, 6-amino-2-chloro-5-nitro-

Inchi:	InChI=1S/C4H3ClN4O3/c5-4-7-2(6)1(9(11)12)3(10)8-4/h(H3,6,7,8,10)
InchiKey:	MJQOUMJPRPRGRF-UHFFFAOYSA-N
Formula:	C4H3ClN4O3
SMILES:	<chem>Nc1nc(Cl)[nH]c(=O)c1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	190.54
CAS:	116434-77-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.85		Crippen Method
logp	-0.568		Crippen Method
mcvol	108.930	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116434776&Units=SI
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

Legend

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

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