

Pyrimidine, 4-amino-6-chloro-5-nitro-

Inchi:	InChI=1S/C4H3ClN4O2/c5-3-2(9(10)11)4(6)8-1-7-3/h1H,(H2,6,7,8)
InchiKey:	BWLOHIMQWHFSQF-UHFFFAOYSA-N
Formula:	C4H3ClN4O2
SMILES:	<chem>Nc1ncnc(Cl)c1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	174.54
CAS:	4316-94-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	0.620		Crippen Method
mcvol	103.060	ml/mol	McGowan Method

Sources

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=C4316943&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/55-808-4/Pyrimidine-4-amino-6-chloro-5-nitro.pdf>

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