

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

Inchi:	InChI=1S/C4H4ClN5O2/c5-3-2(10(11)12)4(9-6)8-1-7-3/h1H,6H2,(H,7,8,9)
InchiKey:	DAEOYVCNUJFQAW-UHFFFAOYSA-N
Formula:	C4H4ClN5O2
SMILES:	NNc1ncnc(Cl)c1[N+](=O)[O-]
Mol. weight [g/mol]:	189.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	0.324		Crippen Method
mcvol	113.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/113-854-8/Pyrimidine-4-chloro-6-hydrazino-5-nitro.pdf>

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