

Acetic acid, 5-amino-6-chloro-4-pyrimidinyl hydrazide

Inchi:	InChI=1S/C6H8ClN5O/c1-3(13)11-12-6-4(8)5(7)9-2-10-6/h2H,8H2,1H3,(H,11,13)(H,9,10)
InchiKey:	QLRSZYIHMUMZQY-UHFFFAOYSA-N
Formula:	C6H8ClN5O
SMILES:	CC(=O)NNc1ncnc(Cl)c1N
Mol. weight [g/mol]:	201.61
CAS:	7597-91-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	0.175		Crippen Method
mcvol	135.350	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7597913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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