

2-Amino-5-chloro-4-pyrimidinecarboxylic acid

Other names:	2-Amino-5-chloropyrimidine-4-carboxylic acid 4-Pyrimidinecarboxylic acid, 2-amino-5-chloro-
Inchi:	InChI=1S/C5H4ClN3O2/c6-2-1-8-5(7)9-3(2)4(10)11/h1H,(H,10,11)(H2,7,8,9)
InchiKey:	PDLZOTZLGNZOFS-UHFFFAOYSA-N
Formula:	C5H4ClN3O2
SMILES:	<chem>Nc1ncc(Cl)c(C(=O)O)n1</chem>
Mol. weight [g/mol]:	173.56
CAS:	45867-11-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	0.410		Crippen Method
mvol	107.170	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=C45867116&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
mvol:	McGowan's characteristic volume

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