

2-Thiazolamine, 5-chloro-

Other names:	Thiazole, 2-amino-5-chloro- 2-Amino-5-chlorothiazole NSC 86106
Inchi:	InChI=1S/C3H3CIN2S/c4-2-1-6-3(5)7-2/h1H,(H2,5,6)
InchiKey:	SWQWTDAWUSBMGA-UHFFFAOYSA-N
Formula:	C3H3CIN2S
SMILES:	<chem>N=c1[nH]cc(Cl)s1</chem>
Mol. weight [g/mol]:	134.59
CAS:	41663-73-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	0.727		Crippen Method
mcvol	82.220	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41663734&Units=SI

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/98-720-4/2-Thiazolamine-5-chloro.pdf>

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