

# 2-(4-chloro-2-oxo-1,3-benzothiazol-3-yl)acetic acid

<b>Inchi:</b>	InChI=1S/C9H6ClNO3S/c10-5-2-1-3-6-8(5)11(4-7(12)13)9(14)15-6/h1-3H,4H2,(H,12,13)
<b>InchiKey:</b>	HYJSGOXICXYZGS-UHFFFAOYSA-N
<b>Formula:</b>	C9H6ClNO3S
<b>SMILES:</b>	O=C(O)Cn1c(=O)sc2cccc(Cl)c21
<b>Mol. weight [g/mol]:</b>	243.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Aqueous Solubility Prediction Method
logp	1.801		Crippen Method
mcvol	150.630	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

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

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