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

Inchi: 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)
InchiKey: HYJSGOXICXYZGS-UHFFFAOYSA-N
Formula: C9H6ClNO3S
SMILES: O=C(O)Cn1c(=O)sc2cccc(Cl)c21
Mol. weight [g/mol]: 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/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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