

# 2-[4-[3-(2-chlorophenothiazin-10-yl)propyl]piperaz

Inchi:  
**acetate**

InChI=1S/C23H28ClN3O2S/c1-18(28)29-16-15-26-13-11-25(12-14-26)9-4-10-27-20-5-2-

InchiKey:

AIUHRQHVSUTGJ-UHFFFAOYSA-N

Formula:

C23H28ClN3O2S

SMILES:

CC(=O)OCCN1CCN(CCCN2c3ccccc3Sc3ccc(Cl)cc32)CC1

Mol. weight [g/mol]:

446.02

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Aqueous Solubility Prediction Method
logp	4.513		Crippen Method
mvol	331.660	ml/mol	McGowan Method

## Sources

**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>

**Crippen Method:**

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

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mvol:** McGowan's characteristic volume

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