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

Inchi: InChI=1S/C23H28ClN3O2S/c1-18(28)29-16-15-26-13-11-25(12-14-26)9-4-10-27-20-5-2-
InchiKey: AIUHRQHVWSUTGJ-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
mcvol	331.660	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
mcvol: McGowan's characteristic volume