2-[4-(4-chlorophenyl)-2-phenyl-1,3-thiazol-5-yl]ace
acid

Inchi: InChI=1S/C17H12ClNO2S/c18-13-8-6-11(7-9-13)16-14(10-15(20)21)22-17(19-16)12-4-2

InchiKey: JIEKMACRVQTPRC-UHFFFAOYSA-N

Formula: C17H12ClNO2S

SMILES: O=C(O)Cc1sc(-c2ccccc2)nc1-c1ccc(Cl)cc1

Mol. weight [g/mol]: 329.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Aqueous Solubility Prediction Method
logp	4.758		Crippen Method
mcvol	229.420	ml/mol	McGowan Method
tf	434.65	K	Aqueous Solubility Prediction Method

Sources

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.