3,3-dimethyl-7-oxo-6-[(2-phenylacetyl)amino]-4-th
acid

Inchi: InChI=1S/C16H18N2O4S/c1-16(2)12(15(21)22)18-13(20)11(14(18)23-16)17-10(19)8-9-6

InchiKey: JGSARLDLIJGVTE-UHFFFAOYSA-N

Formula: C16H18N2O4S

SMILES: CC1(C)SC2C(NC(=O)Cc3ccccc3)C(=O)N2C1C(=O)O

Mol. weight [g/mol]: 334.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Aqueous Solubility Prediction Method
logp	0.861		Crippen Method
mcvol	237.710	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