3,3-dimethyl-7-oxo-6-[[2-(phenoxy)acetyl]amino]-4-acid

Inchi: InChI=1S/C16H18N2O5S/c1-16(2)12(15(21)22)18-13(20)11(14(18)24-16)17-10(19)8-23-

InchiKey: BPLBGHOLXOTWMN-UHFFFAOYSA-N

Formula: C16H18N2O5S

SMILES: CC1(C)SC2C(NC(=O)COc3ccccc3)C(=O)N2C1C(=O)O

Mol. weight [g/mol]: 350.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Aqueous Solubility Prediction Method
logp	0.697		Crippen Method
mcvol	243.580	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