7-[(2-hydroxy-2-phenylacetyl)amino]-3-[(1-methylt
acid

Inchi: InChI=1S/C18H18N6O5S2/c1-23-18(20-21-22-23)31-8-10-7-30-16-11(15(27)24(16)12(10

InchiKey: OLVCFLKTBJRLHI-UHFFFAOYSA-N

Formula: C18H18N6O5S2

SMILES: Cn1nnnc1SCC1=C(C(=O)O)N2C(=O)C(NC(=O)C(O)c3ccccc3)C2SC1

Mol. weight [g/mol]: 462.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.14		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.226		Crippen Method
mcvol	304.270	ml/mol	McGowan Method

Sources

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume