7-[(2-amino-2-cyclohexa-1,4-dien-1-ylacetyl)amino acid

Inchi: InChI=1S/C16H19N3O4S/c1-8-7-24-15-11(14(21)19(15)12(8)16(22)23)18-13(20)10(17)9

InchiKey: RDLPVSKMFDYCOR-UHFFFAOYSA-N

Formula: C16H19N3O4S

SMILES: CC1=C(C(=O)O)N2C(=O)C(NC(=O)C(N)C3=CCC=CC3)C2SC1

Mol. weight [g/mol]: 349.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.349		Crippen Method
mcvol	247.690	ml/mol	McGowan Method

Sources

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

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