

6-[D-(2-amino-2-phenylacetyl)amino]-3,3-dimethyl-2-oxo-1,2,3,4-tetrahydro-1H-pyridine-4-carboxylic acid

Other names:	ampicillin
Inchi:	InChI=1S/C16H19N3O4S/c1-16(2)11(15(22)23)19-13(21)10(14(19)24-16)18-12(20)9(17)25
InchiKey:	AVKUERGKIZMTKX-UHFFFAOYSA-N
Formula:	C16H19N3O4S
SMILES:	CC1(C)SC2C(NC(=O)C([NH3+])c3ccccc3)C(=O)N2C1C(=O)[O-]
Mol. weight [g/mol]:	349.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Cheméo Relay (1.0)
logp	-1.733		Crippen Method
mcvol	247.690	ml/mol	McGowan Method

Sources

Densities and Speeds of Sound of L-Serine with Aqueous Solutions of Antibacterial Drugs at Different Temperatures: Cheméo Relay (1.0):	https://www.doi.org/10.1021/je3006425 https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
Effect of different variables in the solubility of ampicillin and its interaction with ethacridine: ampicillin with glycine and its interaction with glycine: McGowan's Method:	https://www.doi.org/10.1016/j.fluid.2017.11.033 https://www.doi.org/10.1016/j.tca.2012.10.018 http://link.springer.com/article/10.1007/BF02311772 http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solvation behaviour of dipeptides of alanine in aqueous solutions of antibacterial drug ampicillin at different temperatures:	https://www.doi.org/10.1016/j.tca.2013.09.006

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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