7-ACA

7-ACA (**7-aminocephalosporanic acid**) is the core chemical structure for the synthesis of cephalosporin antibiotics and intermediates. It can be obtained by chemoenzymatic hydrolysis of cephalosporin C.[2][3]

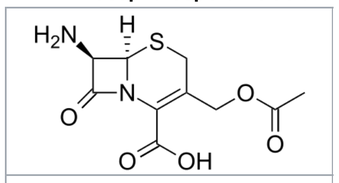
See also

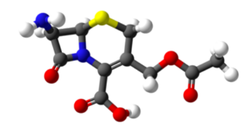
- 6-APA

References

1. 7-ACA at Chemblink (http://www.chemblink.com/products/957-68-6.htm)
2. Tan, Qiang; Zhang, Yewang; Song, Qingxun; Wei, Dongzhi (2010). "Single-pot conversion of cephalosporin C to 7-aminocephalosporanic acid in the absence of hydrogen peroxide". *World Journal of Microbiology & Biotechnology*. **26** (1): 145–152. doi:10.1007/s11274-009-0153-9 (https://doi.org/10.1007%2Fs11274-009-0153-9). S2CID 84749385 (https://api.semanticscholar.org/CorpusID:84749385).
3. Tan, Qiang; Song, Qingxun; Wei, Dongzhi (2006). "Single-pot conversion of cephalosporin C to 7-aminocephalosporanic acid using cell-bound and support-bound enzymes". *Enzyme and Microbial Technology*. **39** (5): 1166–1172. doi:10.1016/j.enzmictec.2006.02.028 (https://doi.org/10.1016%2Fj.enzmictec.2006.02.028).

7-Aminocephalosporanic acid





Names	
Preferred IUPAC name	(6*R*,7*R*)-3-[(Acetyloxy)methyl]-7-amino-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
Other names	7-Aminocephalosporinic acid
Identifiers	
CAS Number	957-68-6 (https://commonchemistry.cas.org/detail?cas_rn=957-68-6) ✓
3D model (JSmol)	Interactive image (https://chemapps.stolaf.edu/jmol/jmol.php?model=O%3DC2N1%2FC%28%3DC%28%5CCS%5BC%40%40H%5D1%5BC%40%40H%5D2N%29COC%28%3DO%29C%29C%28%3DO%29O)
3DMet	B02205 (http://www.3dmet.dna.affrc.go.jp/cgi/show_data.php?acc=B02205)
Abbreviations	7-ACA
Beilstein Reference	622637, 8919572
ChEBI	CHEBI:2255 (https://www.ebi.ac.uk/chebi/searchId.do?chebiId=2255) ✓
ChEMBL	ChEMBL1161449 (https://www.ebi.ac.uk/chembldb/index.php/compound/inspect/ChEMBL1161449) ✓
ChemSpider	390087 (http://www.chemspider.com/Chemical-Structure.390087.html) ✓
ECHA InfoCard	100.012.259 (https://echa.europa.eu/substance-information/-/substanceinfo/100.012.259)
EC Number	213-485-0
KEGG	C07756 (https://www.kegg.jp/entry/C07756) ✓
MeSH	7-Aminocephalosporanic+acid (https://www.nlm.nih.gov/cgi/mesh/2014/MB_cgi?mode=&term=7-Aminocephalosporanic+acid)
PubChem CID	483168 (https://pubchem.ncbi.nlm.nih.gov/compound/483168)
UNII	9XI67897RG (https://fdasis.nlm.nih.gov/srs/srsdirect.jsp?regno=9XI67897RG) ✓
CompTox Dashboard (EPA)	DTXSID9045342 (https://comptox.epa.gov/dashboard/DTXSID9045342)
InChI	InChI=1S/C10H12N2O5S/c1-4(13)17-2-5-3-18-9-6(11)8(14)12(9)7(5)10(15)16/h6,9H,2-3,11H2,1H3,(H,15,16)/t6-,9-/m1/s1 ✓ Key: HSHGZXNAXBPPDL-HZGVNTEJSA-N ✓
SMILES	O=C2N1/C(=C(\CS[C@@H]1[C@@H]2N)COC(=O)C)C(=O)O
Properties	
Chemical formula	$C_{10}H_{12}N_2O_5S$
Molar mass	272.27 g·mol^{-1}
Melting point	300 °C (572 °F; 573 K)[1]
log *P*	-1.87
Acidity (pK_a)	2.59
Basicity (pK_b)	11.41
Hazards	
GHS pictograms	
GHS Signal word	**Danger**
GHS hazard statements	H317, H334
GHS precautionary statements	P261, P280, P342+311

Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).

✗ verify (what is ✓✗?)

Infobox references