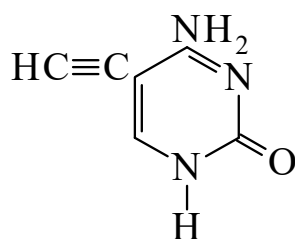




>>Entry Name: 4-Amino-5-ethynyl-2(1H)-pyrimidinone, 9CI

Synonym(s): 5-Ethynylcytosine



CAS Registry Number: 65223-79-2

Molecular Formula: C₆H₅N₃O

Molecular Weight: 135.125

Accurate Mass: 135.043262

Percentage Composition: C 53.33%; H 3.73%; N 31.10%; O 11.84%

Physical Description: Solid

Other Data: No Mp given

>>Derivative: 1-β-D-Ribofuranosyl

Synonym(s): 5-Ethynylcytidine, 9CI

CAS Registry Number: 65223-78-1

Molecular Formula: C₁₁H₁₃N₃O₅

Molecular Weight: 267.241

Accurate Mass: 267.085522

Percentage Composition: C 49.44%; H 4.90%; N 15.72%; O 29.93%

Physical Description: Cryst. (MeOH)

Other Data: No Mp given

>>Derivative: 1-β-D-(2'-Deoxyribofuranosyl)

Synonym(s): 2'-Deoxy-5-ethynylcytidine, 9CI

CAS Registry Number: 69075-47-4

Molecular Formula: C₁₁H₁₃N₃O₄

Molecular Weight: 251.241

Accurate Mass: 251.090607

Percentage Composition: C 52.59%; H 5.22%; N 16.72%; O 25.47%

Melting Point: Mp 155°

>>Derivative: 1-β-D-Arabinofuranosyl

CAS Registry Number: 74954-66-8

Molecular Formula: C₁₁H₁₃N₃O₅

Molecular Weight: 267.241

Accurate Mass: 267.085522

Percentage Composition: C 49.44%; H 4.90%; N 15.72%; O 29.93%

Use/Importance: Shows antiviral activity

Physical Description: Cryst (MeOH)

Melting Point: Mp 265-270°

References:

Barr, P.J. *et al.*, *J.C.S. Perkin I*, 1978, 1263, (*synth, deriv, uv, ir, pmr*)

Bobek, M. *et al.*, *J. Med. Chem.*, 1987, **30**, 2154, (*deriv, synth*)