



>>Entry Name: 2-Phenyl-5-pyrimidinecarboxylic acid, 9CI

CAS Registry Number: 122773-97-1

Molecular Formula: C₁₁H₈N₂O₂

Molecular Weight: 200.196

Accurate Mass: 200.058578

Percentage Composition: C 66.00%; H 4.03%; N 13.99%; O 15.98%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 283-285° (273°)

>>Derivative: Et ester

CAS Registry Number: 85386-14-7

Molecular Formula: C₁₃H₁₂N₂O₂

Molecular Weight: 228.25

Accurate Mass: 228.089878

Percentage Composition: C 68.41%; H 5.30%; N 12.27%; O 14.02%

Physical Description: Cryst. (hexane/CH₂Cl₂)

Melting Point: Mp 95-97° (85-87°)

>>Derivative: Nitrile

Synonym(s): 5-Cyano-2-phenylpyrimidine

CAS Registry Number: 85386-15-8

Molecular Formula: C₁₁H₇N₃

Molecular Weight: 181.196

Accurate Mass: 181.063997

Percentage Composition: C 72.92%; H 3.89%; N 23.19%

Physical Description: Solid

Melting Point: Mp 193-196°

References:

Mamaev, V.P. *et al.*, *Khim. Geterotsikl. Soedin.*, 1988, 371; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1988, **24**, 303, (*synth, nitrile, ir*)

Schenone, P. *et al.*, *J. Het. Chem.*, 1990, **27**, 295, (*synth, uv, ir, pmr*)

Guzmán, A. *et al.*, *J.O.C.*, 1996, **61**, 2470, (*Et ester, synth, ir, pmr, cmr, ms*)