



>>Entry Name: 4-Pyrimidinecarboxylic acid, 9CI

CAS Registry Number: 31462-59-6

Molecular Formula: $C_5H_4N_2O_2$

Molecular Weight: 124.099

Accurate Mass: 124.027278

Percentage Composition: C 48.39%; H 3.25%; N 22.57%; O 25.78%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 240 dec.°

>>Derivative: Me ester

CAS Registry Number: 2450-08-0

Molecular Formula: $C_6H_6N_2O_2$

Molecular Weight: 138.126

Accurate Mass: 138.042928

Percentage Composition: C 52.17%; H 4.38%; N 20.28%; O 23.17%

Physical Description: Cryst. by subl.

Melting Point: Mp 70-71°

Solubility: Sol. H_2O

>>Derivative: Et ester

CAS Registry Number: 62846-82-6

Molecular Formula: $C_7H_8N_2O_2$

Molecular Weight: 152.152

Accurate Mass: 152.058578

Percentage Composition: C 55.26%; H 5.30%; N 18.41%; O 21.03%

Melting Point: Mp 38-40°

Boiling Point: Bp₆ 115-116°

>>Derivative: Amide

CAS Registry Number: 28648-86-4

Molecular Formula: $C_5H_5N_3O$

Molecular Weight: 123.114

Accurate Mass: 123.043262

Percentage Composition: C 48.78%; H 4.09%; N 34.13%; O 13.00%

Physical Description: Cryst. (EtOH)

Solubility: Sol. MeOH, H_2O

>>Derivative: Nitrile

Synonym(s): 4-Cyanopyrimidine

CAS Registry Number: 42839-04-3

Molecular Formula: $C_5H_3N_3$

Molecular Weight: 105.099

Accurate Mass: 105.032697

Percentage Composition: C 57.14%; H 2.88%; N 39.98%

Melting Point: Mp 31°

References:

Gabriel, S. *et al.*, *Ber.*, 1899, **32**, 1536, (*synth*)

Robba, M., *Ann. Chim. (Paris)*, 1960, **5**, 351, (*derivs*)