



>>Entry Name: 5-Pyrimidinecarboxylic acid, 9CI

CAS Registry Number: 4595-61-3

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. (EtOH)

Melting Point: Mp 270°

>>Derivative: Me ester

CAS Registry Number: 34253-01-5

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. (EtOH)

Melting Point: Mp 84°

>>Derivative: Et ester

CAS Registry Number: 40929-50-8

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 16°. Mp 39°

Boiling Point: Bp₁₂ 103°

>>Derivative: Amide

CAS Registry Number: 40929-49-5

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. (MeOH)

Melting Point: Mp 211-213°

>>Derivative: Nitrile

Synonym(s): 5-Cyanopyrimidine

CAS Registry Number: 40805-79-6

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%

Physical Description: Stout needles (EtOH)

Melting Point: Mp 85-86°

Boiling Point: Bp₁₈ 140°

References:

Gabriel, S. *et al.*, *Ber.*, 1904, **37**, 3649, (*synth*)

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

Rho, T. *et al.*, *Synth. Commun.*, 1994, **24**, 253, (*synth, ester*)