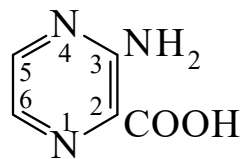




>>Entry Name: 3-Amino-2-pyrazinecarboxylic acid, 9CI

Synonym(s): 3-Aminopyrazinoic acid



CAS Registry Number: 5424-01-1

Molecular Formula:  $C_5H_5N_3O_2$

Molecular Weight: 139.113

Accurate Mass: 139.038177

Percentage Composition: C 43.17%; H 3.62%; N 30.21%; O 23.00%

Melting Point: Mp 205 dec.°

Hazard & Toxicity: Irritant

Aldrich: A7698-2

Fluka: 9334

Sigma: A2891

>>Derivative: Me ester

CAS Registry Number: 16298-03-6

Molecular Formula:  $C_6H_7N_3O_2$

Molecular Weight: 153.14

Accurate Mass: 153.053827

Percentage Composition: C 47.06%; H 4.61%; N 27.44%; O 20.90%

Physical Description: Yellow cryst. ( $H_2O$ )

Melting Point: Mp 172-173°

Aldrich: 27615-4

Fluka: 9333

>>Derivative: Me ester,  $N^4$ -oxide

CAS Registry Number: 17149-35-8

Molecular Formula:  $C_6H_7N_3O_3$

Molecular Weight: 169.14

Accurate Mass: 169.048742

Percentage Composition: C 42.61%; H 4.17%; N 24.84%; O 28.38%

Melting Point: Mp 235-237°

>>Derivative: Et ester

CAS Registry Number: 36526-32-6

Molecular Formula:  $C_7H_9N_3O_2$

Molecular Weight: 167.167

Accurate Mass: 167.069477

Percentage Composition: C 50.30%; H 5.43%; N 25.14%; O 19.14%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 99-100°

>>Derivative: Et ester,  $N^4$ -oxide

CAS Registry Number: 54632-13-2

Molecular Formula:  $C_7H_9N_3O_3$

Molecular Weight: 183.166

Accurate Mass: 183.064392

Percentage Composition: C 45.90%; H 4.95%; N 22.94%; O 26.20%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 194-195°