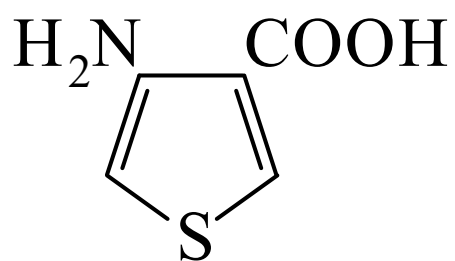




>>Entry Name: 4-Amino-3-thiophenecarboxylic acid, 9CI



CAS Registry Number: 26112-64-1

Molecular Formula: C₅H₅NO₂S

Molecular Weight: 143.166

Accurate Mass: 143.004099

Percentage Composition: C 41.95%; H 3.52%; N 9.78%; O 22.35%; S 22.40%

Physical Description: No phys. props. reported

>>Derivative: Me ester

CAS Registry Number: 39978-14-8

Molecular Formula: C₆H₇NO₂S

Molecular Weight: 157.193

Accurate Mass: 157.019749

Percentage Composition: C 45.85%; H 4.49%; N 8.91%; O 20.36%; S 20.40%

Physical Description: Needles (MeOH/Et₂O) (as hydrochloride)

Melting Point: Mp 203-205° (hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Derivative: Nitrile

Synonym(s): 3-Amino-4-cyanothiazole

CAS Registry Number: 121071-72-5

Molecular Formula: C₅H₄N₂S

Molecular Weight: 124.166

Accurate Mass: 124.009518

Percentage Composition: C 48.37%; H 3.25%; N 22.56%; S 25.83%

Melting Point: Mp 244-246° (as hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Derivative: *N*-Ac

CAS Registry Number: 36945-32-1

Molecular Formula: C₇H₇NO₃S

Molecular Weight: 185.203

Accurate Mass: 185.014664

Percentage Composition: C 45.40%; H 3.81%; N 7.56%; O 25.92%; S 17.31%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 207-208°

>>Derivative: *N*-Ac, Me ester

CAS Registry Number: 36945-29-6

Molecular Formula: C₈H₉NO₃S

Molecular Weight: 199.23

Accurate Mass: 199.030314

Percentage Composition: C 48.23%; H 4.55%; N 7.03%; O 24.09%; S 16.09%

Physical Description: Cryst. (petrol)

Melting Point: Mp 67°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 51485-55-3

Molecular Formula: C₁₂H₉NO₃S

Molecular Weight: 247.274

Accurate Mass: 247.030314

Percentage Composition: C 58.29%; H 3.67%; N 5.66%; O 19.41%; S 12.97%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 215-216°