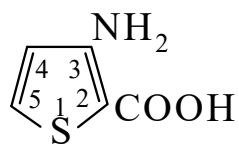




>>Entry Name: 3-Amino-2-thiophenecarboxylic acid, 9CI



CAS Registry Number: 55341-87-2

Related CAS Registry Numbers(s): 78756-27-1

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%

Melting Point: Mp 83 dec.°

>>Derivative: Me ester

CAS Registry Number: 22288-78-4

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%

Melting Point: Mp 65.5°

Boiling Point: Bp_{0.1} 100-102°

Aldrich: 23290-4

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

CAS Registry Number: 22288-79-5

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%

Melting Point: Mp 100°

>>Derivative: Et ester

CAS Registry Number: 31823-64-0

Molecular Formula: C₇H₉NO₂S

Molecular Weight: 171.22

Accurate Mass: 171.035399

Percentage Composition: C 49.10%; H 5.30%; N 8.18%; O 18.69%; S 18.73%

Physical Description: Cryst.

Melting Point: Mp 42-43°

Boiling Point: Bp_{0.3} 109-112°

>>Derivative: Amide

CAS Registry Number: 147123-47-5

Molecular Formula: C₅H₆N₂OS

Molecular Weight: 142.181

Accurate Mass: 142.020083

Percentage Composition: C 42.24%; H 4.25%; N 19.70%; O 11.25%; S 22.55%

Physical Description: Prisms (EtOH or by subl.)

Melting Point: Mp 122-124° (118-120°)

>>Derivative: Nitrile

Synonym(s): 3-Amino-2-cyanothiophene

CAS Registry Number: 56489-05-5

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%

Physical Description: Cryst. (toluene)

Melting Point: Mp 47.5-50°

References: