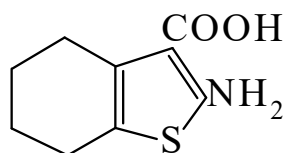




>>Entry Name: 2-Amino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylic acid, 9CI

Synonym(s): 2-Amino-4,5-tetramethylene-3-thiophenecarboxylic acid



CAS Registry Number: 5936-58-3

Molecular Formula: C₉H₁₁NO₂S

Molecular Weight: 197.257

Accurate Mass: 197.051049

Percentage Composition: C 54.80%; H 5.62%; N 7.10%; O 16.22%; S 16.26%

Physical Description: Cryst. (propanol)

Melting Point: Mp 158-160°

>>Derivative: Et ester

CAS Registry Number: 4506-71-2

Molecular Formula: C₁₁H₁₅NO₂S

Molecular Weight: 225.311

Accurate Mass: 225.082349

Percentage Composition: C 58.64%; H 6.71%; N 6.22%; O 14.20%; S 14.23%

Melting Point: Mp 115°

Aldrich: 15918-2

>>Derivative: Et ester; hydrochloride

CAS Registry Number: 76488-06-7

Melting Point: Mp 137-138°

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

CAS Registry Number: 5919-29-9

Molecular Formula: C₁₃H₁₇NO₃S

Molecular Weight: 267.348

Accurate Mass: 267.092914

Percentage Composition: C 58.40%; H 6.41%; N 5.24%; O 17.95%; S 11.99%

Melting Point: Mp 111-113°

Rare Chemicals Library: S54458-2

>>Derivative: Et ester, *N*-benzoyl

CAS Registry Number: 52535-73-6

Molecular Formula: C₁₈H₁₉NO₃S

Molecular Weight: 329.419

Accurate Mass: 329.108564

Percentage Composition: C 65.63%; H 5.81%; N 4.25%; O 14.57%; S 9.73%

Melting Point: Mp 166-168°

>>Derivative: Amide

CAS Registry Number: 4815-28-5

Molecular Formula: C₉H₁₂N₂OS

Molecular Weight: 196.273

Accurate Mass: 196.067033

Percentage Composition: C 55.08%; H 6.16%; N 14.27%; O 8.15%; S 16.34%

Use/Importance: Possesses analgesic props.

Physical Description: Cryst. (EtOH)

Melting Point: Mp 189-190°

Rare Chemicals Library: S54561-9