



>>Entry Name: Benzo[*b*]thiophene-3-carboxylic acid

CAS Registry Number: 5381-25-9

Molecular Formula: C₉H₆O₂S

Molecular Weight: 178.211

Accurate Mass: 178.00885

Percentage Composition: C 60.66%; H 3.39%; O 17.96%; S 17.99%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 179-180°

Other Data: Steam-volatile

>>Derivative: Me ester

CAS Registry Number: 22913-25-3

Molecular Formula: C₁₀H₈O₂S

Molecular Weight: 192.238

Accurate Mass: 192.0245

Percentage Composition: C 62.48%; H 4.19%; O 16.65%; S 16.68%

Physical Description: Oil

Boiling Point: Bp₇₅₀ 285-287°. Bp₁₇ 165°

>>Derivative: Chloride

CAS Registry Number: 39827-12-8

Molecular Formula: C₉H₅ClOS

Molecular Weight: 196.657

Accurate Mass: 195.974962

Percentage Composition: C 54.97%; H 2.56%; Cl 18.03%; O 8.14%; S 16.31%

Melting Point: Mp 50°

Boiling Point: Bp 296-298°

>>Derivative: Amide

Molecular Formula: C₉H₇NOS

Molecular Weight: 177.226

Accurate Mass: 177.024834

Percentage Composition: C 60.99%; H 3.98%; N 7.90%; O 9.03%; S 18.09%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 197-198°

>>Derivative: Nitrile

Synonym(s): 3-Cyanobenzo[*b*]thiophene

CAS Registry Number: 24434-84-2

Molecular Formula: C₉H₅NS

Molecular Weight: 159.211

Accurate Mass: 159.014269

Percentage Composition: C 67.90%; H 3.17%; N 8.80%; S 20.14%

Melting Point: Mp 74°

References:

Matsuki, Y., *Nippon Kagaku Kaishi*, 1966, **87**, 186, (*synth*)

Brabanden, H.J., *J. Het. Chem.*, 1973, **10**, 177

Yuldashev, Kh.Yu., *Khim. Geterotsikl. Soedin.*, 1978, 1039; *CA*, **89**, 215149