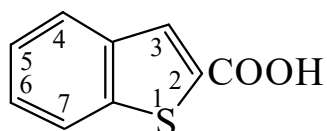




>>Entry Name: Benzo[*b*]thiophene-2-carboxylic acid



CAS Registry Number: 6314-28-9

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. (H₂O or C₆H₆/EtOAc)

Melting Point: Mp 240-241.5°

Solubility: Spar. sol. H₂O

Aldrich: 46746-4

>>Derivative: Me ester

CAS Registry Number: 22913-24-2

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: Cryst. (EtOH)

Melting Point: Mp 72-73°

Boiling Point: Bp₁₃ 176-180°

>>Derivative: Et ester

CAS Registry Number: 17890-55-0

Molecular Formula: C₁₁H₁₀O₂S

Molecular Weight: 206.265

Accurate Mass: 206.04015

Percentage Composition: C 64.05%; H 4.89%; O 15.51%; S 15.55%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 36-37°

>>Derivative: Chloride

CAS Registry Number: 39827-11-7

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%

Physical Description: Leaflets (petrol)

Melting Point: Mp 88-89°

Boiling Point: Bp₁₉ 173-175°

>>Derivative: Amide

CAS Registry Number: 6314-42-7

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: Needles (H₂O)

Melting Point: Mp 177°

>>Derivative: Nitrile

Synonym(s): 2-Cyanobenzo[*b*]thiophene

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%

Physical Description: Yellow oil