



>>Entry Name: 4,5-Dibromo-2-thiophenecarboxylic acid, 9CI

CAS Registry Number: 6324-10-3

Related CAS Registry Numbers(s): 116041-66-8 131818-21-8

Molecular Formula: C₅H₂Br₂O₂S

Molecular Weight: 285.944

Accurate Mass: 283.854222

Percentage Composition: C 21.00%; H 0.70%; Br 55.89%; O 11.19%; S 11.21%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 228-229.5°

Other: PB D10770

>>Derivative: Me ester

CAS Registry Number: 62224-24-2

Molecular Formula: C₆H₄Br₂O₂S

Molecular Weight: 299.97

Accurate Mass: 297.869872

Percentage Composition: C 24.02%; H 1.34%; Br 53.27%; O 10.67%; S 10.69%

Physical Description: Needles (EtOH)

Melting Point: Mp 80° (75-77°)

>>Derivative: Et ester

CAS Registry Number: 62224-25-3

Molecular Formula: C₇H₆Br₂O₂S

Molecular Weight: 313.997

Accurate Mass: 311.885522

Percentage Composition: C 26.78%; H 1.93%; Br 50.89%; O 10.19%; S 10.21%

Melting Point: Mp 55°. Mp 48-49° (43-43.5°)

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 62224-26-4

Molecular Formula: C₉H₁₀Br₂O₂S

Molecular Weight: 342.051

Accurate Mass: 339.916822

Percentage Composition: C 31.60%; H 2.95%; Br 46.72%; O 9.35%; S 9.37%

Melting Point: Mp 29-30°

>>Derivative: Chloride

CAS Registry Number: 21815-07-6

Molecular Formula: C₅HBr₂ClOS

Molecular Weight: 304.389

Accurate Mass: 301.820334

Percentage Composition: C 19.73%; H 0.33%; Br 52.50%; Cl 11.65%; O 5.26%; S 10.53%

Melting Point: Mp 36°

Boiling Point: Bp₁₅ 75-77°

>>Derivative: Amide

CAS Registry Number: 171851-27-7

Molecular Formula: C₅H₃Br₂NOS

Molecular Weight: 284.959

Accurate Mass: 282.870206

Percentage Composition: C 21.07%; H 1.06%; Br 56.08%; N 4.92%; O 5.61%; S 11.25%

Physical Description: Needles (H₂O)

Melting Point: Mp 167°