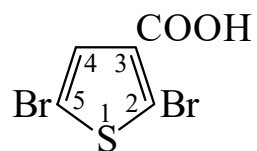




>>Entry Name: 2,5-Dibromo-3-thiophenecarboxylic acid, 8Cl



CAS Registry Number: 7311-70-8

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. (H₂O)

Melting Point: Mp 178° (175-176°)

>>Derivative: Me ester

CAS Registry Number: 77014-10-9

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: Cryst. (MeOH)

Melting Point: Mp 60-61°

>>Derivative: Amide

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: Cryst. (H₂O)

Melting Point: Mp 147-148°

>>Derivative: Nitrile

Synonym(s): 2,5-Dibromo-3-thiophenecarbonitrile

CAS Registry Number: 18792-01-3

Molecular Formula: C₅HBr₂NS

Molecular Weight: 266.944

Accurate Mass: 264.859641

Percentage Composition: C 22.50%; H 0.38%; Br 59.87%; N 5.25%; S 12.01%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 76°

References:

Campaigne, E. *et al.*, *J.A.C.S.*, 1954, **76**, 2445, (*synth, amide*)

Fournari, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 4115, (*synth, nitrile*)

Bowie, J.H. *et al.*, *J. Chin. Biochem. Soc.*, 1967, 616, (*ms*)