



>>Entry Name: Benzo[*b*]thiophene-3-carboxaldehyde, 9CI

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

CAS Registry Number: 5381-20-4

Molecular Formula: C₉H₆OS

Molecular Weight: 162.212

Accurate Mass: 162.013935

Percentage Composition: C 66.64%; H 3.73%; O 9.86%; S 19.77%

Physical Description: Cryst. (EtOH or petrol)

Melting Point: Mp 58°

Boiling Point: Bp₁₅ 162-163°

>>Derivative: Oxime

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. (petrol)

Melting Point: Mp 90°

>>Derivative: Semicarbazone

Molecular Formula: C₁₀H₉N₃OS

Molecular Weight: 219.267

Percentage Composition: C 54.78%; H 4.14%; N 19.16%; O 7.30%; S 14.62%

Physical Description: Fine needles (EtOH)

Melting Point: Mp 256° (dec. from 233°)

>>Derivative: Phenylhydrazone

Physical Description: Solid

Melting Point: Mp 115°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Solid

Melting Point: Mp 287°

References:

Cagniant, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1949, 382, (*synth*)

Weston, A.W. *et al.*, *J.A.C.S.*, 1950, **72**, 1422, (*synth*)

Gheisas, V.V., *J.O.C.*, 1957, **22**, 703, (*synth, uv*)

Matsuki, Y. *et al.*, *Nippon Kagaku Zasshi*, 1966, **87**, 186, (*synth, uv*)

Kucharczyk, N. *et al.*, *Coll. Czech. Chem. Comm.*, 1969, **34**, 2959, (*uv, ir*)

Shafiee, A. *et al.*, *J. Het. Chem.*, 1976, **13**, 141, (*synth, pmr, ms*)

Benassi, R. *et al.*, *J.C.S. Perkin 2*, 1983, 911, (*pmr, cmr*)