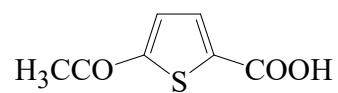




>>Entry Name: 5-Acetyl-2-thiophenecarboxylic acid, 9CI



CAS Registry Number: 4066-41-5

Molecular Formula: C₇H₆O₃S

Molecular Weight: 170.189

Accurate Mass: 170.003765

Percentage Composition: C 49.40%; H 3.55%; O 28.20%; S 18.84%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 205-208°

pKa Value: pK_a 3 (H₂O) pK_a 4.3 (EtOH aq.)

>>Derivative: Oxime

CAS Registry Number: 98279-55-1

Molecular Formula: C₇H₇NO₃S

Molecular Weight: 185.203

Accurate Mass: 185.014664

Percentage Composition: C 45.40%; H 3.81%; N 7.56%; O 25.92%; S 17.31%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 236°

>>Derivative: Et ester

CAS Registry Number: 33148-82-2

Molecular Formula: C₉H₁₀O₃S

Molecular Weight: 198.242

Accurate Mass: 198.035065

Percentage Composition: C 54.53%; H 5.08%; O 24.21%; S 16.18%

Physical Description: Cryst.

Melting Point: Mp 54-54.5°

>>Derivative: Chloride

CAS Registry Number: 89692-69-3

Molecular Formula: C₇H₅ClO₂S

Molecular Weight: 188.634

Accurate Mass: 187.969877

Percentage Composition: C 44.57%; H 2.67%; Cl 18.79%; O 16.96%; S 17.00%

Physical Description: Cryst.

Melting Point: Mp 77-79°

References:

- Gol'dfarb, Ya.L. *et al.*, *Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1959, 2021; 1960, 2238; *Bull. Acad. Sci. USSR, Phys. Ser. (Engl. Transl.)*, 1959, 1925; 1960, 2071, (*synth*)
Schloegl, K. *et al.*, *Annalen*, 1962, **651**, 1, (*synth, Et ester, chloride*)
Spinelli, D. *et al.*, *J. Chem. Res., Miniprint*, 1993, **8**, 1873, (*props*)
Abarbri, M. *et al.*, *J.O.C.*, 2000, **65**, 4618-4634, (*synth, uv, pmr, ms*)