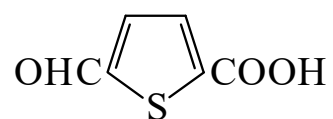




>>Entry Name: 5-Formyl-2-thiophenecarboxylic acid



CAS Registry Number: 4565-31-5

Molecular Formula: C₆H₄O₃S

Molecular Weight: 156.162

Accurate Mass: 155.988115

Percentage Composition: C 46.15%; H 2.58%; O 30.74%; S 20.53%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 165-167°

>>Derivative: Nitrile

Synonym(s): 5-Formyl-2-thiophenecarbonitrile, 9CI. 5-Cyano-2-thiophenecarboxaldehyde. 2-Cyano-5-formylthiophene

CAS Registry Number: 21512-16-3

Molecular Formula: C₆H₃NOS

Molecular Weight: 137.162

Accurate Mass: 136.993534

Percentage Composition: C 52.54%; H 2.20%; N 10.21%; O 11.66%; S 23.38%

Physical Description: Cryst.

Melting Point: Mp 96-97° (94°). Mp 89°

Boiling Point: Bp_{1.2} 130-135°

>>Derivative: Nitrile, thiosemicarbazone

Synonym(s): Citenazone, INN. Hoe 105

CAS Registry Number: 21512-15-2

Molecular Formula: C₇H₆N₄S₂

Molecular Weight: 210.283

Accurate Mass: 210.003386

Percentage Composition: C 39.98%; H 2.88%; N 26.64%; S 30.50%

Use/Importance: Antiviral (for smallpox), antitubercular agent

Development Status: No longer marketed

Melting Point: Mp 234 dec.°

References:

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Gogte, V.N. *et al.*, *Tetrahedron*, 1967, **23**, 2443, (*synth*)

U.K. Pat., 1968, Hoechst, 1 127 064; *CA*, **70**, 47284, (*Citenazone*)

Winkelmann, E. *et al.*, *Arzneim.-Forsch.*, 1972, **22**, 1704; 1713; 1717, (*pharmacol*, *Citenazone*)

Dubus, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1976, 628, (*nitrile*)

Carpenter, A.J. *et al.*, *Tetrahedron*, 1985, **41**, 3803, (*synth*, *pmr*, *ms*)