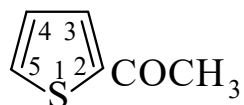




>>Entry Name: 2-Acetylthiophene

ENTRY UNDER REVIEW

Synonym(s): 1-(2-Thienyl)ethanone, 9CI. Methyl 2-thienyl ketone. 2-Acetothenone



CAS Registry Number: 88-15-3

Related CAS Registry Numbers(s): 39709-34-7

Molecular Formula: C₆H₆OS

Molecular Weight: 126.179

Accurate Mass: 126.013935

Percentage Composition: C 57.11%; H 4.79%; O 12.68%; S 25.41%

Biological Source: Isol. from above-ground parts of *Bidens pilosa*

Use/Importance: Organoleptic which contributes to several aromas

Physical Description: Liq.

Melting Point: Mp 9°

Boiling Point: Bp 213-214°. Bp₁₃ 94.5-96.5°

Density: d²⁴ 1.167

Hazard & Toxicity: LD₅₀ (mus, ipr) 40 mg/kg

Aldrich: W50350-9

Fluka: 1490

Sigma: A0385

>>Derivative: Oxime, (E)-

CAS Registry Number: 92313-54-7

Molecular Formula: C₆H₇NOS

Molecular Weight: 141.193

Accurate Mass: 141.024834

Percentage Composition: C 51.04%; H 5.00%; N 9.92%; O 11.33%; S 22.71%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 113-114°

>>Derivative: Oxime, (Z)-

CAS Registry Number: 92313-45-6

Molecular Formula: C₆H₇NOS

Molecular Weight: 141.193

Accurate Mass: 141.024834

Percentage Composition: C 51.04%; H 5.00%; N 9.92%; O 11.33%; S 22.71%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 84-85°

>>Derivative: Phenylhydrazone

CAS Registry Number: 55968-17-7

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 96°

>>Derivative: Semicarbazone

CAS Registry Number: 3771-70-8

Physical Description: Plates (C₆H₆)

Melting Point: Mp 190-191°

References: