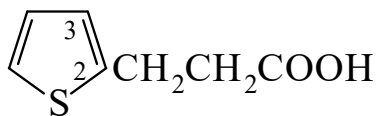




>>Entry Name: **3-(2-Thienyl)propanoic acid**

Synonym(s): 2-Thiophenepropanoic acid, 9CI



CAS Registry Number: 5928-51-8

Related CAS Registry Numbers(s): 65121-27-9

Molecular Formula: C₇H₈O₂S

Molecular Weight: 156.205

Accurate Mass: 156.0245

Percentage Composition: C 53.82%; H 5.16%; O 20.49%; S 20.53%

Physical Description: Long needles (petrol)

Melting Point: Mp 48.5-49.5° (44-45°)

Boiling Point: Bp₁₂ 151°

pKa Value: pK_{a1} 6.91 (80% 2-methoxyethanol)

>>Derivative: Me ester

CAS Registry Number: 16862-05-8

Molecular Formula: C₈H₁₀O₂S

Molecular Weight: 170.232

Accurate Mass: 170.04015

Percentage Composition: C 56.45%; H 5.92%; O 18.80%; S 18.84%

Physical Description: Liq.

Boiling Point: Bp₅ 50°

Refractive Index: n_D²⁰ 1.5140

>>Derivative: Et ester

CAS Registry Number: 64107-46-6

Molecular Formula: C₉H₁₂O₂S

Molecular Weight: 184.259

Accurate Mass: 184.0558

Percentage Composition: C 58.67%; H 6.56%; O 17.37%; S 17.40%

Physical Description: Liq.

Boiling Point: Bp_{11.3} 122-122.5°

Density: d^{20.5} 1.103

Refractive Index: n_D^{19.6} 1.5041

>>Derivative: Chloride

CAS Registry Number: 5834-04-8

Molecular Formula: C₇H₇ClOS

Molecular Weight: 174.65

Accurate Mass: 173.990612

Percentage Composition: C 48.14%; H 4.04%; Cl 20.30%; O 9.16%; S 18.36%

Physical Description: Liq.

Boiling Point: Bp₁₅ 121°

Refractive Index: n_D^{20.2} 1.5400

Hazard & Toxicity: Lachrymator

>>Derivative: Amide

CAS Registry Number: 26359-22-8

Molecular Formula: C₇H₉NOS

Molecular Weight: 155.22

Accurate Mass: 155.040484

Percentage Composition: C 54.17%; H 5.84%; N 9.02%; O 10.31%; S 20.66%

Physical Description: Pearly spangles or needles (C₆H₆/petrol)

Melting Point: Mp 102° (99-100°)

References: