



>>Entry Name: 2-Thiopheneacetic acid, 9Cl, 8Cl

Synonym(s): 2-Thienylacetic acid



CAS Registry Number: 1918-77-0

Molecular Formula: C₆H₆O₂S

Molecular Weight: 142.178

Accurate Mass: 142.00885

Percentage Composition: C 50.69%; H 4.25%; O 22.51%; S 22.55%

Physical Description: Cryst. (CCl₄/petrol)

Melting Point: Mp 76°

Solubility: Sol. hot H₂O

pK_a Value: pK_a 3.89 (25°)

Aldrich: 19594-4

Fluka: 89015

Sigma: T3896

>>Derivative: Me ester

CAS Registry Number: 19432-68-9

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: Liq.

Boiling Point: Bp₂₃ 115-118°

Fluka: 89019

>>Derivative: Et ester

CAS Registry Number: 57382-97-5

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: Bp₂₆ 124-129°

Aldrich: 25764-8

>>Derivative: Chloride

CAS Registry Number: 39098-97-0

Molecular Formula: C₆H₅ClOS

Molecular Weight: 160.624

Accurate Mass: 159.974962

Percentage Composition: C 44.87%; H 3.14%; Cl 22.07%; O 9.96%; S 19.96%

Physical Description: Liq.

Boiling Point: Bp_{0.05} 39°

Aldrich: 19599-5

Fluka: 88973

>>Derivative: Amide

CAS Registry Number: 4461-29-4

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. (H₂O)

Melting Point: Mp 146-147°

Rare Chemicals Library: S9067-1