



>>Entry Name: Benzenesulfinic acid, 9Cl

Synonym(s): Phenylsulfinic acid

CAS Registry Number: 618-41-7

PhSO₂H

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%

General Statement: Esters and other derivatives are chiral

Use/Importance: Used as a 5mM aq. soln. for gravimetric detn. of Th, Zr; photometric detn. of quinones

Physical Description: Prisms

Melting Point: Mp 83-84°

pKa Value: pK_a 1.29 (20°)

Other Data: Dec. at *ca.* 100°

>>Derivative: Na salt

CAS Registry Number: 873-55-2

Extra CAS Registry Numbers(s): 25932-11-0

Melting Point: Mp 300°

Aldrich: 12357-9

Fluka: 12610

Sigma: B2029

>>Derivative: Me ester (±-)

CAS Registry Number: 670-98-4

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%

Boiling Point: Bp_{0.45} 76-78°. Bp_{0.04} 59-60°

Hazard & Toxicity: Skin irritant

Aldrich: 46089-3

>>Derivative: Chloride (±-)

CAS Registry Number: 4972-29-6

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: Plates

Melting Point: Mp 38°

Boiling Point: Bp_{0.04} 62-63°

Other Data: Hydrol. by H₂O

Hazard & Toxicity: Explodes after prolonged storage in glass

>>Derivative: Amide (±-)

CAS Registry Number: 16066-31-2

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%

Melting Point: Mp 121°

>>Derivative: Dimethylamide (±-)

CAS Registry Number: 5539-54-8

Molecular Formula: C₈H₁₁NOS

Molecular Weight: 169.247

Accurate Mass: 169.056134

Percentage Composition: C 56.77%; H 6.55%; N 8.28%; O 9.45%; S 18.95%

Boiling Point: Bp_{2.5} 90° (lit. gives a pressure range)