



>>Entry Name: Benzenesulfonic acid, 9CI

Synonym(s): Phenylsulfonic acid

CAS Registry Number: 98-11-3

Related CAS Registry Numbers(s): 3198-32-1 39510-76-4

PhSO₃H

Molecular Formula: C₆H₆O₃S

Molecular Weight: 158.178

Accurate Mass: 158.003765

Percentage Composition: C 45.56%; H 3.82%; O 30.34%; S 20.27%

Physical Description: Plates + 1½ H₂O

Melting Point: Mp 43-44° (anhyd. 65-66°)

pKa Value: pK_a -2.7

Other Data: Deliquescent

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 890 mg/kg

Aldrich: 13507-0

Fluka: 12640

Sigma: B3129

>>Derivative: Na salt

CAS Registry Number: 515-42-4

Physical Description: Leaflets + 1H₂O

Melting Point: Mp 450° (dec.)

Aldrich: 14728-1

Fluka: 12690

Rare Chemicals Library: S44007-8

Sigma: B3254

>>Derivative: Me ester

CAS Registry Number: 80-18-2

Molecular Formula: C₇H₈O₃S

Molecular Weight: 172.204

Accurate Mass: 172.019415

Percentage Composition: C 48.82%; H 4.68%; O 27.87%; S 18.62%

Boiling Point: Bp₁₅ 150°

Density: d₄¹⁷ 1.273

Hazard & Toxicity: Fl. p. >74°

Rare Chemicals Library: S54479-5

>>Derivative: Et ester

CAS Registry Number: 515-46-8

Molecular Formula: C₈H₁₀O₃S

Molecular Weight: 186.231

Accurate Mass: 186.035065

Percentage Composition: C 51.60%; H 5.41%; O 25.77%; S 17.22%

Boiling Point: Bp₁₅ 156°

Solubility: Spar. sol. H₂O

Density: d₄¹⁷ 1.219

Rare Chemicals Library: S54478-7

>>Derivative: Butyl ester

CAS Registry Number: 80-44-4

Molecular Formula: C₁₀H₁₄O₃S

Molecular Weight: 214.285

Accurate Mass: 214.066365

Percentage Composition: C 56.05%; H 6.58%; O 22.40%; S 14.96%

Boiling Point: Bp 134-141°

Rare Chemicals Library: S70614-0