



>>Entry Name: [1,1'-Biphenyl]-4-sulfonic acid, 9Cl

Synonym(s): 4-Phenylbenzenesulfonic acid

CAS Registry Number: 2113-68-0

Molecular Formula: C₁₂H₁₀O₃S

Molecular Weight: 234.275

Accurate Mass: 234.035065

Percentage Composition: C 61.52%; H 4.30%; O 20.49%; S 13.69%

Physical Description: Cryst.

Melting Point: Mp 138° (117-119°)

Rare Chemicals Library: S44651-3

>>Derivative: Me ester

Molecular Formula: C₁₃H₁₂O₃S

Molecular Weight: 248.302

Accurate Mass: 248.050715

Percentage Composition: C 62.88%; H 4.87%; O 19.33%; S 12.91%

Physical Description: Cryst. (petrol)

Melting Point: Mp 76-77°

>>Derivative: Chloride

CAS Registry Number: 1623-93-4

Molecular Formula: C₁₂H₉ClO₂S

Molecular Weight: 252.721

Accurate Mass: 252.001177

Percentage Composition: C 57.03%; H 3.59%; Cl 14.03%; O 12.66%; S 12.69%

Melting Point: Mp 115°. Mp 142-143°

Fluka: 14442

>>Derivative: Amide

Molecular Formula: C₁₂H₁₁NO₂S

Molecular Weight: 233.29

Accurate Mass: 233.051049

Percentage Composition: C 61.78%; H 4.75%; N 6.00%; O 13.72%; S 13.75%

Physical Description: Cryst.

Melting Point: Mp 228°

References:

Gebauer-Fülneegg, E. *et al.*, *Monatsh. Chem.*, 1928, **49**, 46, (*chloride*)

Pollak, J. *et al.*, *Monatsh. Chem.*, 1930, **35**, 358, (*synth*)

Dannley, R.L. *et al.*, *J.A.C.S.*, 1954, **76**, 2997, (*ester*)

Schultz, R.G., *J.O.C.*, 1961, **26**, 5195, (*synth*)

Roemmele, R.C. *et al.*, *J.O.C.*, 1988, **53**, 2367, (*synth, pmr, ir*)