



>>Entry Name: 2,5-Dibromobenzenesulfonic acid, 9Cl

CAS Registry Number: 63137-37-1

Related CAS Registry Numbers(s): 35495-22-8 38484-96-7

Molecular Formula: C₆H₄Br₂O₃S

Molecular Weight: 315.97

Accurate Mass: 313.864787

Percentage Composition: C 22.81%; H 1.28%; Br 50.58%; O 15.19%; S 10.15%

Physical Description: Cryst. + 2 or 3H₂O (H₂O)

Melting Point: Mp 128° (anhyd.)

>>Derivative: Chloride

CAS Registry Number: 23886-64-8

Molecular Formula: C₆H₃Br₂ClO₂S

Molecular Weight: 334.415

Accurate Mass: 331.830899

Percentage Composition: C 21.55%; H 0.90%; Br 47.79%; Cl 10.60%; O 9.57%; S 9.59%

Physical Description: Prisms (Et₂O or C₆H₆/petrol)

Melting Point: Mp 71-71.5°

>>Derivative: Amide

CAS Registry Number: 7467-11-0

Molecular Formula: C₆H₅Br₂NO₂S

Molecular Weight: 314.985

Accurate Mass: 312.880771

Percentage Composition: C 22.88%; H 1.60%; Br 50.74%; N 4.45%; O 10.16%; S 10.18%

Physical Description: Needles (EtOH)

Melting Point: Mp 194°

>>Derivative: Anilide

Molecular Formula: C₁₂H₉Br₂NO₂S

Molecular Weight: 391.083

Accurate Mass: 388.912071

Percentage Composition: C 36.85%; H 2.32%; Br 40.86%; N 3.58%; O 8.18%; S 8.20%

Melting Point: Mp 144-145°

References:

Bahlmann, A., *Annalen*, 1877, **186**, 307

Borss, H., *Annalen*, 1877, **187**, 350

Lukashevich, V.O., *Dokl. Akad. Nauk SSSR*, 1954, **99**, 995-998; *CA*, **50**, 217g, (*synth*)

Eriksson, A. *et al.*, *Acta Chem. Scand.*, 1972, **26**, 1591-1598, (*ir*)

Lundgren, J.O. *et al.*, *Acta Cryst. B*, 1972, **28**, 475-481; 1979, **35**, 780-783, (*trihydrate, cryst struct*)