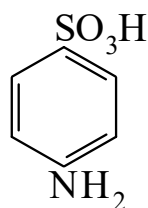




>>Entry Name: 4-Aminobenzenesulfonic acid, 9CI

Synonym(s): Aniline-*p*-sulfonic acid. Sulfanilic acid



CAS Registry Number: 121-57-3

Related CAS Registry Numbers(s): 127-56-0 515-74-2 6106-22-5 6209-17-2 22484-64-6 31884-76-1

Molecular Formula: C₆H₇NO₃S

Molecular Weight: 173.192

Accurate Mass: 173.014664

Percentage Composition: C 41.61%; H 4.07%; N 8.09%; O 27.71%; S 18.51%

Use/Importance: Used as a 0.8% soln. in 25% AcOH for photometric detn. of NO₂⁽⁻⁾ (Griess method), Ce(IV) (λ_{max} 540 nm)

Physical Description: Cryst. + 2H₂O

pKa Value: pK_{a1} 3.24 (25°)

Other Data: Also used as Zn salt, Sulfanilate zinc, USAN

Hazard & Toxicity: Eye and skin irritant. Low acute toxicity

Aldrich: 24042-7

Fluka: 86092

Sigma: S5643

>>Derivative: Me ester

CAS Registry Number: 55034-26-9

Molecular Formula: C₇H₉NO₃S

Molecular Weight: 187.219

Accurate Mass: 187.030314

Percentage Composition: C 44.91%; H 4.85%; N 7.48%; O 25.64%; S 17.13%

Melting Point: Mp 92°

>>Derivative: Amide

Synonym(s): 4-Aminobenzenesulfonamide. Prontosil album. Many other names. **Sulfanilamide**, INN

CAS Registry Number: 63-74-1

Molecular Formula: C₆H₈N₂O₂S

Molecular Weight: 172.207

Accurate Mass: 172.030648

Percentage Composition: C 41.85%; H 4.68%; N 16.27%; O 18.58%; S 18.62%

Use/Importance: Antibacterial chiefly of historical importance. Numerous derivs. have antibacterial props. Used for photometric detn. of NO₂⁽⁻⁾ and NO₃⁽⁻⁾

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 165-166°

Solubility: Sol. H₂O

pKa Value: pK_{a1} 10.58 (20°, 0.1M KCl)

Calculated Log P Data: Log P -0.57 (calc)

Other Data: Can be diazotised

Hazard & Toxicity: Human teratogenic effects. Exp. reprod. effects. LD₅₀ (rat, orl) 3900 mg/kg

Aldrich: 24034-6

Fluka: 86060

Sigma: S9251