



>>Entry Name: 4-Aminobenzenethiol, 9CI

Synonym(s): *p*-Aminophenyl mercaptan. *p*-Aminothiophenol. *p*-Mercaptoaniline

CAS Registry Number: 1193-02-8

Molecular Formula: C₆H₇NS

Molecular Weight: 125.194

Accurate Mass: 125.029919

Percentage Composition: C 57.56%; H 5.64%; N 11.19%; S 25.61%

Use/Importance: Corrosion inhibitor for metal surfaces

Physical Description: Granular cryst.

Melting Point: Mp 46°

Boiling Point: Bp₁₅ 142°

pKa Value: pK_a 7.47 (20°, 20% EtOH aq.)

Other Data: Steam-volatile

Aldrich: A8100-5

Fluka: 9493

Sigma: A8395

>>Derivative: Hydrochloride

Physical Description: Cryst. (EtOH)

Melting Point: Mp 197°

>>Derivative: *N*-Ac

CAS Registry Number: 1126-81-4

Molecular Formula: C₈H₉NOS

Molecular Weight: 167.231

Accurate Mass: 167.040484

Percentage Composition: C 57.46%; H 5.42%; N 8.38%; O 9.57%; S 19.17%

Physical Description: Scales (cryst. <70°) or yellow leaflets (cryst. >70°)

Melting Point: Mp 154° (both forms)

Aldrich: A820-1

>>Derivative: *N,S*-Di-Ac

Molecular Formula: C₁₀H₁₁NO₂S

Molecular Weight: 209.268

Accurate Mass: 209.051049

Percentage Composition: C 57.40%; H 5.30%; N 6.69%; O 15.29%; S 15.32%

Physical Description: Leaflets (H₂O)

Melting Point: Mp 146-147°

>>Derivative: *N*-Me

Synonym(s): 4-(Methylamino)benzenethiol

Molecular Formula: C₇H₉NS

Molecular Weight: 139.221

Accurate Mass: 139.045569

Percentage Composition: C 60.39%; H 6.52%; N 10.06%; S 23.03%

Boiling Point: Bp₁₅ 155°

>>Derivative: *N,N*-Di-Me

Synonym(s): 4-(Dimethylamino)benzenethiol

CAS Registry Number: 4946-22-9

Molecular Formula: C₈H₁₁NS

Molecular Weight: 153.248

Accurate Mass: 153.061219

Percentage Composition: C 62.70%; H 7.23%; N 9.14%; S 20.92%

Melting Point: Mp 28.5°

Boiling Point: Bp₂₅ 162-168°. Bp_{9,5} 113.5-117° (lit. gives a pressure range)