



>>Entry Name: 3-Aminobenzenethiol, 9CI

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

CAS Registry Number: 22948-02-3

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%

Boiling Point: Bp₁₆ 180-190°

pKa Value: pK_a 6.95 (20°, 20% EtOH aq.)

Aldrich: 14348-0

>>Derivative: Hydrochloride

Melting Point: Mp 232°

>>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: Cryst. (C₆H₆)

Melting Point: Mp 97°

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

Synonym(s): 3-(Dimethylamino)benzenethiol

CAS Registry Number: 33284-28-5

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%

Boiling Point: Bp_{2.5} 100°. Bp_{0.6} 82-83°

pKa Value: pK_a 6.99 (20°, 20% EtOH aq.)

>>Derivative: *S*-Me

Synonym(s): 3-(Methylthio)aniline. *m*-Thioanisidine

CAS Registry Number: 1783-81-9

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%

Physical Description: Pale-yellow oil

Boiling Point: Bp₁₆ 163-165°

Aldrich: 14488-6

Fluka: 67789

>>Derivative: *N,N,S*-Tri-Me

Synonym(s): 1-(Dimethylamino)-3-(methylthio)benzene

CAS Registry Number: 2552-33-2

Molecular Formula: C₉H₁₃NS

Molecular Weight: 167.274

Accurate Mass: 167.076869

Percentage Composition: C 64.62%; H 7.83%; N 8.37%; S 19.17%

Boiling Point: Bp₁₀ 165-167°. Bp_{0.03} 63-64°