



-->Entry Name: 3-Aminobenzenethiol, 9CI
Synonym(s): m-Aminophenyl mercaptan, m-Aminothiophenol, m-Mercaptaniline
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: Bp₁₀ 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. (C₁₀H₁₁)
Melting Point: Mp 97°

-->Derivative: N,N-Di-Me
Synonym(s): 3-(Dimethylamino)benzenethiol

CAS Registry Number: 33284-28-5
Molecular Formula: C₉H₁₁NS
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_{1.3} 100°; Bp₁₀ 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: C₇H₇NS
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: Bp₁₀ 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: C₉H₁₁NS
Molecular Weight: 167.274
Accurate Mass: 167.070869
Percentage Composition: C 64.62%; H 7.83%; N 8.37%; S 19.17%
Boiling Point: Bp₁₀ 165-167°; Bp₁₀ 63-64°

-->Derivative: S-Et
Synonym(s): 3-(Ethylthio)aniline

CAS Registry Number: 1783-82-0
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: Bp₁ 103°

-->Derivative: Disulfide

References:
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