



>>Entry Name: 2-Amino-6-benzothiazolecarboxylic acid, 9CI

CAS Registry Number: 93-85-6

Related CAS Registry Numbers(s): 18330-76-2

Molecular Formula: $C_8H_6N_2O_2S$

Molecular Weight: 194.214

Accurate Mass: 194.014998

Percentage Composition: C 49.48%; H 3.11%; N 14.42%; O 16.48%; S 16.51%

Physical Description: Solid

Melting Point: Mp 300°. Mp 193°

>>Derivative: Me ester

CAS Registry Number: 66947-92-0

Molecular Formula: $C_9H_8N_2O_2S$

Molecular Weight: 208.24

Accurate Mass: 208.030648

Percentage Composition: C 51.91%; H 3.87%; N 13.45%; O 15.37%; S 15.40%

Melting Point: Mp 244-245°

>>Derivative: Et ester

CAS Registry Number: 50850-93-6

Molecular Formula: $C_{10}H_{10}N_2O_2S$

Molecular Weight: 222.267

Accurate Mass: 222.046298

Percentage Composition: C 54.04%; H 4.53%; N 12.60%; O 14.40%; S 14.43%

Melting Point: Mp 241°

>>Derivative: Nitrile

Synonym(s): 2-Amino-6-cyanobenzothiazole

CAS Registry Number: 19759-66-1

Molecular Formula: $C_8H_5N_3S$

Molecular Weight: 175.214

Accurate Mass: 175.020417

Percentage Composition: C 54.84%; H 2.88%; N 23.98%; S 18.30%

Melting Point: Mp 203-204°

>>Derivative: *N*-Ac

CAS Registry Number: 100817-94-5

Molecular Formula: $C_{10}H_8N_2O_3S$

Molecular Weight: 236.251

Accurate Mass: 236.025563

Percentage Composition: C 50.84%; H 3.41%; N 11.86%; O 20.32%; S 13.57%

Melting Point: Mp 236°

>>Derivative: *N*-Me

Molecular Formula: $C_9H_8N_2O_2S$

Molecular Weight: 208.24

Accurate Mass: 208.030648

Percentage Composition: C 51.91%; H 3.87%; N 13.45%; O 15.37%; S 15.40%

Physical Description: Cryst. (EtOH/EtOAc)

Melting Point: Mp 298°

>>Derivative: *N*-Me, Et ester

Molecular Formula: $C_{11}H_{12}N_2O_2S$

Molecular Weight: 236.294

Accurate Mass: 236.061948

Percentage Composition: C 55.91%; H 5.12%; N 11.86%; O 13.54%; S 13.57%

Physical Description: Plates (EtOH/EtOAc)

Melting Point: Mp 169°