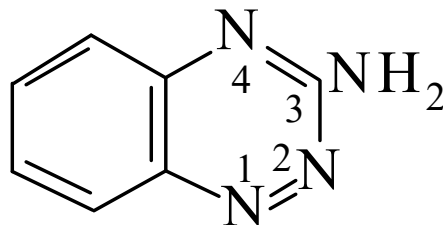




>>Entry Name: 3-Amino-1,2,4-benzotriazine, 8Cl

Synonym(s): 1,2,4-Benzotriazin-3-amine, 9Cl



CAS Registry Number: 20028-80-2

Molecular Formula: C₇H₆N₄

Molecular Weight: 146.151

Accurate Mass: 146.059246

Percentage Composition: C 57.53%; H 4.14%; N 38.33%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 207°

>>Derivative: 1-*N*-Oxide

CAS Registry Number: 5424-06-6

Molecular Formula: C₇H₆N₄O

Molecular Weight: 162.151

Accurate Mass: 162.054161

Percentage Composition: C 51.85%; H 3.73%; N 34.55%; O 9.87%

Physical Description: Yellow plates (AcOH or EtOH)

Melting Point: Mp 275° (271°)

Rare Chemicals Library: S59694-9

>>Derivative: 2-*N*-Oxide

CAS Registry Number: 27238-43-3

Molecular Formula: C₇H₆N₄O

Molecular Weight: 162.151

Accurate Mass: 162.054161

Percentage Composition: C 51.85%; H 3.73%; N 34.55%; O 9.87%

Physical Description: Yellow needles (AcOH or EtOH)

Melting Point: Mp 200° (187°)

>>Derivative: 1,4-Dioxide

Synonym(s): Tirapazamine. SR 4233. Win 59075

CAS Registry Number: 27314-97-2

Molecular Formula: C₇H₆N₄O₂

Molecular Weight: 178.15

Accurate Mass: 178.049076

Percentage Composition: C 47.19%; H 3.39%; N 31.45%; O 17.96%

Use/Importance: Antineoplastic agent showing selective toxicity towards hypoxic cells. Radiosensitiser

Physical Description: Orange-red needles (MeOH)

Melting Point: Mp 220 dec.°

Calculated Log P Data: Log P -2.89 (calc)

Sigma: A9938

>>Derivative: 4-Acetoxy, 1-oxide

Synonym(s): 4-Acetyloxy-1,2,4-benzotriazin-3(4*H*)-imine 1-oxide, 9Cl

CAS Registry Number: 59399-02-9

Molecular Formula: C₉H₈N₄O₃

Molecular Weight: 220.187

Accurate Mass: 220.059641

Percentage Composition: C 49.09%; H 3.66%; N 25.45%; O 21.80%

Use/Importance: Bactericide