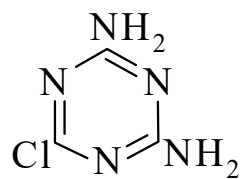




>>Entry Name: **2,4-Diamino-6-chloro-1,3,5-triazine**

Synonym(s): 6-Chloro-1,3,5-triazine-2,4-diamine, 9Cl



CAS Registry Number: 3397-62-4

Molecular Formula: C<sub>3</sub>H<sub>4</sub>ClN<sub>5</sub>

Molecular Weight: 145.551

Accurate Mass: 145.015522

Percentage Composition: C 24.76%; H 2.77%; Cl 24.36%; N 48.12%

Biological Use/Importance: Various *N*-subst. derivs. used as herbicides

Physical Description: Needles (DMF aq.)

Other Data: Evolves NH<sub>3</sub> on heating, forming polymer

Aldrich: C3330-1

>>Derivative: *N*-Et

CAS Registry Number: 1007-28-9

Molecular Formula: C<sub>3</sub>H<sub>8</sub>ClN<sub>5</sub>

Molecular Weight: 173.604

Accurate Mass: 173.046822

Percentage Composition: C 34.59%; H 4.64%; Cl 20.42%; N 40.34%

Metabolism: Metab. of simazine and atrazine in plants and soil microorganisms

Physical Description: Cryst. (H<sub>2</sub>O)

Melting Point: Mp 177-179°

>>Derivative: 2,4-*N*-Di-Et

Synonym(s): Simazine, ANSI, BSI, ISO, WSSA, CAT, JMAF, Aquazine, Azotop, Gesatop, Herbatoxol S, Herbazin, Herbex, Hungazin DT, **Primatol**‡, Tafazine, Yrodazin, Weedex

CAS Registry Number: 122-34-9

Molecular Formula: C<sub>7</sub>H<sub>12</sub>ClN<sub>5</sub>

Molecular Weight: 201.658

Accurate Mass: 201.078122

Percentage Composition: C 41.69%; H 6.00%; Cl 17.58%; N 34.73%

Biological Use/Importance: Pre-emergence herbicide

Physical Description: Cryst.

Melting Point: Mp 228-229°

pKa Value: pK<sub>a</sub> 1.7 (21°,basic)

**Hazard & Toxicity:** LD<sub>50</sub> (rat, orl) >5000 mg/kg

Rare Chemicals Library: S44237-2

Supelco: 4-9089

>>Derivative: 2,2,4-*N*-Tri-Et

Synonym(s): Trietazine, ANSI, BSI, ISO, JMAF, Aventox, Bronox, Remtal

CAS Registry Number: 1912-26-1

Molecular Formula: C<sub>9</sub>H<sub>16</sub>ClN<sub>5</sub>

Molecular Weight: 229.712

Accurate Mass: 229.109422

Percentage Composition: C 47.06%; H 7.02%; Cl 15.43%; N 30.49%

Use/Importance: Herbicide

Physical Description: Cryst. solid

Melting Point: Mp 100-101°

**Hazard & Toxicity:** LD<sub>50</sub> (rat, orl) 594 mg/kg