



>>Entry Name: Nitroguanidine, 9Cl, 8Cl

Synonym(s): Picrite

CAS Registry Number: 556-88-7

$(\text{H}_2\text{N})_2\text{C}=\text{NNO}_2$

Molecular Formula: $\text{CH}_4\text{N}_4\text{O}_2$

Molecular Weight: 104.068

Accurate Mass: 104.033426

Percentage Composition: C 11.54%; H 3.87%; N 53.84%; O 30.75%

Source/Synthesis: Manuf. by dehydration of guanidine nitrate with H_2SO_4

Use/Importance: Secondary high explosive used in gun and rocket propellants

Physical Description: Two forms: long, thin, flat needles or prisms (H_2O) (more stable, α -form), fan-like clusters of small, thin, elongated plates (H_2O)

Melting Point: Mp 232 dec. $^\circ$ (220 $^\circ$ dec.)

Solubility: Sol. conc. acids; spar. sol. MeOH, EtOH; prac. insol. Et_2O ; spar. sol. hot H_2O

pKa Value: $\text{pK}_{\text{a}1}$ -0.55; $\text{pK}_{\text{a}2}$ 12.2 (25 $^\circ$, acid)

Other Data: Both forms dec. on melting $\rightarrow \text{NH}_3$

Hazard & Toxicity: Shock- or heat-sensitive explosive. LD_{50} (mus, ipr) 48 mg/kg

Aldrich: N1735-1

Fluka: 73350

>>Derivative: Hydrochloride

Physical Description: Plates, prisms or needles (HCl aq.)

>>Derivative: Nitrate

Physical Description: Plates (hot conc. HNO_3)

Melting Point: Mp 140 (147 $^\circ$) dec. $^\circ$

>>Derivative: *N*'-Ac

Molecular Formula: $\text{C}_3\text{H}_6\text{N}_4\text{O}_3$

Molecular Weight: 146.105

Accurate Mass: 146.043991

Percentage Composition: C 24.66%; H 4.14%; N 38.35%; O 32.85%

Physical Description: Cryst. (MeCN)

Melting Point: Mp 214.5-215.3 $^\circ$

>>Derivative: *N*'-Me

Synonym(s): *N*'-Methyl-*N*-nitroguanidine

CAS Registry Number: 4245-76-5

Molecular Formula: $\text{C}_2\text{H}_6\text{N}_4\text{O}_2$

Molecular Weight: 118.095

Accurate Mass: 118.049076

Percentage Composition: C 20.34%; H 5.12%; N 47.44%; O 27.10%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 160-161 $^\circ$

Aldrich: 34212-2

Rare Chemicals Library: S36366-9

>>Derivative: *N*'-Et

Synonym(s): *N*'-Ethyl-*N*-nitroguanidine

CAS Registry Number: 39197-62-1

Molecular Formula: $\text{C}_3\text{H}_8\text{N}_4\text{O}_2$

Molecular Weight: 132.122

Accurate Mass: 132.064726

Percentage Composition: C 27.27%; H 6.10%; N 42.41%; O 24.22%

Physical Description: Cubes or needles (EtOH aq.)

Melting Point: Mp 148-149 dec. $^\circ$