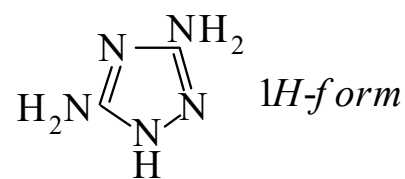




>>Entry Name: 1,2,4-Triazole-3,5-diamine, 9Cl

Synonym(s): 3,5-Diamino-1,2,4-triazole. Guanazole $\ddagger$. NSC 1895



CAS Registry Number: 1455-77-2

Molecular Formula: $\text{C}_2\text{H}_5\text{N}_5$

Molecular Weight: 99.095

Accurate Mass: 99.054495

Percentage Composition: C 24.24%; H 5.09%; N 70.67%

Use/Importance: Antineoplastic agent

Physical Description: Prisms (H_2O)

Melting Point: Mp 206°

pKa Value: $\text{p}K_{\text{a}1}$ 4.43; $\text{p}K_{\text{a}2}$ 12.12 (20°)

Aldrich: D2620-2

Fluka: 33410

Sigma: D7761

>>Derivative: Hydrochloride

CAS Registry Number: 6415-36-7

Melting Point: Mp 100°

>>Derivative: Hydrochloride (1:2)

Melting Point: Mp 145°

>>Derivative: Picrate

Physical Description: Yellow cryst. or flat needles (H_2O)

Melting Point: Mp 245°. Mp 249-251 dec.°

>>Derivative: 3-*N*-Ac

Molecular Formula: $\text{C}_4\text{H}_7\text{N}_5\text{O}$

Molecular Weight: 141.132

Accurate Mass: 141.06506

Percentage Composition: C 34.04%; H 5.00%; N 49.62%; O 11.34%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 296°

>>Derivative: 3,5-Di-*N*-Ac

CAS Registry Number: 60010-81-3

Molecular Formula: $\text{C}_6\text{H}_9\text{N}_5\text{O}_2$

Molecular Weight: 183.169

Accurate Mass: 183.075625

Percentage Composition: C 39.34%; H 4.95%; N 38.23%; O 17.47%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 330°