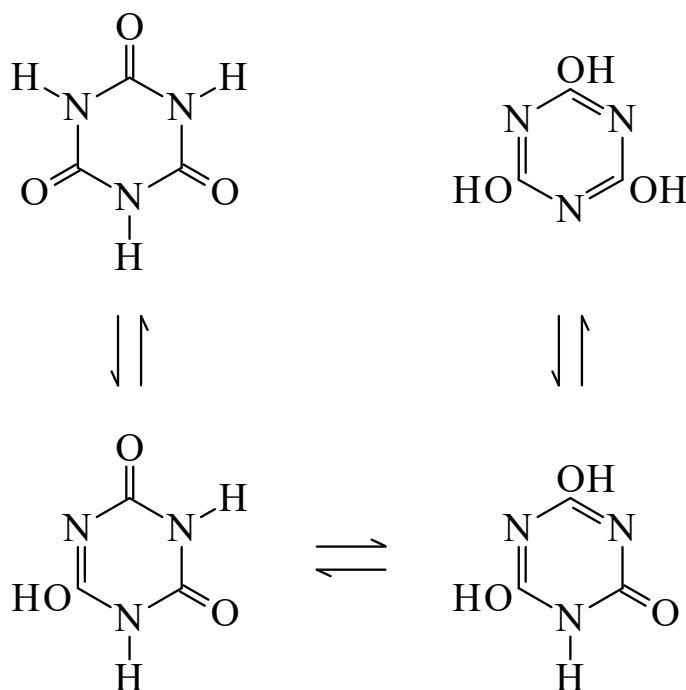




>>Entry Name: Cyanuric acid

Synonym(s): 1,3,5-Triazine-2,4,6(1*H*,3*H*,5*H*)-trione, 9Cl. *s*-Triazine-2,4,6-triol, 8Cl. Isocyanuric acid. Trihydroxycyanidine



CAS Registry Number: 108-80-5

Related CAS Registry Numbers(s): 504-19-8 37640-57-6

Molecular Formula: C₃H₃N₃O₃

Molecular Weight: 129.075

Accurate Mass: 129.017442

Percentage Composition: C 27.92%; H 2.34%; N 32.55%; O 37.19%

General Statement: Tri-*NH*-form predominates. Derivs. of the tri-*OH* tautomer are referred to as cyanurates and of the tri-*NH* form as isocyanurates

Use/Importance: Commercially available. Used in rubber, resin manuf. Herbicide. Ethers (cyanuric esters) are hypnotics and anticonvulsants

Physical Description: Off-white cryst. + 2H₂O (H₂O)

Melting Point: Mp 360°

Boiling Point: Subl._{0.0001} 380-400°. Subl._{0.02} 150-180°

Solubility: Sol. hot EtOH, mod. sol. H₂O

Density: d⁰ 1.768

pKa Value: pK_a 4.74 (25°,H₂O)

Other Data: Dec. to cyanic acid on heating without melting. Reacts as mono-, di- or tribasic acid

Hazard & Toxicity: Reacts violently with EtOH. Forms explosive by-product with chlorine. Eye and skin irritant. LD₅₀ (rat, orl) 7700 mg/kg

Aldrich: 18580-9

Fluka: 28640

>>Variant: Tri-*NH*-form

Molecular Formula: C₃H₃N₃O₃

Molecular Weight: 129.075

Accurate Mass: 129.017442

Percentage Composition: C 27.92%; H 2.34%; N 32.55%; O 37.19%

>>Derivative: *N*¹-Me

Synonym(s): 1-Methyl-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione

CAS Registry Number: 6726-47-2

Molecular Formula: C₄H₅N₃O₃

Molecular Weight: 143.102

Accurate Mass: 143.033092

Percentage Composition: C 33.57%; H 3.52%; N 29.36%; O 33.54%

Melting Point: Mp 285-286°