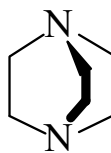




>>Entry Name: 1,4-Diazabicyclo[2.2.2]octane

Synonym(s): Triethylenediamine. Dabco



CAS Registry Number: 280-57-9

Molecular Formula: C₆H₁₂N₂

Molecular Weight: 112.174

Accurate Mass: 112.100048

Percentage Composition: C 64.24%; H 10.78%; N 24.97%

Use/Importance: Reagent for the cleavage of β-keto esters and geminal diesters and dehydrohalogenation reactions. Also a cyclisation catalyst and catalyst for urethane foam prepn. Nonnucleophilic base

Physical Description: Hygroscopic cryst.

Melting Point: Mp 158°

Boiling Point: Bp 174°

pKa Value: pK_{a1} 8.82; pK_{a2} 2.97 (25°)

Other Data: Sublimes readily at r.t.

Hazard & Toxicity: Forms explosive 1:1 complex with H₂O₂. Eye and skin irritant. Sensitiser and allergen. LD₅₀ (rat, orl) 1700 mg/kg

Aldrich: D2780-2

Fluka: 33480

Sigma: D2522

>>Derivative: Hydrochloride

Physical Description: Long deliquescent needles

Melting Point: Mp 320 dec.°

>>Derivative: Br₂ complex

CAS Registry Number: 5770-70-7

Use/Importance: Reagent for the oxidn. of aromatic and secondary alcohols

Physical Description: Yellow cryst.

Melting Point: Mp 155-160 dec.°

Other Data: Stable to light, air and H₂O

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