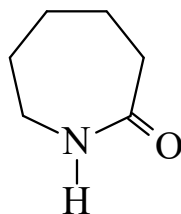




>>Entry Name: Hexahydro-2*H*-azepin-2-one, 9CI

Synonym(s): ϵ -Caprolactam. Hexanolactam. 6-Aminohexanoic acid lactam. 6-Aminocaproic acid lactam



CAS Registry Number: 105-60-2

Related CAS Registry Numbers(s): 2123-24-2

Molecular Formula: C₆H₁₁NO

Molecular Weight: 113.159

Accurate Mass: 113.084064

Percentage Composition: C 63.69%; H 9.80%; N 12.38%; O 14.14%

Use/Importance: Used in manuf. of nylon-type polymers, esp. nylon-6. Cross-linking agent for polyurethanes. Important industrial chemical, 47th in order of volume for USA in 1994 (production 0.84 million tons/year)

Physical Description: Leaflets (petrol)

Melting Point: Mp 68-70°

Boiling Point: Bp 267°. Bp₁₂ 139°

Solubility: Sol. H₂O, org. solvs.

Other Data: Ceiling temp. for polym., *T*_c 220°

Hazard & Toxicity: Eye, skin and respiratory tract irritant. LD₅₀ (rat, orl) 1210 mg/kg. LC₅₀ (rat, ihl) 300 mg m⁻³ (2h exposure). OES: long-term 1 mg m⁻³; short-term 3 mg m⁻³ (dust); long-term 5 ppm; short-term 10 ppm (vapour)

Aldrich: C220-4

Fluka: 21500

Rare Chemicals Library: S44882-6

Sigma: C3907

>>Derivative: Na salt

CAS Registry Number: 2123-24-2

Use/Importance: Initiator for polym. of caprolactam

Physical Description: Powder

>>Derivative: *N*-Ac

CAS Registry Number: 1888-91-1

Molecular Formula: C₈H₁₃NO₂

Molecular Weight: 155.196

Accurate Mass: 155.094629

Percentage Composition: C 61.91%; H 8.44%; N 9.03%; O 20.62%

Boiling Point: Bp₂₆ 134-135°

Refractive Index: n_D²⁰ 1.4890

Aldrich: 28301-0

Fluka: 981

>>Derivative: *N*-Benzoyl

CAS Registry Number: 6248-28-8

Molecular Formula: C₁₃H₁₅NO₂

Molecular Weight: 217.267

Accurate Mass: 217.110279

Percentage Composition: C 71.87%; H 6.96%; N 6.45%; O 14.73%

Use/Importance: Polymerisation catalyst, has laundry/bleaching applications

Physical Description: Plates (Me₂CO)

Melting Point: Mp 69-71°

Solubility: Sol. H₂O (1.48g/l H₂O, 25°).