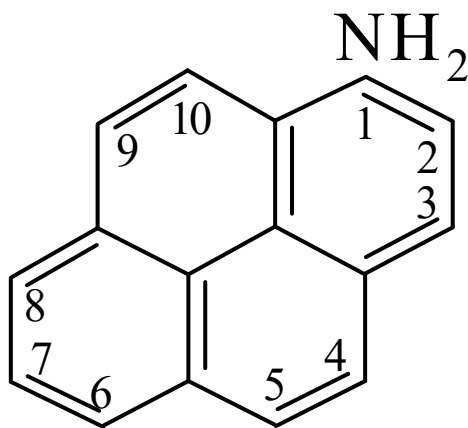




>>Entry Name: 1-Aminopyrene

Synonym(s): 1-Pyrenamine, 9CI



CAS Registry Number: 1606-67-3

Molecular Formula: C₁₆H₁₁N

Molecular Weight: 217.27

Accurate Mass: 217.089149

Percentage Composition: C 88.45%; H 5.10%; N 6.45%

Source/Synthesis: Isol. from coal tar

Use/Importance: Used as 0.05% soln. in conc. H₂SO₄ for photometric detn. of NO₂⁽⁻⁾, NO₃⁽⁻⁾

Physical Description: Pale-yellow needles (hexane)

Melting Point: Mp 117-118°

Solubility: Sol. C₆H₆, Et₂O; insol. H₂O

Other Data: Conc. H₂SO₄ → colourless soln. with violet-blue fluor.

Hazard & Toxicity: Mutagen. LD₅₀ (rat, orl) 1070 mg/kg

Aldrich: A7790-3

Fluka: 9339

Rare Chemicals Library: S26576-4

Sigma: A9265

>>Derivative: N-Ac

CAS Registry Number: 64709-54-2

Molecular Formula: C₁₈H₁₃NO

Molecular Weight: 259.307

Accurate Mass: 259.099714

Percentage Composition: C 83.38%; H 5.05%; N 5.40%; O 6.17%

Physical Description: Needles (AcOH)

Melting Point: Mp 260°

Aldrich: A750-7

>>Derivative: N-Me

CAS Registry Number: 22965-22-6

Molecular Formula: C₁₇H₁₃N

Molecular Weight: 231.296

Accurate Mass: 231.104799

Percentage Composition: C 88.28%; H 5.66%; N 6.06%

Melting Point: Mp 82-83°

References:

- Aldrich Library of NMR Spectra*, 2nd edn., 1983, **1**, 1066B, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1256B, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1161D, (*ir*)
Vollmann, H. *et al.*, *Annalen*, 1937, **531**, 1
Jones, R.N., *J.A.C.S.*, 1945, **67**, 2127, (*uv*)
Lund, H. *et al.*, *CA*, 1946, **40**, 6072
Weigel, W. *et al.*, *Annalen*, 1961, **647**, 108