



>>Entry Name: 1,5-Pentanediamine, 9CI

Synonym(s): Pentamethylenediamine. 1,5-Diaminopentane. Cadaverine

CAS Registry Number: 462-94-2

$\text{H}_2\text{NCH}_2(\text{CH}_2)_3\text{CH}_2\text{NH}_2$

Molecular Formula: $\text{C}_5\text{H}_{14}\text{N}_2$

Molecular Weight: 102.179

Accurate Mass: 102.115698

Percentage Composition: C 58.77%; H 13.81%; N 27.42%

Biological Source: Found in nature as bacterial decarboxylation prod. of Lysine [BCS45-Z](#), e.g. in putrefaction. Anal sac secretion of the red fox *Vulpes vulpes*

Use/Importance: Monomer for polyamides

Physical Description: Syrupy fuming liq.

Boiling Point: Bp 178-180°

Density: d^{20}_4 0.843

pKa Value: $\text{p}K_{\text{a}1}$ 10.92; $\text{p}K_{\text{a}2}$ 10.05 (25°, 0.5M KNO_3)

Refractive Index: n^{20}_{D} 1.4582

Hazard & Toxicity: Skin irritant

Aldrich: D2260-6

Fluka: 33211

Sigma: C8382

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 1476-39-7

Physical Description: Needles (H_2O)

Melting Point: Mp 226°. Mp 260-262°

Aldrich: 27182-9

Fluka: 33220

Sigma: C0500

>>Derivative: *N*-Benzoyl

CAS Registry Number: 29833-52-1

Molecular Formula: $\text{C}_{12}\text{H}_{18}\text{N}_2\text{O}$

Molecular Weight: 206.287

Accurate Mass: 206.141913

Percentage Composition: C 69.87%; H 8.79%; N 13.58%; O 7.76%

Physical Description: Oil

Boiling Point: $\text{Bp}_{0.5}$ 202°

>>Derivative: *N,N'*-Dibenzoyl

CAS Registry Number: 31991-79-4

Molecular Formula: $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_2$

Molecular Weight: 310.395

Accurate Mass: 310.168128

Percentage Composition: C 73.52%; H 7.14%; N 9.03%; O 10.31%

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 135°

>>Derivative: *N,N'*-Bis(4-nitrobenzoyl)

CAS Registry Number: 81852-10-0

Physical Description: Cryst. (Me_2CO aq.)

Melting Point: Mp 185-185.5°