



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

Synonym(s): Pentamethylene glycol

CAS Registry Number: 111-29-5

HOCH₂CH₂CH₂CH₂CH₂OH

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

Percentage Composition: C 57.66%; H 11.61%; O 30.72%

Source/Synthesis: Manuf. by hydrogenation of glutaric acid or glutaraldehyde

Use/Importance: Used in manuf. of pharmaceuticals and pesticides. Monomer for polyamides and polyurethanes

Physical Description: Oil with bitter taste

Melting Point: Mp -18°

Boiling Point: Bp 238-239°. Bp₁₂ 134°

Solubility: Sol. H₂O, EtOH, Me₂CO

Density: d₁₅¹¹ 0.999

Refractive Index: n_D²⁰ 1.4499

Hazard & Toxicity: Eye and skin irritant

Aldrich: P770-3

Fluka: 76892

>>Derivative: Diformyl

CAS Registry Number: 5436-53-3

Molecular Formula: C₇H₁₂O₄

Molecular Weight: 160.169

Accurate Mass: 160.07356

Percentage Composition: C 52.49%; H 7.55%; O 39.96%

Physical Description: Liq.

Boiling Point: Bp₂₀ 122-123°

>>Derivative: Di-Ac

CAS Registry Number: 6963-44-6

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Physical Description: Liq. with fruity odour

Melting Point: Fp 2°

Boiling Point: Bp 241°. Bp₃ 122-123°

>>Derivative: Bisphenylurethane

Physical Description: Needles (EtOH or EtOH/CHCl₃)

Melting Point: Mp 176°

>>Derivative: Bis-4-nitrobenzoyl

CAS Registry Number: 22104-39-8

Physical Description: Cryst. (C₆H₆ or Me₂CO aq.)

Melting Point: Mp 104.5°

>>Derivative: Mono-Me ether

Synonym(s): 5-Methoxy-1-pentanol, 9CI

CAS Registry Number: 4799-62-6

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Physical Description: Liq.

Boiling Point: Bp₅₀ 118°