



>>Entry Name: 1,6-Hexanediol, 9CI, 8CI

Synonym(s): Hexamethylene glycol

CAS Registry Number: 629-11-8

Extra CAS Registry Numbers(s): 26762-52-7

HOH₂C(CH₂)₄CH₂OH

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

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

Source/Synthesis: Manuf. by redn. of dimethyl hexanedioate

Use/Importance: Monomer used in the manuf. of polyesters and polyurethanes

Physical Description: Needles (H₂O)

Melting Point: Mp 42°. Mp 59°

Boiling Point: Bp 250°. Bp₁₇ 152°

Solubility: Sol. H₂O

Hazard & Toxicity: Fl. p. 96°. Eye irritant. LD₅₀ (rat, orl) 3730 mg/kg

Aldrich: 24011-7

Fluka: 52800

>>Derivative: Mono-Ac

CAS Registry Number: 68750-24-3

Molecular Formula: C₈H₁₆O₃

Molecular Weight: 160.213

Accurate Mass: 160.109945

Percentage Composition: C 59.98%; H 10.07%; O 29.96%

Boiling Point: Bp₄ 100-103°

>>Derivative: Di-Ac

CAS Registry Number: 6222-17-9

Molecular Formula: C₁₀H₁₈O₄

Molecular Weight: 202.25

Accurate Mass: 202.12051

Percentage Composition: C 59.39%; H 8.97%; O 31.64%

Boiling Point: Bp₆ 103-105°

>>Derivative: Di-2-propenoyl

Synonym(s): 1,6-Bis(2-propenoyloxy)hexane

CAS Registry Number: 13048-33-4

Molecular Formula: C₁₂H₁₈O₄

Molecular Weight: 226.272

Accurate Mass: 226.12051

Percentage Composition: C 63.70%; H 8.02%; O 28.28%

Use/Importance: Monomer

Physical Description: Liq.

Boiling Point: Bp₁ 130°

>>Derivative: Dibenzoyl

CAS Registry Number: 22915-73-7

Molecular Formula: C₂₀H₂₂O₄

Molecular Weight: 326.391

Accurate Mass: 326.15181

Percentage Composition: C 73.60%; H 6.79%; O 19.61%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 56°