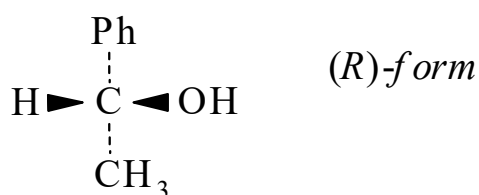




>>Entry Name: 1-Phenylethanol

ENTRY UNDER REVIEW

Synonym(s): α -Methylbenzenemethanol, 9CI. α -Methylbenzyl alcohol, 8CI. Methylphenylcarbinol. α -Hydroxyethylbenzene. *sec*-Phenethyl alcohol. 1-(Phenylethyl) alcohol. Styrallyl alcohol. FEMA 2685



CAS Registry Number: 98-85-1

Related CAS Registry Numbers(s): 3299-05-6 4013-34-7

Molecular Formula: C₈H₁₀O

Molecular Weight: 122.166

Accurate Mass: 122.073165

Percentage Composition: C 78.65%; H 8.25%; O 13.10%

Biological Source: Present in tea aroma, mushroom volatiles, etc.

Use/Importance: Perfumery ingredient and flavouring agent

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 400 mg/kg. LD₅₀ (rbt, skn) 2500 mg/kg

Aldrich: W26851-8

>>Variant: (R)-form

CAS Registry Number: 1517-69-7

Molecular Formula: C₈H₁₀O

Molecular Weight: 122.166

Accurate Mass: 122.073165

Percentage Composition: C 78.65%; H 8.25%; O 13.10%

Physical Description: Oil

Boiling Point: Bp 202-204°. Bp₁ 75°

Optical Rotation: [α]_D²⁵+54.8 (c, 0.9 in CHCl₃) (97% ee)

Density: d₄¹³ 1.019

Refractive Index: n_D²⁰ 1.5270

Aldrich: 23742-6

Fluka: 77848

Sigma: P4277

>>Derivative: Ac

CAS Registry Number: 16197-92-5

Extra CAS Registry Numbers(s): 93-92-5

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Use/Importance: Perfumery ingredient

Physical Description: Oil

Boiling Point: Bp₁₈ 109°

Optical Rotation: [α]_D¹²+127.6 (neat)

>>Derivative: Benzoyl

CAS Registry Number: 65915-69-7

Molecular Formula: C₁₅H₁₄O₂

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Physical Description: Oil

Optical Rotation: [α]_D²⁵-20.7 (c, 2.28 in EtOH) (95% op)