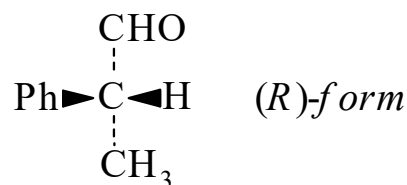




>>Entry Name: 2-Phenylpropanal

ENTRY UNDER REVIEW

Synonym(s): α -Methylbenzeneacetaldehyde, 9CI. Hydratropaldehyde, 8CI. Hydratropic aldehyde. 2-Phenylpropionaldehyde. FEMA 2886



CAS Registry Number: 93-53-8

Related CAS Registry Numbers(s): 90-87-9 59647-78-8

Molecular Formula: C₉H₁₀O

Molecular Weight: 134.177

Accurate Mass: 134.073165

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Physical Description: Liq. with sweet pungent taste suggestive of apricot

Hazard & Toxicity: LD₅₀ (rat, orl) 2800 mg/kg

Aldrich: 24136-9

>>Variant: (R)-form

CAS Registry Number: 38235-74-4

Molecular Formula: C₉H₁₀O

Molecular Weight: 134.177

Accurate Mass: 134.073165

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Physical Description: Liq.

Boiling Point: Bp₅ 85°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -238$ (neat) (100% op). $[\alpha]_{\text{D}}^{20} -288.3$ (c, 0.5 in C₆H₆) (91% ee)

>>Variant: (S)-form

CAS Registry Number: 33530-47-1

Molecular Formula: C₉H₁₀O

Molecular Weight: 134.177

Accurate Mass: 134.073165

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Physical Description: Liq.

Boiling Point: Bp₅ 85°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +314.6$ (c, 0.45 in C₆H₆) (99.4% ee)

>>Derivative: Di-Me acetal

Synonym(s): (2,2-Dimethoxy-1-methylethyl)benzene, 9CI. 1,1-Dimethoxy-2-phenylpropane

CAS Registry Number: 103593-60-8

Molecular Formula: C₁₁H₁₆O₂

Molecular Weight: 180.246

Accurate Mass: 180.11503

Percentage Composition: C 73.30%; H 8.95%; O 17.75%

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{22} +3.3$ (c, 1.01 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 34713-70-7

Molecular Formula: C₉H₁₀O

Molecular Weight: 134.177

Accurate Mass: 134.073165

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Use/Importance: Perfumery and flavour ingredient

Physical Description: Liq.

Boiling Point: Bp 202-205°. Bp₁₂ 92-92.5°

Refractive Index: n_D²⁰ 1.5170

Fluka: 53790