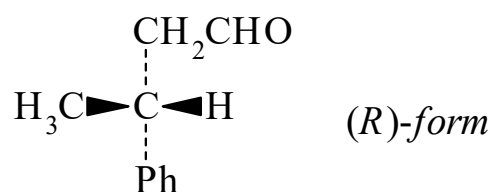




>>Entry Name: 3-Phenylbutanal

Synonym(s): β -Methylbenzenepropanal, 9Cl. 3-Phenylbutyraldehyde. β -Methylhydrocinnamaldehyde



CAS Registry Number: 16251-77-7

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}$

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Aldrich: 28902-7

>>Variant: (R)-form

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}$

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Boiling Point: $\text{Bp}_{0.02} 35^\circ$

Optical Rotation: $[\alpha]_{\text{D}}^{20} -35.8$ (c, 1.20 in C_6H_6) (80% e.e)

>>Variant: ($\pm$)-form

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}$

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Physical Description: Liq.

Boiling Point: $\text{Bp}_9 110^\circ$

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 25611-38-5

Melting Point: $\text{Mp} 111\text{-}112^\circ$

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 926A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1280C, (*ir*)

Org. Synth., 1971, **51**, 17, (*synth*)

Ahlbrecht, H. *et al.*, *Chem. Ber.*, 1989, **122**, 1995, (*synth, pmr, cmr*)