



>>Entry Name: 2-Methyl-4-phenyl-2-butanol, 8CI

ENTRY UNDER REVIEW

Synonym(s): α,α -Dimethylbenzenepropanol, 9CI. Dimethylphenylethylcarbinol. FEMA 3629

CAS Registry Number: 103-05-9

$\text{PhCH}_2\text{CH}_2\text{C}(\text{CH}_3)_2\text{OH}$

Molecular Formula: $\text{C}_{11}\text{H}_{16}\text{O}$

Molecular Weight: 164.247

Accurate Mass: 164.120115

Percentage Composition: C 80.44%; H 9.82%; O 9.74%

Use/Importance: Used in perfumery formulations

Physical Description: Needles or liq. with lily-like odour

Melting Point: Mp 29-30°

Boiling Point: Bp 238°. Bp₁₇ 128°. Bp₃ 71-94°

Refractive Index: n_D^{21} 1.5077

Hazard & Toxicity: LD₅₀ (rat, orl) 2200 mg/kg. LD₅₀ (rbt, skn) 3500 mg/kg

Aldrich: B1800-6

>>Derivative: Phenylurethane

Physical Description: Cryst. (petrol)

Melting Point: Mp 139.1-140.1°

>>Derivative: Ac

Synonym(s): 3-Acetoxy-3-methyl-1-phenylbutane. Centifolia. Phenyl-*tert*-amyl acetate. FEMA 2735

CAS Registry Number: 103-07-1

Molecular Formula: $\text{C}_{13}\text{H}_{18}\text{O}_2$

Molecular Weight: 206.284

Accurate Mass: 206.13068

Percentage Composition: C 75.69%; H 8.79%; O 15.51%

Use/Importance: Used in perfumery

Physical Description: Liq. with a jasmine and hyacin-like odour

Boiling Point: Bp 244°. Bp 275°

>>Derivative: 2-Methylpropanoyl

Synonym(s): FEMA 2736

CAS Registry Number: 10031-71-7

Molecular Formula: $\text{C}_{15}\text{H}_{22}\text{O}_2$

Molecular Weight: 234.338

Accurate Mass: 234.16198

Percentage Composition: C 76.88%; H 9.46%; O 13.66%

Physical Description: Liq.

Boiling Point: Bp 250°

References:

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