



>>Entry Name: 2-Methyl-1-phenyl-2-propanol

Synonym(s): α,α -Dimethylbenzeneethanol, 9CI. α,α -Dimethylphenethyl alcohol, 8CI. Benzyldimethylcarbinol. FEMA 2393

CAS Registry Number: 100-86-7

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

Molecular Formula: $\text{C}_{10}\text{H}_{14}\text{O}$

Molecular Weight: 150.22

Accurate Mass: 150.104465

Percentage Composition: C 79.96%; H 9.39%; O 10.65%

Biological Source: Present in cocoa

Use/Importance: Flavouring agent. Used in floral perfumes. Alkali-stable, used in soap perfumes

Physical Description: Needles or oil with floral-herbaceous odour

Melting Point: Mp 24°

Boiling Point: Bp 214-216°. Bp₁ 58°

Refractive Index: n_{D}^{20} 1.5170 (supercooled liq.)

Hazard & Toxicity: LD₅₀ (rat, orl) 1280 mg/kg

Aldrich: 17027-5

Fluka: 68710

Rare Chemicals Library: S55931-8

>>Derivative: Ac

Synonym(s): FEMA 2392

CAS Registry Number: 151-05-3

Molecular Formula: $\text{C}_{12}\text{H}_{16}\text{O}_2$

Molecular Weight: 192.257

Accurate Mass: 192.11503

Percentage Composition: C 74.97%; H 8.39%; O 16.64%

Use/Importance: Used in perfumery. Flavouring agent

Physical Description: Liq. with flowery, woody odour

Melting Point: Mp 30°

Boiling Point: Bp₁₀ 102-103°

Refractive Index: n_{D}^{20} 1.4923 (supercooled liq.)

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 3300 mg/kg

Rare Chemicals Library: S52802-1

>>Derivative: Butanoyl

Synonym(s): FEMA 2394

CAS Registry Number: 10094-34-5

Molecular Formula: $\text{C}_{14}\text{H}_{20}\text{O}_2$

Molecular Weight: 220.311

Accurate Mass: 220.14633

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Use/Importance: Used in perfumery. Flavouring agent

Physical Description: Liq. with fruity, herbal odour and plum-like flavour

Boiling Point: Bp₃ 96°

Hazard & Toxicity: n_{D}^{20} 1.4880

Rare Chemicals Library: S52811-0

>>Derivative: Benzoyl

CAS Registry Number: 19284-03-8

Molecular Formula: $\text{C}_{17}\text{H}_{18}\text{O}_2$

Molecular Weight: 254.328

Accurate Mass: 254.13068

Percentage Composition: C 80.28%; H 7.13%; O 12.58%

Boiling Point: Bp_{0.15} 105°

>>Derivative: Formyl

Synonym(s): α,α -Dimethylphenethyl formate. FEMA 2395