



>>Entry Name: **Benzyl alcohol**, BAN, INN, USAN

ENTRY UNDER REVIEW

Synonym(s): Benzenemethanol, 9CI. Phenylmethanol. Hydroxymethylbenzene. Phenylcarbinol. α -Hydroxytoluene. **Peruvina**. Benzenecarbinol. FEMA 2137

CAS Registry Number: 100-51-6

Related CAS Registry Numbers(s): 20194-18-7

PhCH₂OH

Molecular Formula: C₇H₈O

Molecular Weight: 108.14

Accurate Mass: 108.057515

Percentage Composition: C 77.75%; H 7.46%; O 14.80%

Biological Source: Constit. of jasmin and other ethereal oils, both free and as esters. Also present in cherry, orange juice, mandarin peel oil, guava fruit, feijon fruit, pineapple, leek, cinnamon, cloves, mustard, fermented tea, basil and red sage. Flavouring ingredient

Use/Importance: Dyeing assistant used in colour film development preservative. Used in perfumery and flavour industries and as an antimicrobial preservative in pharmaceuticals and cosmetics

Physical Description: Liq.

Melting Point: Fp -15.2°

Boiling Point: Bp 205.3°. Bp₁₀ 93°

Solubility: Mod. sol. H₂O

Density: d₂₀²⁰ 1.045. d₁₅¹⁵ 1.05

pKa Value: pK_a 15.4 (25°)

Refractive Index: n_D²⁰ 1.5396

Hazard & Toxicity: Fl. p. 93/96/101°, autoignition temp. 436°. Mixt. with 58% H₂SO₄ dec. explosively at 180°. Eye and skin irritant. Ingestion or inhalation can cause adverse gastrointestinal and CNS effects. LD₅₀ (rat, orl) 1230 mg/kg

Aldrich: 10800-6

Fluka: 13170

Sigma: B2263

Supelco: S48-2137

>>Derivative: *O*-Sulfate

Synonym(s): Benzyl sulfate

Molecular Formula: C₇H₈O₄S

Molecular Weight: 188.204

Accurate Mass: 188.01433

Percentage Composition: C 44.67%; H 4.28%; O 34.00%; S 17.04%

Biological Source: Constit. of various plant spp.

Use/Importance: Flavour component

>>Derivative: *O*-Glucopyranoside

see Benzyl glucopyranoside, [BZF33-M](#)

>>Derivative: *O*-[β -D-Glucopyranosyl-(1 $\rightarrow$ 6)- β -D-glucopyranoside]

Synonym(s): Benzyl gentiobioside

CAS Registry Number: 56775-64-5

Molecular Formula: C₁₉H₂₈O₁₁

Molecular Weight: 432.424

Accurate Mass: 432.163165

Percentage Composition: C 52.77%; H 6.53%; O 40.70%

Biological Source: Constit. of tomato cell cultures (*Lycopersicon esculentum* Solanaceae)

Optical Rotation: [α]_D -76.2 (c, 0.01 in H₂O)

>>Derivative: *O*-[β -D-Apiofuranosyl-(1 $\rightarrow$ 2)- β -D-glucopyranoside]

Molecular Formula: C₁₈H₂₆O₁₀

Molecular Weight: 402.397

Accurate Mass: 402.1526

Percentage Composition: C 53.73%; H 6.51%; O 39.76%

Biological Source: Constit. of *Scutellaria baicalensis*