



>>Entry Name: Phenylacetaldehyde

ENTRY UNDER REVIEW

Synonym(s): Benzeneacetaldehyde, 9Cl. α -Toluic aldehyde. Phenylethanal. FEMA 2874

CAS Registry Number: 122-78-1

PhCH₂CHO

Molecular Formula: C₈H₈O

Molecular Weight: 120.151

Accurate Mass: 120.057515

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Biological Source: Found in some essential oils, e.g. *Citrus* spp., *Tagetes minuta* and in the mushroom *Phallus impudicus*

Use/Importance: Perfumery and flavouring ingredient

Physical Description: Liq. with hyacinth odour

Boiling Point: Bp 195°. Bp₁₀ 78°

Density: d₄¹⁵ 1.027

Refractive Index: n_D²⁰ 1.5290

Other Data: Forms complexes with metals. Polym. on standing to odourless trimer

Hazard & Toxicity: Fl. p. 68/71/88°. Human skin irritant. LD₅₀ (rat, orl) 1550 mg/kg

Aldrich: W28740-7

Fluka: 77800

Sigma: P0145

>>Derivative: Oxime

CAS Registry Number: 7028-48-0

Molecular Formula: C₈H₉NO

Molecular Weight: 135.165

Accurate Mass: 135.068414

Percentage Composition: C 71.09%; H 6.71%; N 10.36%; O 11.84%

Biosynthesis: Testosterone-dependant urinary metab. of phenylalanine isol. from guinea pigs

Use/Importance: Intermed. in the plant biosynthesis of glucosinolates (mustard oil glycosides)

Physical Description: Cryst. (MeOH)

Melting Point: Mp 98.5°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2074-04-6

Physical Description: Light-yellow needles (EtOH)

Melting Point: Mp 189-190°

Rare Chemicals Library: S85251-1

>>Derivative: Di-Me acetal

Synonym(s): (2,2-Dimethoxyethyl)benzene, 9Cl. 1,1-Dimethoxy-2-phenylethane. Viridine. FEMA 2876

CAS Registry Number: 101-48-4

Molecular Formula: C₁₀H₁₄O₂

Molecular Weight: 166.219

Accurate Mass: 166.09938

Percentage Composition: C 72.26%; H 8.49%; O 19.25%

Use/Importance: Important perfumery ingredient

Physical Description: Oil

Boiling Point: Bp₇₅₄ 219-221°

Density: d₀¹⁸ 1.004

Aldrich: P1660-5

Fluka: 77811