



>>Entry Name: Phenylacetic acid

ENTRY UNDER REVIEW

Synonym(s): Benzeneacetic acid, 9CI. Phenylethanoic acid. α -Toluic acid. FEMA 2878

CAS Registry Number: 103-82-2

Related CAS Registry Numbers(s): 114-70-5

PhCH₂COOH

Molecular Formula: C₈H₈O₂

Molecular Weight: 136.15

Accurate Mass: 136.05243

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Biological Source: Found in essential oils, e.g. neroli, rose oil, free and as esters. Also prod. by microorganisms e.g. by *Fusarium oxysporum* and by *Glomerella cingulata*.

Volatile component of tail gland secretion from red deer *Cervus elaphus*

Use/Importance: Used as 1M soln. in CHCl₃ for selective extraction separation of Cu and U (CHCl₃). Important industrial intermediate. Perfumery and flavouring ingredient.

Incorporation in fermentation of penicillin results in production of Benzylpenicillin [CJX81-O](#)

Biological Use/Importance: Phytotoxin, germination inhibitor

Physical Description: Plates (petrol) with sweet taste at low conc. and rose-like odour

Melting Point: Mp 77-78.5°

Boiling Point: Bp 265.5°. Bp_{0.01} 65-70°

pKa Value: pK_a 4.31 (H₂O)

Hazard & Toxicity: Fl. p. 102°. LD₅₀ (rat, orl) 2250 mg/kg. Exp. teratogenic effects

Aldrich: W28780-6

Fluka: 78490

Sigma: P4514

>>Derivative: α -L-Rhamnopyranosyl ester

Synonym(s): Phenylacetyl α -L-rhamnopyranoside

Molecular Formula: C₁₄H₁₈O₆

Molecular Weight: 282.293

Accurate Mass: 282.11034

Percentage Composition: C 59.57%; H 6.43%; O 34.01%

Biological Source: Prod. by *Streptomyces* sp

Melting Point: Mp 85 dec.°

Optical Rotation: [α]_D²⁰ -52 (c, 1 in MeOH)

UV: [neutral] $\lambda_{\max}$ 206 (log ϵ 3.48); 258 (log ϵ 2.58) (MeOH)

>>Derivative: Me ester

Synonym(s): FEMA 2733

CAS Registry Number: 101-41-7

Molecular Formula: C₉H₁₀O₂

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Biological Source: Odoriferous constit. of many plants. Present in cocoa, coffee and strawberry

Use/Importance: Perfumery and flavouring ingredient

Physical Description: Liq. with sweet honey-like flavour

Boiling Point: Bp 215°. Bp₅₀ 131-132°

Density: d₁₆¹⁶ 1.063

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 2550 mg/kg

Aldrich: W27330-9

Fluka: 78540