>>**Entry Name: Phenylacetic acid**
ENTRY UNDER REVIEW
Synonym(s): Benzeneacetic acid, 9Cl. Phenylethanoic acid. α-Toluic acid. FEMA 2878

CAS Registry Number: 103-82-2
Related CAS Registry Numbers(s): 114-70-5

$PhCH_2COOH$

Molecular Formula: $C_8H_8O_2$
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 1*M* soln. in $CHCl_3$ for selective extraction separation of Cu and U ($CHCl_3$). 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 (H_2O)
Hazard & Toxicity: Fl. p. 102°. LD_{50} (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: $C_{14}H_{18}O_6$
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: $[\alpha]_D^{20}$ –52 (c, 1 in MeOH)
UV: [neutral] λ_{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: $C_9H_{10}O_2$
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°. Bp_{50} 131-132°
Density: d_{16}^{16} 1.063
Hazard & Toxicity: Skin irritant. LD_{50} (rat, orl) 2550 mg/kg

Aldrich: W27330-9
Fluka: 78540