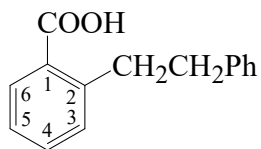




>>Entry Name: 2-(2-Phenylethyl)benzoic acid, 9CI

Synonym(s): 2-Phenethylbenzoic acid, 8CI. Bibenzyl-2-carboxylic acid



CAS Registry Number: 4890-85-1

Molecular Formula: C₁₅H₁₄O₂

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 132-133°

Boiling Point: Bp 259°

Aldrich: 15151-3

>>Derivative: Et ester

Molecular Formula: C₁₇H₁₈O₂

Molecular Weight: 254.328

Accurate Mass: 254.13068

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

Physical Description: Pale yellow oil

Boiling Point: Bp₁₈ 205°

>>Derivative: Chloride

Molecular Formula: C₁₅H₁₃ClO

Molecular Weight: 244.72

Accurate Mass: 244.065492

Percentage Composition: C 73.62%; H 5.35%; Cl 14.49%; O 6.54%

Physical Description: Cryst.

Melting Point: Mp 50-55°

>>Derivative: Amide

CAS Registry Number: 36795-31-0

Molecular Formula: C₁₅H₁₅NO

Molecular Weight: 225.29

Accurate Mass: 225.115364

Percentage Composition: C 79.97%; H 6.71%; N 6.22%; O 7.10%

Physical Description: Needles (propanol)

Melting Point: Mp 128°

>>Derivative: Nitrile

CAS Registry Number: 5505-00-0

Molecular Formula: C₁₅H₁₃N

Molecular Weight: 207.274

Accurate Mass: 207.104799

Percentage Composition: C 86.92%; H 6.32%; N 6.76%

Physical Description: Oil

Boiling Point: Bp₄ 168°

References: