



>>Entry Name: 5-Phenylpentanoic acid

Synonym(s): Benzenepentanoic acid, 9Cl. 5-Phenylvaleric acid

CAS Registry Number: 2270-20-4

PhCH2CH2CH2CH2COOH

Molecular Formula: C₁₁H₁₄O₂

Molecular Weight: 178.23

Accurate Mass: 178.09938

Percentage Composition: C 74.13%; H 7.92%; O 17.95%

Physical Description: Plates (H₂O), prisms (petrol)

Melting Point: Mp 58-59°

Boiling Point: Bp_{0.02} 113-114°

pKa Value: pK_{a1} 4.88 (20°)

Aldrich: P3760-2

Fluka: 79284

>>Derivative: Me ester

CAS Registry Number: 20620-59-1

Molecular Formula: C₁₂H₁₆O₂

Molecular Weight: 192.257

Accurate Mass: 192.11503

Percentage Composition: C 74.97%; H 8.39%; O 16.64%

Boiling Point: Bp₃₅ 173°

Rare Chemicals Library: S43134-6

>>Derivative: Amide

CAS Registry Number: 36603-28-8

Molecular Formula: C₁₁H₁₅NO

Molecular Weight: 177.246

Accurate Mass: 177.115364

Percentage Composition: C 74.54%; H 8.53%; N 7.90%; O 9.03%

Melting Point: Mp 109°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-4-phenylbutane

CAS Registry Number: 7726-45-6

Molecular Formula: C₁₁H₁₃N

Molecular Weight: 159.23

Accurate Mass: 159.104799

Percentage Composition: C 82.97%; H 8.23%; N 8.80%

Boiling Point: Bp₁₇ 157-161°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 988C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 141B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1318B, (*ir*)

Walter, M. *et al.*, *Helv. Chim. Acta*, 1961, **44**, 1546, (*synth*)

ShklyaeV, V.S. *et al.*, *CA*, 1968, **68**, 86917, (*synth*)

Baer, T.A. *et al.*, *Tet. Lett.*, 1976, 4697, (*synth*)