



>>Entry Name: 6-Phenylhexanoic acid, 8Cl

Synonym(s): 6-Phenylcaproic acid

CAS Registry Number: 5581-75-9

Ph(CH₂)₅COOH

Molecular Formula: C₁₂H₁₆O₂

Molecular Weight: 192.257

Accurate Mass: 192.11503

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

Physical Description: Cryst. or liq.

Melting Point: Mp 22-24°

Boiling Point: Bp₁₁ 186-188°

Aldrich: 33360-3

>>Derivative: Et ester

CAS Registry Number: 52692-51-0

Molecular Formula: C₁₄H₂₀O₂

Molecular Weight: 220.311

Accurate Mass: 220.14633

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Boiling Point: Bp₁₂ 162-164°

>>Derivative: Chloride

CAS Registry Number: 21389-46-8

Molecular Formula: C₁₂H₁₅ClO

Molecular Weight: 210.703

Accurate Mass: 210.081142

Percentage Composition: C 68.41%; H 7.18%; Cl 16.83%; O 7.59%

Boiling Point: Bp₁₁ 151-152°

>>Derivative: Amide

CAS Registry Number: 31274-14-3

Molecular Formula: C₁₂H₁₇NO

Molecular Weight: 191.272

Accurate Mass: 191.131014

Percentage Composition: C 75.35%; H 8.96%; N 7.32%; O 8.36%

Melting Point: Mp 90°

>>Derivative: Nitrile

CAS Registry Number: 17777-31-0

Molecular Formula: C₁₂H₁₅N

Molecular Weight: 173.257

Accurate Mass: 173.120449

Percentage Composition: C 83.19%; H 8.73%; N 8.08%

Boiling Point: Bp₁₃ 161-163°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 989B, (*nmr*)

v. Braun, J., *Ber.*, 1911, **44**, 2867, (*synth*)

Staudinger, H. *et al.*, *Ber.*, 1923, **56**, 711, (*synth*)

Huisgen, R. *et al.*, *Annalen*, 1954, **586**, 52, (*synth*)