



>>Entry Name: 5-Chloropentanoic acid, 9Cl

CAS Registry Number: 1119-46-6

ClCH₂CH₂CH₂CH₂COOH

Molecular Formula: C₅H₉ClO₂

Molecular Weight: 136.578

Accurate Mass: 136.029107

Percentage Composition: C 43.97%; H 6.64%; Cl 25.96%; O 23.43%

Physical Description: Cryst.

Melting Point: Mp 18°

Boiling Point: Bp 230°. Bp₁₁ 128-131°

Density: d₄²⁵ 1.34

Other Data: Acc. to one reference partly dec. on dist. at 12 mm, but this may have been an impure sample

Aldrich: C7290-0

Fluka: 26580

>>Derivative: Me ester

CAS Registry Number: 14273-86-0

Molecular Formula: C₆H₁₁ClO₂

Molecular Weight: 150.604

Accurate Mass: 150.044757

Percentage Composition: C 47.85%; H 7.36%; Cl 23.54%; O 21.25%

Boiling Point: Bp₁₈ 89-92°. Bp₁₀ 77°

Aldrich: 13598-4

>>Derivative: Chloride

CAS Registry Number: 1575-61-7

Molecular Formula: C₅H₈Cl₂O

Molecular Weight: 155.023

Accurate Mass: 153.995219

Percentage Composition: C 38.74%; H 5.20%; Cl 45.74%; O 10.32%

Refractive Index: n_D²⁰ 1.4640

Aldrich: 12524-5

Fluka: 26585

>>Derivative: Nitrile

Synonym(s): 1-Chloro-4-cyanobutane

CAS Registry Number: 6280-87-1

Molecular Formula: C₅H₈ClN

Molecular Weight: 117.578

Accurate Mass: 117.034526

Percentage Composition: C 51.08%; H 6.86%; Cl 30.15%; N 11.91%

Refractive Index: n_D²⁰ 1.4460

Aldrich: C7300-1

Fluka: 26590

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 801A; 1021B; 1370A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 512D; 728D; 851A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 592D; 711A; 809C, (*ir*)

U.S. Pat., 1946, 2 398 430; *CA*, **40**, 3768, (*synth*)

Kuhnle, J.A. *et al.*, *Chem. Comm.*, 1972, 287, (*synth*)