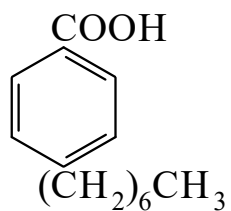




>>Entry Name: 4-Heptylbenzoic acid, 9CI



CAS Registry Number: 38350-87-7

Molecular Formula: C₁₄H₂₀O₂

Molecular Weight: 220.311

Accurate Mass: 220.14633

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

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 101.5°

Aldrich: 23064-2

Fluka: 51970

>>Derivative: 4-Cyanophenyl ester

CAS Registry Number: 38690-76-5

Molecular Formula: C₂₁H₂₃NO₂

Molecular Weight: 321.418

Accurate Mass: 321.172879

Percentage Composition: C 78.47%; H 7.21%; N 4.36%; O 9.96%

Use/Importance: Component of r.t. nematic liq. cryst. mixts.

Melting Point: Mp 40°. Mp 44-45°

Aldrich: 18031-9

Rare Chemicals Library: S26645-0

>>Derivative: Chloride

CAS Registry Number: 50606-96-7

Molecular Formula: C₁₄H₁₉ClO

Molecular Weight: 238.756

Accurate Mass: 238.112442

Percentage Composition: C 70.43%; H 8.02%; Cl 14.85%; O 6.70%

Physical Description: Liq.

Boiling Point: Bp₅ 160°

Refractive Index: n_D²⁰ 1.5218

Aldrich: 22205-4

References:

Zaki, A. *et al.*, *J.C.S.*, 1942, 307-308, (*synth*)

Ignasiak, S. *et al.*, *Mol. Cryst. Liq. Cryst.*, 1975, **30**, 125; *CA*, **83**, 146621p, (*4-cyanophenyl ester*)

Newbert, M.E. *et al.*, *Org. Synth.*, 1983, **61**, 8, (*chloride*)

Nakai, H. *et al.*, *J. Med. Chem.*, 1988, **31**, 84-91, (*ms, synth*)

Blake, A.J. *et al.*, *Acta Cryst. C*, 1995, **51**, 2666, (*cryst struct*)