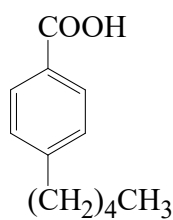




>>Entry Name: 4-Pentylbenzoic acid, 9Cl, 8Cl



CAS Registry Number: 26311-45-5

Related CAS Registry Numbers(s): 44763-65-7 51128-24-6 53132-06-2 73329-05-2

Molecular Formula: C₁₂H₁₆O₂

Molecular Weight: 192.257

Accurate Mass: 192.11503

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

Use/Importance: Exhibits liq. cryst. props.

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 86-88°. Mp 126-127°

Other Data: Melts to form liq. cryst. mesomorph which changes sharply to isotropic liq. at 126-127°

>>Derivative: Me ester

CAS Registry Number: 26311-44-4

Molecular Formula: C₁₃H₁₈O₂

Molecular Weight: 206.284

Accurate Mass: 206.13068

Percentage Composition: C 75.69%; H 8.79%; O 15.51%

Use/Importance: Exhibits liq. cryst. props.

Boiling Point: Bp₂ 119-121°

Refractive Index: n_D²⁰ 1.5010

>>Derivative: Et ester

CAS Registry Number: 75681-67-3

Molecular Formula: C₁₄H₂₀O₂

Molecular Weight: 220.311

Accurate Mass: 220.14633

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

Physical Description: Liq.

>>Derivative: 4-Cyanophenyl ester

CAS Registry Number: 49763-64-6

Molecular Formula: C₁₉H₁₉NO₂

Molecular Weight: 293.365

Accurate Mass: 293.141579

Percentage Composition: C 77.79%; H 6.53%; N 4.77%; O 10.91%

Use/Importance: Exhibits liq. cryst. props.

Melting Point: Mp 64.5° (55.5°)

Other Data: Many other 4-substituted phenyl esters reported with potential liq. cryst. applications

>>Derivative: Chloride

CAS Registry Number: 49763-65-7

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: Bp₁₀ 144-145°

>>Derivative: Amide

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%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 147-148°