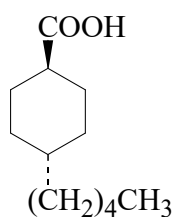




>>Entry Name: 4-Pentylcyclohexanecarboxylic acid, 9CI



CAS Registry Number: 38792-89-1

Extra CAS Registry Numbers(s): 67589-84-8

Molecular Formula: C₁₂H₂₂O₂

Molecular Weight: 198.305

Accurate Mass: 198.16198

Percentage Composition: C 72.68%; H 11.18%; O 16.14%

>>**Variant:** (1*RS*,4*RS*)-form

Synonym(s): *trans*-form

CAS Registry Number: 38289-29-1

Molecular Formula: C₁₂H₂₂O₂

Molecular Weight: 198.305

Accurate Mass: 198.16198

Percentage Composition: C 72.68%; H 11.18%; O 16.14%

Use/Importance: Intermed. for liq. crystal compounds

Physical Description: Cryst. (petrol)

Melting Point: Mp 53.7°

Other Data: Nematic phase at 101°

>>**Derivative:** 4-Methoxyphenyl ester

CAS Registry Number: 67589-52-0

Molecular Formula: C₁₉H₂₈O₃

Molecular Weight: 304.428

Accurate Mass: 304.203845

Percentage Composition: C 74.96%; H 9.27%; O 15.77%

Use/Importance: Nematic liq. crystal

Melting Point: Mp 36°

Other Data: Nematic phase at 63.5°

>>**Derivative:** Nitrile

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

Molecular Formula: C₁₂H₂₁N

Molecular Weight: 179.305

Accurate Mass: 179.167399

Percentage Composition: C 80.38%; H 11.80%; N 7.81%

Use/Importance: Nematic liq. crystal

Melting Point: Mp 30-35°

References:

Schubert, H. *et al.*, *Z. Chem.*, 1972, **12**, 219-220, (*synth, props*)

Deutscher, H.J. *et al.*, *J. Prakt. Chem.*, 1978, **320**, 191-205, (*4-methoxyphenyl ester, synth, props*)

Gray, G.W. *et al.*, *Mol. Cryst. Liq. Cryst.*, 1979, **53**, 147-166, (*synth, props*)