



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

CAS Registry Number: 2438-05-3

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Use/Importance: Used in liq. cryst.

Physical Description: Prisms or leaflets (H₂O)

Melting Point: Mp 141°

Other Data: Steam-volatile

Aldrich: 33297-6

>>Derivative: Chloride

CAS Registry Number: 52710-27-7

Molecular Formula: C₁₀H₁₁ClO

Molecular Weight: 182.649

Accurate Mass: 182.049842

Percentage Composition: C 65.76%; H 6.07%; Cl 19.41%; O 8.76%

Boiling Point: Bp₂₀ 135-136°

Density: d 1.1

Refractive Index: n_D²⁰ 1.5394

Aldrich: 24945-9

>>Derivative: Nitrile

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

CAS Registry Number: 60484-66-4

Molecular Formula: C₁₀H₁₁N

Molecular Weight: 145.204

Accurate Mass: 145.089149

Percentage Composition: C 82.72%; H 7.64%; N 9.65%

Boiling Point: Bp 227°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1073B, (*nmr*)

Widman, O., *Ber.*, 1889, **22**, 2278, (*synth*)

Buechi, J. *et al.*, *Arzneim.-Forsch.*, 1972, **22**, 1071, (*use*)

Schubert, H. *et al.*, *Z. Chem.*, 1972, **12**, 219, (*use*)

Deutscher, H.J. *et al.*, *J. Prakt. Chem.*, 1978, **320**, 191, (*use*)