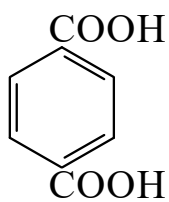




>>Entry Name: 1,4-Benzenedicarboxylic acid, 9CI

Synonym(s): Terephthalic acid, 8CI. *p*-Phthalic acid



CAS Registry Number: 100-21-0

Related CAS Registry Numbers(s): 3856-02-8 10028-70-3 60088-54-2

Molecular Formula: C₈H₆O₄

Molecular Weight: 166.133

Accurate Mass: 166.02661

Percentage Composition: C 57.84%; H 3.64%; O 38.52%

Biological Source: Isol. from pods of *Cassia roxburghii* and *Tephrosia hamiltonii*. Manuf. by oxidn. of *p*-xylene

Use/Importance: Acid and derivs. are important feedstocks for polymerisations, used for making polyester resins, e.g. terylene, for fibres and films. Important industrial chemical, 24th in order of volume for USA in 1994 (production 4.32 million tons/year)

Physical Description: Cryst.

Boiling Point: Subl. *ca.* ° 300

Solubility: Prac. insol. H₂O, CHCl₃, Et₂O, AcOH; mod. sol. hot EtOH; sol. Py, DMSO, DMF

pKa Value: p*K*_{a1} 3.54; p*K*_{a2} 4.34 (25°)

Hazard & Toxicity: Eye irritant. Low acute mammalian tox.

Aldrich: 18536-1

Fluka: 86420

Sigma: T7774

>>Derivative: Mono-Me ester

CAS Registry Number: 1679-64-7

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Physical Description: Needles (H₂O)

Boiling Point: Subl. *ca.* ° 230

Aldrich: 32838-3

Fluka: 86448

>>Derivative: Di-Me ester

Synonym(s): Dimethyl terephthalate

CAS Registry Number: 120-61-6

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Biological Source: Isol. from flowers of *Cytisus scoparius*

Use/Importance: Leading intermed for industrial prodn. of polyesters

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 141-142°

Boiling Point: Bp 284°

Solubility: Sl. sol. H₂O, EtOH; sol. Et₂O, CHCl₃

Other Data: Sublimes. Steam-volatile

Hazard & Toxicity: Fl. p. 153° (oc), autoignition temp. 518°. Eye irritant

Aldrich: 18512-4

Fluka: 86440

Rare Chemicals Library: S44253-4