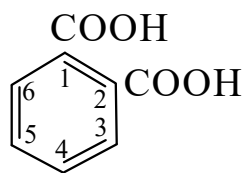




>>Entry Name: **1,2-Benzenedicarboxylic acid**, 9CI

Synonym(s): Phthalic acid, 8CI. Alizarinic acid. **Naphthalinic acid**‡. Phthalinic acid



CAS Registry Number: 88-99-3

Related CAS Registry Numbers(s): 131-15-7 523-24-0 3198-29-6 4409-98-7 10197-71-4 15968-01-1 28553-12-0 79723-02-7 102904-15-4

Molecular Formula: C₈H₆O₄

Molecular Weight: 166.133

Accurate Mass: 166.02661

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

Source/Synthesis: Obt. industrially by oxidn. of 1,2-Dimethylbenzene [BLQ00-J](#) and Naphthalene [BNK69-U](#)

Biological Source: Found in *Gibberella fujikuroi*

Use/Importance: Esters are important plasticisers. Used for gravimetric detn. of Pb. Used as aq. soln. in buffer solns.; alkalimetric standard (as K salt)

Physical Description: Plates (H₂O)

Melting Point: Mp 210 dec.°. Mp 234°

Solubility: Sol. hot H₂O, alkalis; mod. sol. H₂O, EtOH; spar. sol. Et₂O

pKa Value: pK_{a1} 2.95; pK_{a2} 5.41 (25°,H₂O)

Other Data: Forms anhydride at Mp. Frequent reports of the isol. of phthalate esters as nat. prods. are in prob. all cases erroneous because of their ubiquitous presence in solvs., laboratory plastics, etc. as plasticisers

Hazard & Toxicity: Fl. p. 168°. Violent reaction on heating with NaNO₂. Skin and mucous membrane irritant. Low acute mammalian toxicity

Aldrich: 40291-5

Fluka: 80011

Rare Chemicals Library: S3912-9

Sigma: P2944

Supelco: R30-1285

>>Derivative: Mono-K salt

CAS Registry Number: 877-24-7

Melting Point: Mp 295-300 dec.°

Aldrich: 17992-2

Fluka: 60360

Sigma: P3792

>>Derivative: Mono-Me ester

Synonym(s): Monomethyl phthalate

CAS Registry Number: 4376-18-5

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 (C₆H₆)

Melting Point: Mp 85°

Aldrich: 31764-0

Fluka: 80160

Rare Chemicals Library: S38821-1

>>Derivative: Di-Me ester

Synonym(s): Dimethyl phthalate, BSI, ISO. DMP

CAS Registry Number: 131-11-3

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Use/Importance: Insect repellent. Plasticiser for cellulose acetate and nitrocellulose

Physical Description: Liq.

Melting Point: Mp 0°

Boiling Point: Bp 282.4°. Bp₂ 116-116.5°

Solubility: Insol. H₂O; misc. EtOH, Et₂O

Density: d₂₅²⁵ 1.189

Refractive Index: n