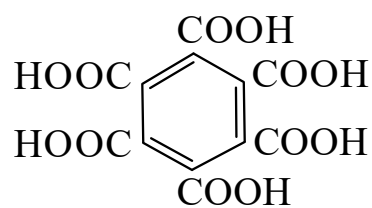




>>Entry Name: Benzenehexacarboxylic acid, 9CI

Synonym(s): Mellitic acid



CAS Registry Number: 517-60-2

Molecular Formula: C₁₂H₆O₁₂

Molecular Weight: 342.172

Accurate Mass: 341.98593

Percentage Composition: C 42.12%; H 1.77%; O 56.11%

Biological Source: Found in many coal and wood products. The Al salt is known as the mineral honeystone

Physical Description: Needles (EtOH)

Melting Point: Mp 286-288 dec.°

pKa Value: pK_{a1} 0.8; pK_{a2} 2.26; pK_{a3} 3.52; pK_{a4} 5.15; pK_{a5} 6.52; pK_{a6} 7.71 (25°)

Aldrich: M270-5

Fluka: 63652

Rare Chemicals Library: S44223-2

>>Derivative: Tetra-Me ester

Molecular Formula: C₁₆H₁₄O₁₂

Molecular Weight: 398.279

Accurate Mass: 398.04853

Percentage Composition: C 48.25%; H 3.54%; O 48.21%

Melting Point: Mp 70-110°

>>Derivative: Penta-Me ester

Molecular Formula: C₁₇H₁₆O₁₂

Molecular Weight: 412.306

Accurate Mass: 412.06418

Percentage Composition: C 49.52%; H 3.91%; O 46.57%

Physical Description: Needles (H₂O)

Melting Point: Mp 141-144°

>>Derivative: Hexa-Me ester

CAS Registry Number: 6237-59-8

Molecular Formula: C₁₈H₁₈O₁₂

Molecular Weight: 426.333

Accurate Mass: 426.07983

Percentage Composition: C 50.71%; H 4.26%; O 45.03%

Melting Point: Mp 72-73°

>>Derivative: Hexaisopropyl ester

CAS Registry Number: 91621-00-0

Molecular Formula: C₃₀H₄₂O₁₂

Molecular Weight: 594.655

Accurate Mass: 594.26763

Percentage Composition: C 60.59%; H 7.12%; O 32.29%

Physical Description: Cryst.

Melting Point: Mp 122-123°