



>>Entry Name: 2,4-Hexadienedioic acid, 9CI

Synonym(s): 1,3-Butadiene-1,4-dicarboxylic acid. Muconic acid

CAS Registry Number: 505-70-4

HOOCCH=CHCH=CHCOOH

Molecular Formula: C<sub>6</sub>H<sub>6</sub>O<sub>4</sub>

Molecular Weight: 142.111

Accurate Mass: 142.02661

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

>>Variant: (E,E)-form

CAS Registry Number: 3588-17-8

Molecular Formula: C<sub>6</sub>H<sub>6</sub>O<sub>4</sub>

Molecular Weight: 142.111

Accurate Mass: 142.02661

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

Physical Description: Prisms (H<sub>2</sub>O)

Melting Point: Mp 301°

Other Data: Undergoes radical polym.

Aldrich: M9000-3

Fluka: 70000

Sigma: M6262

>>Derivative: Di-Me ester

CAS Registry Number: 1119-43-3

Molecular Formula: C<sub>8</sub>H<sub>10</sub>O<sub>4</sub>

Molecular Weight: 170.165

Accurate Mass: 170.05791

Percentage Composition: C 56.47%; H 5.92%; O 37.61%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 159°

>>Derivative: Di-Et ester

CAS Registry Number: 6032-74-2

Molecular Formula: C<sub>10</sub>H<sub>14</sub>O<sub>4</sub>

Molecular Weight: 198.218

Accurate Mass: 198.08921

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

Physical Description: Cryst. (hexane)

Melting Point: Mp 60-61°

Other Data: Undergoes radical and anionic polym. Q/e values for copolym., Q 1.94, e +1.39

>>Derivative: Diamide

CAS Registry Number: 5867-86-7

Molecular Formula: C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 140.141

Accurate Mass: 140.058578

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Plates (H<sub>2</sub>O)

Melting Point: Mp 294-295 dec.°

>>Variant: (E,Z)-form

CAS Registry Number: 1119-73-9

Molecular Formula: C<sub>6</sub>H<sub>6</sub>O<sub>4</sub>

Molecular Weight: 142.111

Accurate Mass: 142.02661

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

Physical Description: Needles (H<sub>2</sub>O)

Melting Point: Mp 190-191°