



>>Entry Name: 3-Hexenedioic acid, 9CI

Synonym(s): 2-Butene-1,4-dicarboxylic acid. β -Hydromuconic acid

CAS Registry Number: 4436-74-2

HOOCCH₂CH=CHCH₂COOH

Molecular Formula: C₆H₈O₄

Molecular Weight: 144.127

Accurate Mass: 144.04226

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Aldrich: H1785-6

Fluka: 53020

Sigma: D2635

>>Variant: (*E*)-form

Molecular Formula: C₆H₈O₄

Molecular Weight: 144.127

Accurate Mass: 144.04226

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Physical Description: Prisms (H₂O)

Melting Point: Mp 197-198°

pKa Value: p*K*_a 3.99 (25°)

>>Derivative: Di-Me ester

CAS Registry Number: 25126-93-6

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Melting Point: Mp 5°

Boiling Point: Bp₁₄ 125°

>>Derivative: Dichloride

CAS Registry Number: 58823-57-7

Molecular Formula: C₆H₆Cl₂O₂

Molecular Weight: 181.018

Accurate Mass: 179.974484

Percentage Composition: C 39.81%; H 3.34%; Cl 39.17%; O 17.68%

Use/Importance: Monomer used in synth. of polyesters and polyamides

>>Derivative: Diamide

Molecular Formula: C₆H₁₀N₂O₂

Molecular Weight: 142.157

Accurate Mass: 142.074228

Percentage Composition: C 50.69%; H 7.09%; N 19.71%; O 22.51%

Physical Description: Needles

Melting Point: Mp 210 dec.°

>>Derivative: Dinitrile

Synonym(s): 1,4-Dicyano-2-butene

CAS Registry Number: 1119-85-3

Melting Point: Mp 76°

Aldrich: D7720-6