



>>Entry Name: 1-Acetoxybutadiene

Synonym(s): 1,3-Butadien-1-ol acetate, 9Cl, 8Cl

CAS Registry Number: 1515-76-0



Molecular Formula: $\text{C}_6\text{H}_8\text{O}_2$

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Use/Importance: Diels-Alder diene

Hazard & Toxicity: Skin irritant. LD₅₀ (rbt, skn) 420 mg/kg. LD₅₀ (rat, orl) 710 mg/kg

Aldrich: 22086-8

Fluka: 824

>>Variant: (E)-form

CAS Registry Number: 35694-20-3

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_2$

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Melting Point: Mp -55--60° (approx.)

Boiling Point: Bp₃₂ 55-55.3°

>>Variant: (Z)-form

CAS Registry Number: 35694-19-0

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_2$

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Melting Point: Mp -78°

Boiling Point: Bp₃₂ 53.2-54.2°

References: