



>>Entry Name: 1-Acetoxybutadiene

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

CAS Registry Number: 1515-76-0

$\text{H}_2\text{C}=\text{CHCH}=\text{CHOAc}$

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:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 967B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 636D, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 668A, (ir)

Hagemeyer, H.J. *et al.*, *Ind. Eng. Chem.*, 1949, **41**, 2920, (synth)

Georgieff, K.K. *et al.*, *Can. J. Chem.*, 1960, **38**, 1070, (synth, ir, uv)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 7; **3**, 104; **9**, 56, (use)

Rautenstrauch, V., *Helv. Chim. Acta*, 1972, **55**, 594, (synth, pmr, ir)

Gressier, J.-C. *et al.*, *Makromol. Chem.*, 1974, **176**, 341, (synth, ir, pmr)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, ABM250