



>>Entry Name: Isopropyl acetate, 8CI

ENTRY UNDER REVIEW

Synonym(s): 1-Methylethyl acetate, 9CI. FEMA 2926

CAS Registry Number: 108-21-4

$\text{H}_3\text{CCOOCH}(\text{CH}_3)_2$

Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}_2$

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Biological Source: Isol. from ripening melons and grape oil. Also present in cheddar cheese, soybean, beer, red wine, white wine and plum brandy. Flavouring agent

Use/Importance: Solvent

Physical Description: Colourless liq. with sweet apple-like flavour on dil

Boiling Point: $\text{Bp}_{734.299988}$ 88-91°

Solubility: Spar. sol. H_2O , misc. EtOH, Et_2O

Hazard & Toxicity: Highly flammable, fl. p. 2/4°, autoignition temp. 460°. Eye and respiratory tract irritant. High vapour conc. narcotic. LD_{50} (rat, orl) 3000 mg/kg, OES: short-term 200 ppm

Aldrich: 18547-7

Fluka: 45970

References:

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Minato, H. *et al.*, *Chem. Lett.*, 1977, 413, (synth)

Benoit, F.M. *et al.*, *Org. Mass Spectrom.*, 1977, **12**, 78, (ms)

Yabumoto, K. *et al.*, *Food Chem.*, 1978, **3**, 7, (isol)

Couperos, P.A. *et al.*, *Org. Magn. Reson.*, 1978, **11**, 590, (cmr)

Ergorov, I.A. *et al.*, *Prikl. Biokhim. Mikrobiol.*, 1978, **14**, 135, (isol)

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