



>>Entry Name: Acetic acid, 9CI, USAN

ENTRY UNDER REVIEW

Synonym(s): Ethanoic acid. Methanecarboxylic acid. FEMA 2006

CAS Registry Number: 64-19-7

Related CAS Registry Numbers(s): 71-50-1 758-12-3 1186-52-3

H_3CCOOH

Molecular Formula: $\text{C}_2\text{H}_4\text{O}_2$

Molecular Weight: 60.052

Accurate Mass: 60.02113

Percentage Composition: C 40.00%; H 6.71%; O 53.28%

General Statement: Many esters (acetates) are known apart from those cross-referenced below. Most are recorded as Ac derivs. of the relevant alcohols. Salts are included in the *Dictionary of Inorganic Compounds*

Source/Synthesis: Metabolic intermed., bacterial oxidn. prod. of Ethanol [BGT97-X](#), known since ancient times as dil. soln. (vinegar). Major constituent of human and present in other primate vaginal secretions. Manuf. industrially by oxidn. of naphtha, Acetaldehyde [DFR74-T](#) or Butane [BGV93-D](#) or (since 1970) by the Monsanto process involving methanol carbonylation over an Rh or Ir catalyst, which now (1996) accounts for =60% of world production

Use/Importance: Industrial and lab. solv., used for preserving foods. Major petrochemical used in manuf. of cellulose acetate, vinyl acetate and other acetate esters and also 1,4-Benzenedicarboxylic acid [DSP80-V](#). Solv. in prodn. of 1,4-Benzenedicarboxylic acid [DSP80-V](#). Used as component of buffers; as masking agent for Al, La, Cr(III), Pb, Th; lead(IV) acetate used for photometric detn. of H_2O (λ_{max} 400 nm) in pure solvs. 34th in order of volume for USA in 1994 (production 1.91 million tons/year). Pharmaceutical aid

Physical Description: Liq. or cryst. with pungent vinegar odour

Melting Point: Mp 16.7°

Boiling Point: Bp₃₁ 30°. Bp 118°

Solubility: Misc. H_2O , EtOH, Et₂O; sol. most org. solvs.; insol. CS₂

Density: d_4^{20} 1.049

pKa Value: pK_a 4.76 (20°, H_2O) pK_a 4.78 (25°)

Refractive Index: n_D^{20} 1.3718 n_D^{25} 1.3696

Other Data: Vp 15.5 mmHg (25°). Molecular Fp depression 39, molecular Bp elevation 29.9. Dissolves elemental S

Hazard & Toxicity: Flammable, fl. p. 39°, autoignition temp. 463°. Reacts violently with some oxidants. Corrosive and irritating to all tissues. Exp. reprod. effects. OES: long-term 10 ppm; short-term 15 ppm

Aldrich: 31859-0

Fluka: 45730

Sigma: J6294

Supelco: 4-6928

>>Derivative: Me ester

see Methyl acetate, [DCK28-E](#)

>>Derivative: Et ester

see Ethyl acetate, [CTW40-O](#)

>>Derivative: Vinyl ester

see Ethenol, [CTS73-G](#)

>>Derivative: Isopropyl ester

see Isopropyl acetate, [CVH43-I](#)

>>Derivative: Benzyl ester

see Benzyl acetate, [CWL26-G](#)

>>Derivative: Ph ester

see Phenyl acetate, [MTL83-G](#)

>>Derivative: Fluoride

see Acetyl fluoride, [DFT06-K](#)

>>Derivative: Chloride