



>>Entry Name: Acetaldehyde, 9CI

Synonym(s): Ethanal

CAS Registry Number: 75-07-0

Related CAS Registry Numbers(s): 631-59-4 1019-57-4 1632-89-9 25473-09-0

H₃CCHO

Molecular Formula: C₂H₄O

Molecular Weight: 44.053

Accurate Mass: 44.026215

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

General Statement: For enol form see Ethenol [CTS73-G](#)

Biological Source: Manuf. by hydration of Acetylene [DFS79-D](#), oxidn. of Ethanol [BGT97-X](#) etc. Intermed. in respiration. Toxic intermed. in ethanol metab. in humans.

Widely distributed in essential oils and other plant products

Use/Importance: Chemical intermed. used in manuf. of 2,2-Bis(hydroxymethyl)-1,3-propanediol [DDT03-T](#), Peracetic acid [DDW29-U](#) acid, pyridines. Declining as source of Acetic acid [DFR91-W](#). Various acetals are used in perfumery

Physical Description: Liq. with a pungent fruity odour

Melting Point: Mp -121°

Boiling Point: Bp 21°

Solubility: Misc. H₂O, org. solvs.

Density: d₄²⁰ 0.778

pKa Value: pK_{a1} 13.57 (25°,hydrate)

Refractive Index: n_D²⁰ 1.3316

Other Data: Vp 900 mmHg (25°). Readily polymerises. At low temps., cationic or anionic polym. gives poly(acetaldehyde). At higher temps. cyclisation to the cyclic trimer, paraldehyde, and the cyclic tetramer, metaldehyde, occurs. The trimer may be formed on standing; redistn. regenerates acetaldehyde. Ceiling temp. for polym. T_c-39° (pure liq.). Crit. point 181.5°/63.2 atm.

Hazard & Toxicity: Extremely flammable, fl. p.-38°, autoignition temp. 140/175°. Reacts violently with a range of organic and inorganic substances. Possible human carcinogen. Skin and severe eye irritant. A systemic irritant by inhalation. High vapour conc. narcotic preceded by sore throat and headache. Exp. carcinogen and teratogen. Exp. reprod. effects

Aldrich: 40278-8

Fluka: 71

Sigma: A5076

Supelco: S48-2003

>>Derivative: Oxime

Synonym(s): Acetaldoxime. Aldoxime. Ethylidenehydroxylamine

CAS Registry Number: 107-29-9

Molecular Formula: C₂H₅NO

Molecular Weight: 59.068

Accurate Mass: 59.037114

Percentage Composition: C 40.67%; H 8.53%; N 23.71%; O 27.09%

Use/Importance: Colorimetric reagent for Co, Cu, Ni

Physical Description: Needles

Melting Point: Mp 47°

Boiling Point: Bp 115°

Solubility: Sol. H₂O, CHCl₃, EtOH, Et₂O

Refractive Index: n_D²² 1.4258 (Z-form)

Other Data: Mp refers to (E)-form which is the crystalline isomer. (Z)-form is liq.

Hazard & Toxicity: Highly flammable, fl. p. <22°

Aldrich: 40776-3

Fluka: 150

Sigma: A0375

>>Derivative: Semicarbazone

CAS Registry Number: 591-86-6

Molecular Formula: C₃H₇N₃O

Molecular Weight: 101.108

Accurate Mass: 101.058912

Percentage Composition: C 35.64%; H 6.98%; N 41.56%; O 15.82%

Physical Description: Needles (H₂O or EtOH)

Melting Point: Mp 163°