



>>>**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

H<sub>3</sub>CCHO

**Molecular Formula:** C<sub>2</sub>H<sub>4</sub>O

**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. H<sub>2</sub>O, org. solvs.

**Density:** d<sub>4</sub><sup>20</sup> 0.778

**pKa Value:** pK<sub>a1</sub> 13.57 (25°,hydrate)

**Refractive Index:** n<sub>D</sub><sup>20</sup> 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<sub>c</sub>-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:** C<sub>2</sub>H<sub>5</sub>NO

**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. H<sub>2</sub>O, CHCl<sub>3</sub>, EtOH, Et<sub>2</sub>O

**Refractive Index:** n<sub>D</sub><sup>22</sup> 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:** C<sub>3</sub>H<sub>7</sub>N<sub>3</sub>O

**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 (H<sub>2</sub>O or EtOH)

**Melting Point:** Mp 163°