



>>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_3CCHO

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

Molecular Weight: 44.053

Accurate Mass: 44.026215

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

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_2O , org. solvs.

Density: d_4^{20} 0.778

pKa Value: $\text{p}K_{\text{a}1}$ 13.57 (25° , hydrate)

Refractive Index: n_D^{20} 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 $181.5^\circ/63.2$ atm.

Hazard & Toxicity: Extremely flammable, fl. p. -38° , autoignition temp. $140/175^\circ$. 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