>>**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: C_2H_4O
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: pK_{a1} 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°/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