>>**Entry Name: Acetaldehyde,** 9Cl
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%
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_2O, org. solvs.
Density: $d_4^{2\text{C}}$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

>>**Derivative:** Oxime
Synonym(s): Acetaldoxime. Aldoxime. Ethylidenehydroxylamine

CAS Registry Number: 107-29-9

Molecular Formula: C_2H_5NO
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_2O, $CHCl_3$, EtOH, Et_2O
Refractive Index: n_D^{22} 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: $C_3H_7N_3O$
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_2O or EtOH)
Melting Point: Mp 163°