



>>Entry Name: 2-Propenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): Acraldehyde. Acrolein, BSI, WSSA. Acrylaldehyde. Formylethylene. Aqualin. Magnacide H

CAS Registry Number: 107-02-8

$\text{H}_2\text{C}=\text{CHCHO}$

Molecular Formula: $\text{C}_3\text{H}_4\text{O}$

Molecular Weight: 56.064

Accurate Mass: 56.026215

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Biological Source: Present in fruit aromas, black tea and prod. by microorganisms, e.g. *Clostridium perfringens*. Manuf. by catalytic oxidation of 1-Propene [BGX51-Z](#)

Use/Importance: Synthetic reagent. used in manuf. of Methionine [HJR27-B](#), Glycerol [BGV25-K](#) and Pentanedial [BGW32-P](#). Aquatic herbicide and algicide used in water treatment. Undergoes radical and anionic homopolym. and copolym. with vinylic and acrylic comonomers. Q/e values for copolym., Q 0.80, e +1.31

Physical Description: Strongly lachrymatory liq.

Melting Point: Mp -87°

Boiling Point: Bp 52°

Solubility: V. sol. H_2O ; sol. EtOH, Et_2O , Me_2CO

Density: d_4^{20} 0.841

Refractive Index: n_D^{20} 1.3998

Other Data: Vp 220 mmHg (20°). Unstable, polymerises to a white translucent solid Disacryl. Hydroquinone is used as a stabiliser to prevent autoxidn. and polym.

Hazard & Toxicity: Highly flammable, fl. p. -26° , autoignition temp. $220/235^\circ$. Can undergo violent acid- and base-catalysed polym. Irritating to all tissues. Vesicant. Inhalation may cause pulmonary oedema. Potent lachrymator. OES: long-term 0.1 ppm; short-term 0.3 ppm

Aldrich: 11022-1

Fluka: 1680

Sigma: A7199

Supelco: 4-8501

>>Derivative: Trimer

Synonym(s): 2,4,6-Triethenyl-1,3,5-trioxane, 9CI. 2,4,6-Trivinyl-s-trioxane, 8CI. Metacrolein

CAS Registry Number: 588-01-2

Molecular Formula: $\text{C}_9\text{H}_{12}\text{O}_3$

Molecular Weight: 168.192

Accurate Mass: 168.078645

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Physical Description: Plates (EtOH)

Melting Point: Mp 50°

Solubility: Sol. EtOH, Et_2O

>>Derivative: Oxime

CAS Registry Number: 5314-33-0

Molecular Formula: $\text{C}_3\text{H}_5\text{NO}$

Molecular Weight: 71.079

Accurate Mass: 71.037114

Percentage Composition: C 50.69%; H 7.09%; N 19.71%; O 22.51%

Boiling Point: Bp₉ 35°

>>Derivative: Dimethylhydrazone

CAS Registry Number: 25368-52-9

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2$

Molecular Weight: 98.147

Accurate Mass: 98.084398

Percentage Composition: C 61.19%; H 10.27%; N 28.54%

Physical Description: Liq.

Boiling Point: Bp₁₀₀ 80°