



>>Entry Name: Ethenol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Vinyl alcohol

CAS Registry Number: 557-75-5

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

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%

General Statement: The enol tautomer of Acetaldehyde [DFR74-T](#), not known in the free state. Keto/enol equilib. = 3×10^{-7} at 25°

Use/Importance: Polymers of the alcohol and its esters are used in synthetic resins. The polymer, polyvinyl alcohol, is obt. indirectly (see below)

>>Derivative: Ac

Synonym(s): Ethenyl acetate, 9CI. Vinyl acetate

CAS Registry Number: 108-05-4

Molecular Formula: $\text{C}_4\text{H}_6\text{O}_2$

Molecular Weight: 86.09

Accurate Mass: 86.03678

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Source/Synthesis: Manuf. by reaction of ethylene with acetic acid in the presence of PdCl_2

Use/Importance: Used to manuf. lacquers and resins. Polymerisation followed by hydrol. gives polyvinyl alcohol (adhesive). Reagent for synth. of vinyl esters by ester interchange and for diene synth. Important industrial chemical, 40th in order of volume for USA in 1994 (production 1.51 million tons/year)

Physical Description: Liq. with a characteristic odour

Melting Point: Fp -100° (-93°)

Boiling Point: Bp 72°

Solubility: Misc. EtOH, Et_2O ; spar. sol. H_2O

Density: d^{20}_4 0.931

Refractive Index: n^{20}_D 1.3959

Other Data: Vp 89 mmHg (20°). Radical polym. gives poly(vinyl acetate); copolymers with acrylates, maleates and ethylene are also produced. Q/e for copolym., Q 0.026, e -0.88 . Coml. samples are stabilised with hydroquinone or diphenylamine. Rate for radical polym., k_p $1012 \text{ L mol}^{-1} \text{ s}^{-1}$, k_t $5.9 \times 10^{-5} \text{ L mol}^{-1} \text{ s}^{-1}$ (25°). Copolym. with vinyl chloride: r_{VAC} 0.23, r_{VC} 1.68 (typical values, 60°); Q 0.026; e -0.22 . Also copolym with vinylidene chloide: r_{VOC} 6.0, r_{VAC} 0.1 (typical values); Q 0.026; e -0.22

Hazard & Toxicity: Highly flammable, fl. p. -8° , autoignition temp. 385° . May polymerise violently. Skin and eye irritant. LD₅₀ (rat, orl) 2920 mg/kg. Exp. reprod. effects. OES: long-term 10 ppm; short-term 20 ppm

Aldrich: V150-3

Fluka: 46060

Sigma: V9382

Supelco: R43-4100

>>Derivative: Benzoyl

Synonym(s): Ethenyl benzoate, 9CI. Vinyl benzoate

CAS Registry Number: 769-78-8

Molecular Formula: $\text{C}_9\text{H}_8\text{O}_2$

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Use/Importance: Polymers are used in lacquers. Speciality monomer. Used in cosmetics

Physical Description: Liq.

Boiling Point: Bp 203° . Bp₂₀ $95-96^\circ$

Density: d^{20}_4 1.068

Other Data: Q/e values for copolym., Q 0.030, e -0.77 . Rate for radical polym., k_p $185 \text{ L mol}^{-1} \text{ s}^{-1}$, k_t $4.02 \times 10^{-4} \text{ L mol}^{-1} \text{ s}^{-1}$ (C_6H_6 , 30°)

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 3250 mg/kg

Aldrich: 40309-1

Fluka: 12485

>>Derivative: Me ether

see Methyl vinyl ether, [DDM93-L](#)

>>Derivative: Et ether