



>>Entry Name: 2-Propenoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Acrylic acid

CAS Registry Number: 79-10-7

Related CAS Registry Numbers(s): 6292-01-9 7446-81-3 9003-05-8 9003-06-9 10192-85-5 10344-93-1 14643-87-9

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

Molecular Formula: $\text{C}_3\text{H}_4\text{O}_2$

Molecular Weight: 72.063

Accurate Mass: 72.02113

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Biological Source: Found in green algae. Manuf. by oxidn. of 1-Propene BGX51-Z or by reaction of $\text{Ni}(\text{CO})_4$ with Acetylene DFS79-D and H_2O

Use/Importance: Undergoes free-radical polym. in aq. soln. to give polyacrylates, acrylic resins etc. USA production in 1999 1.39 million tons

Physical Description: Corrosive liq. with acrid odour and fumes

Melting Point: Mp 13°

Boiling Point: Bp 141° (polymerises)

Solubility: Misc. H_2O , EtOH, Et₂O; sol. Me₂CO; BERDY SOL: Fairly sol. H_2O

Density: d_4^{16} 1.062

pKa Value: $\text{p}K_a$ 4.25 (25°)

Refractive Index: n_D^{20} 1.4424

Other Data: Vp 4 mmHg (25°). Polym. readily in the presence of O_2 . Acrylic acid and its esters usually contain hydroquinone monomethyl ether as polym. inhibitor. Q/e values for copolym., Q 0.83, e +0.88. Copolym. with vinyl chloride: r_{AA} 6.8; r_{VC} 0.107 (typical values, 60°); Q 1.15; e 0.77

Hazard & Toxicity: Flammable, fl. p. 52° , autoignition temp. 438° . May polym. exothermically (possibly violently). Irritant to all tissues. LD₅₀ (rat, orl) 33.5 mg/kg. LD₅₀ (rbt, skn) 280 mg/kg. Exp. teratogen (ipr route). OES: long-term 10 ppm; short-term 20 ppm (Sk)

Aldrich: 14723-0

Fluka: 1730

>>Derivative: Me ester

Synonym(s): Methyl acrylate

CAS Registry Number: 96-33-3

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%

Use/Importance: Dienophile. Used in regiospecific synth. of aromatics. Monomer for acrylic polymers

Physical Description: Liq.

Melting Point: Mp -76.5°

Boiling Point: Bp 80.7°

Solubility: Sl. sol. H_2O ; sol. EtOH, Et₂O, Me₂CO

Density: d^{20} 0.953

Refractive Index: n_D^{20} 1.3984

Other Data: Vp 68 mmHg (20°). Polym. on long standing. Q/e values for copolym., Q 0.45, e +0.64. Rate for radical polym., $k_p = 720 \text{ L mol}^{-1} \text{ s}^{-1}$, $k_t = 4.3 \times 10^6 \text{ L mol}^{-1} \text{ s}^{-1}$ (30°). Copolym. with vinylidene chloride, r_{VDC} 0.74, r_{MA} 0.30 (typical values), Q 0.42, e 0.60. Copolym. with vinyl chloride: r_{MA} 4.4; r_{VC} 0.12 (typical values 50°): Q 0.42; e 0.60

Hazard & Toxicity: Highly flammable, fl. p. -3° (oc), autoignition temp. 468° . Can polym. violently if not inhibited. Peroxidisable. Adverse olfactory, eye and respiratory effects by inhalation. Skin and eye irritant. Exp. lung, liver and kidney injury following chronic exposure. OES: long-term 10 ppm

Aldrich: M2730-1

Fluka: 1800

>>Derivative: Et ester

Synonym(s): Ethyl acrylate. FEMA 2418

CAS Registry Number: 140-88-5

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_2$

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Use/Importance: Polym. feedstock, odorant for natural gas, synthetic reagent

Physical Description: Liq. with acid odour

Melting Point: Mp -71.2°

Boiling Point: Bp 99.8°

Solubility: Sl. sol. H_2O ; sol. EtOH, Et₂O, CHCl_3

Density: d