>>**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

H_2C=CHCOOH

Molecular Formula: $C_3H_4O_2$
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 $Ni(CO)_4$ 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, Et_2O; sol. Me_2CO; BERDY SOL: Fairly sol. H_2O
Density: d_4^{16}1.062
pKa Value: pK_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. LD_{50} (rat, orl) 33.5 mg/kg. LD_{50} (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: $C_4H_6O_2$
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, Et_2O, Me_2CO
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 L mol^{-1} s^{-1}, k_t = 4.3 x 10^6 L mol^{-1} 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: $C_5H_8O_2$
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, Et_2O, $CHCl_3$
Density: d