



>>Entry Name: 1-Chloro-2-propanone, 9CI

Synonym(s): Chloroacetone. Monochloroacetone

CAS Registry Number: 78-95-5

$\text{H}_3\text{CCOCH}_2\text{Cl}$

Molecular Formula: $\text{C}_3\text{H}_5\text{ClO}$

Molecular Weight: 92.525

Accurate Mass: 92.002892

Percentage Composition: C 38.94%; H 5.45%; Cl 38.32%; O 17.29%

Physical Description: Liq.

Boiling Point: Bp 119°

Solubility: Sol. H_2O

Density: d^{16}_4 1.162

pKa Value: pK_a 16.5

Refractive Index: n^{25}_D 1.4300

Hazard & Toxicity: Toxic by skin contact. May polymerise explosively on storage. Severe eye and respiratory tract irritant. Lachrymator and vesicant. LD₅₀ (rat, orl) 100 mg/kg. LD₅₀ (rbt, skn) 141 mg/kg. LC₅₀ (rat, ihl) 262 ppm (1h exposure)

Aldrich: 16747-9

Fluka: 22820

>>Derivative: Oxime

CAS Registry Number: 671-59-0

Molecular Formula: $\text{C}_3\text{H}_6\text{ClNO}$

Molecular Weight: 107.539

Accurate Mass: 107.013791

Percentage Composition: C 33.51%; H 5.62%; Cl 32.97%; N 13.02%; O 14.88%

Physical Description: Liq.

Boiling Point: Bp₇₃₀ 171°. Bp₉ 71°

>>Derivative: Semicarbazone

CAS Registry Number: 53646-01-8

Melting Point: Mp 150°

Other Data: Unstable, dec. by boiling H_2O or EtOH

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 71094-29-6

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 124-125.5°

>>Derivative: Di-Me acetal

Synonym(s): 1-Chloro-2,2-dimethoxypropane, 9CI

CAS Registry Number: 32730-70-4

Molecular Formula: $\text{C}_5\text{H}_{11}\text{ClO}_2$

Molecular Weight: 138.593

Accurate Mass: 138.044757

Percentage Composition: C 43.33%; H 8.00%; Cl 25.58%; O 23.09%

Physical Description: Liq.

Boiling Point: Bp 132-134°. Bp₁₅ 50°

>>Derivative: Di-Et acetal

Synonym(s): 1-Chloro-2,2-diethoxypropane, 9CI

CAS Registry Number: 63594-18-3

Molecular Formula: $\text{C}_7\text{H}_{15}\text{ClO}_2$

Molecular Weight: 166.647

Accurate Mass: 166.076057

Percentage Composition: C 50.45%; H 9.07%; Cl 21.27%; O 19.20%

Physical Description: Liq.

Boiling Point: Bp 162-163°. Bp₁₂ 57°