



>>Entry Name: Diazoacetic acid

CAS Registry Number: 503-68-4

$\text{N}_2=\text{CHCOOH}$

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

Molecular Weight: 86.05

Accurate Mass: 86.011628

Percentage Composition: C 27.92%; H 2.34%; N 32.55%; O 37.19%

General Statement: Free acid unknown

Hazard & Toxicity: Explosion hazard

>>Derivative: Me ester

Synonym(s): Methyl diazoacetate

CAS Registry Number: 6832-16-2

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

Molecular Weight: 100.077

Accurate Mass: 100.027278

Percentage Composition: C 36.01%; H 4.03%; N 27.99%; O 31.97%

Physical Description: Yellow liq.

Boiling Point: Bp_{721} 129°. Bp_{10} 33°

Hazard & Toxicity: Explodes on heating

>>Derivative: Et ester

Synonym(s): Diazoacetic ester. Ethyl diazoacetate

CAS Registry Number: 623-73-4

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

Molecular Weight: 114.104

Accurate Mass: 114.042928

Percentage Composition: C 42.11%; H 5.30%; N 24.55%; O 28.04%

Use/Importance: Reagent for ring expansions and β -keto ester synth.

Physical Description: Yellow oil with pungent odour

Melting Point: Mp -22°

Boiling Point: Bp_{720} 141°. Bp_{13} 44.5-46.5°

Refractive Index: n_D^{25} 1.4620

Hazard & Toxicity: Dec. explosively with conc. HCl or conc. H_2SO_4 . Can explode on dist., even *in vacuo*. Irritant. LD_{50} (rat, orl) 400 mg/kg. Exp. carcinogen

Aldrich: E2220-1

Fluka: 33501

>>Derivative: Butyl ester

Synonym(s): Butyl diazoacetate

CAS Registry Number: 24761-88-4

Molecular Formula: $\text{C}_6\text{H}_{10}\text{N}_2\text{O}_2$

Molecular Weight: 142.157

Accurate Mass: 142.074228

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

Boiling Point: Bp_8 53-54°

>>Derivative: 2-Methylpropyl ester

Synonym(s): 2-Methylpropyl diazoacetate

CAS Registry Number: 50639-30-0

Molecular Formula: $\text{C}_6\text{H}_{10}\text{N}_2\text{O}_2$

Molecular Weight: 142.157

Accurate Mass: 142.074228

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

Boiling Point: Bp_8 58-60°