



>>Entry Name: 2,3-Pentanedione, 9CI

ENTRY UNDER REVIEW

Synonym(s): Ethyl methyl diketone. FEMA 2841

CAS Registry Number: 600-14-6

$\text{H}_3\text{CCOCOCH}_2\text{CH}_3$

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: Flavour ingredient

Physical Description: Yellow liq.

Melting Point: Mp -52°

Boiling Point: Bp 108°

Solubility: Sol. H_2O

Density: d_4^{19} 0.957

Refractive Index: n_D^{19} 1.4014

Hazard & Toxicity: Skin irritant

Aldrich: W28410-6

Fluka: 76910

Rare Chemicals Library: S56492-3

>>Derivative: 2-Oxime

CAS Registry Number: 32818-79-4

Molecular Formula: $\text{C}_5\text{H}_9\text{NO}_2$

Molecular Weight: 115.132

Accurate Mass: 115.063329

Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%

Physical Description: Leaflets

Melting Point: Mp $69-71^\circ$

Hazard & Toxicity: LD_{50} (mus, ipr) 350 mg/kg

>>Derivative: 3-Oxime

CAS Registry Number: 609-29-0

Molecular Formula: $\text{C}_5\text{H}_9\text{NO}_2$

Molecular Weight: 115.132

Accurate Mass: 115.063329

Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%

Physical Description: Leaflets

Melting Point: Mp $58-59^\circ$

Boiling Point: Bp $183-187^\circ$ part. dec.

Hazard & Toxicity: LD_{50} (mus, ipr) 601 mg/kg

>>Derivative: Dioxime

Synonym(s): Ethylmethylglyoxime

CAS Registry Number: 4775-86-4

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2\text{O}_2$

Molecular Weight: 130.146

Accurate Mass: 130.074228

Percentage Composition: C 46.14%; H 7.74%; N 21.52%; O 24.59%

Use/Importance: Used for extraction-photometric detn. of Ni

Physical Description: Needles (EtOH)

Melting Point: Mp $172-173$ part. subl. $^\circ$

pKa Value: $\text{p}K_{\text{a}1}$ 10.51; $\text{p}K_{\text{a}2}$ 12.02