

## SAFETY DATA SHEET

Version 8.2  
Revision Date 09/23/2021  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Acetylacetone for analysis EMSURE®  
Product Number : 1.09600  
Catalogue No. : 109600  
Brand : Millipore  
Index-No. : 606-029-00-0  
CAS-No. : 123-54-6

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Reagent for analysis

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226  
Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 3), H331  
Acute toxicity, Dermal (Category 3), H311  
Short-term (acute) aquatic hazard (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word

Danger

|                            |                                                                                                          |
|----------------------------|----------------------------------------------------------------------------------------------------------|
| Hazard statement(s)        |                                                                                                          |
| H226                       | Flammable liquid and vapor.                                                                              |
| H302                       | Harmful if swallowed.                                                                                    |
| H311 + H331                | Toxic in contact with skin or if inhaled.                                                                |
| H402                       | Harmful to aquatic life.                                                                                 |
| Precautionary statement(s) |                                                                                                          |
| P210                       | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.                                      |
| P233                       | Keep container tightly closed.                                                                           |
| P240                       | Ground/bond container and receiving equipment.                                                           |
| P241                       | Use explosion-proof electrical/ ventilating/ lighting/ equipment.                                        |
| P242                       | Use only non-sparking tools.                                                                             |
| P243                       | Take precautionary measures against static discharge.                                                    |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.                                                    |
| P264                       | Wash skin thoroughly after handling.                                                                     |
| P270                       | Do not eat, drink or smoke when using this product.                                                      |
| P271                       | Use only outdoors or in a well-ventilated area.                                                          |
| P273                       | Avoid release to the environment.                                                                        |
| P280                       | Wear protective gloves/ eye protection/ face protection.                                                 |
| P301 + P312 + P330         | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.                              |
| P303 + P361 + P353         | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.     |
| P304 + P340 + P311         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| P362                       | Take off contaminated clothing and wash before reuse.                                                    |
| P370 + P378                | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.                     |
| P403 + P233                | Store in a well-ventilated place. Keep container tightly closed.                                         |
| P403 + P235                | Store in a well-ventilated place. Keep cool.                                                             |
| P405                       | Store locked up.                                                                                         |
| P501                       | Dispose of contents/ container to an approved waste disposal plant.                                      |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                                |
|------------------|------------------------------------------------|
| Formula          | : C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> |
| Molecular weight | : 100.12 g/mol                                 |
| CAS-No.          | : 123-54-6                                     |
| EC-No.           | : 204-634-0                                    |
| Index-No.        | : 606-029-00-0                                 |

| Component            | Classification                                                                                   | Concentration |
|----------------------|--------------------------------------------------------------------------------------------------|---------------|
| <b>Acetylacetone</b> |                                                                                                  |               |
|                      | Flam. Liq. 3; Acute Tox. 4;<br>Acute Tox. 3; Aquatic<br>Acute 3; H226, H302,<br>H331, H311, H402 | <= 100 %      |

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Foam Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### 5.2 Special hazards arising from the substance or mixture

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### 5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

### **6.2 Environmental precautions**

Do not let product enter drains. Risk of explosion.

### **6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### **Advice on protection against fire and explosion**

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### **Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

#### **Storage class**

Storage class (TRGS 510): 3: Flammable liquids

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

| Component     | CAS-No.  | Value                          | Control parameters | Basis                                   |
|---------------|----------|--------------------------------|--------------------|-----------------------------------------|
| Acetylacetone | 123-54-6 | TWA                            | 25 ppm             | USA. ACGIH Threshold Limit Values (TLV) |
|               | Remarks  | Danger of cutaneous absorption |                    |                                         |

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### Personal protective equipment

#### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

#### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 240 min

Material tested: Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 10 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

#### Body Protection

Flame retardant antistatic protective clothing.

#### Respiratory protection

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

#### Control of environmental exposure

Do not let product enter drains. Risk of explosion.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |                  |
|---------------|------------------|
| a) Appearance | Form: liquid     |
|               | Color: colorless |

Millipore - 1.09600

Page 5 of 11

|                                                 |                                                                                                     |
|-------------------------------------------------|-----------------------------------------------------------------------------------------------------|
| b) Odor                                         | ester-like                                                                                          |
| c) Odor Threshold                               | No data available                                                                                   |
| d) pH                                           | No data available                                                                                   |
| e) Melting point/freezing point                 | Melting point/range: ca.-47.5 - -17.6 °C (ca.-53.5 - 0.3 °F) at 1,013 hPa - OECD Test Guideline 102 |
| f) Initial boiling point and boiling range      | 139.5 °C 283.1 °F at 1,013 hPa - OECD Test Guideline 103                                            |
| g) Flash point                                  | 35 °C (95 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9                               |
| h) Evaporation rate                             | No data available                                                                                   |
| i) Flammability (solid, gas)                    | No data available                                                                                   |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 11.4 %(V)<br>Lower explosion limit: 1.7 %(V)                                 |
| k) Vapor pressure                               | 7.9 hPa at 20 °C (68 °F) - OECD Test Guideline 104                                                  |
| l) Vapor density                                | No data available                                                                                   |
| m) Density                                      | 0.972 g/cm <sup>3</sup> at 25 °C (77 °F)                                                            |
| Relative density                                | 0.97 at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.3                                    |
| n) Water solubility                             | ca.153.8 g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.6 - completely soluble       |
| o) Partition coefficient: n-octanol/water       | log Pow: ca.0.68 at 40 °C (104 °F) - OECD Test Guideline 117 - Bioaccumulation is not expected.     |
| p) Autoignition temperature                     | No data available                                                                                   |
| q) Decomposition temperature                    | Distillable in an undecomposed state at normal pressure.                                            |
| r) Viscosity                                    | No data available                                                                                   |
| s) Explosive properties                         | No data available                                                                                   |
| t) Oxidizing properties                         | none                                                                                                |

## 9.2 Other safety information

|                 |                                                                             |
|-----------------|-----------------------------------------------------------------------------|
| Surface tension | 72 mN/m at 1g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.5 |
|-----------------|-----------------------------------------------------------------------------|

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Acids

Bases

Amines

Aldehydes

anhydrides

Oxidizing agents

Hydrogen fluoride

Halogenated compounds

Cyanides

Isocyanates

alkalines

bases

Risk of ignition or formation of inflammable gases or vapours with:

hydrides

nitrides

Alkali metals

### 10.4 Conditions to avoid

Heating.

### 10.5 Incompatible materials

Mild steel, Zinc, Copper, Nickel, various alloys

### 10.6 Hazardous decomposition products

Peroxides

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - female - 570 mg/kg

Remarks: (ECHA)

LC50 Inhalation - Rat - male and female - 4 h - 5.0305 mg/l

(OECD Test Guideline 403)

Symptoms: mucosal irritations, Cough

LD50 Dermal - Rabbit - female - 790 mg/kg

Remarks: (ECHA)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

Remarks: (ECHA)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: slight irritation

Remarks: (ECHA)

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative  
(OECD Test Guideline 429)

### **Germ cell mutagenicity**

Laboratory experiments have shown mutagenic effects.

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 473

Result: positive

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 479

Result: positive

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: inhalation (vapor)

Method: US-EPA

Result: negative

Test Type: comet assay

Species: Rat

Cell type: Liver cells

Application Route: Oral

Result: negative

Remarks: (ECHA)

### **Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

Ingestion of excessive amounts by pregnant animals resulted in maternal and fetal toxicity.

No data available

### **Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

Repeated dose toxicity - Rabbit - male and female - Dermal - 9 Days - NOAEL (No observed adverse effect level) - 244 mg/kg - LOAEL (Lowest observed adverse effect level) - 975 mg/kg

Remarks: (ECHA)

Inhalation may provoke the following symptoms:, Dizziness, Suffocation

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Systemic effects:

Dizziness

Headache

Shortness of breath

respiratory arrest

Unconsciousness

Damage to:

Liver

Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

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**SECTION 12: Ecological information****12.1 Toxicity**

|                                                     |                                                                                                                    |
|-----------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|
| Toxicity to fish                                    | flow-through test LC50 - Pimephales promelas (fathead minnow) - 104 mg/l - 96 h<br>(OECD Test Guideline 203)       |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - 25.9 mg/l - 48 h<br>(OECD Test Guideline 202)                      |
| Toxicity to algae                                   | static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 83.22 mg/l - 72 h<br>(OECD Test Guideline 201) |
| Toxicity to bacteria                                | static test EC50 - activated sludge - 107.6 mg/l - 3 h<br>(OECD Test Guideline 209)                                |

Millipore - 1.09600

Page 9 of 11

## 12.2 Persistence and degradability

Biodegradability      aerobic - Exposure time 28 d  
Result: 83 - 100 % - Readily biodegradable.  
(OECD Test Guideline 301C)

Ratio BOD/ThBOD      5.6 %  
Remarks: (Lit.)

## 12.3 Bioaccumulative potential

No data available

## 12.4 Mobility in soil

No data available

## 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Other adverse effects

Discharge into the environment must be avoided.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### DOT (US)

UN number: 2310    Class: 3 (6.1)    Packing group: III  
Proper shipping name: Pentane-2,4-dione  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 2310    Class: 3 (6.1)    Packing group: III    EMS-No: F-E, S-D  
Proper shipping name: PENTANE-2,4-DIONE

### IATA

UN number: 2310    Class: 3 (6.1)    Packing group: III  
Proper shipping name: Pentane-2,4-dione

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## SECTION 15: Regulatory information

### SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### **Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

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### **SECTION 16: Other information**

#### **Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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