

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 07/22/2015

Version 1.5

SECTION 1.Identification

Product identifier

Product number 800023

Product name Acetylacetone for synthesis

CAS-No. 123-54-6

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

Identified uses Chemical for synthesis

Details of the supplier of the safety data sheet

Company EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821,

United States of America | General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)

Emergency telephone 800-424-9300 CHEMTREC (USA)

+1-703-527-3887 CHEMTREC (International)

24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 3, H226 Acute toxicity, Category 4, Oral, H302

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

GHS-Labeling

Hazard pictograms





Signal Word Warning

Hazard Statements
H226 Flammable liquid and vapor.
H302 Harmful if swallowed.

Precautionary Statements

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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.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

P301 + P312 IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.

P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing.

Rinse skin with water/ shower.

P330 Rinse mouth.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.

P403 + P235 Store in a well-ventilated place. Keep cool.

P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula $CH_3COCH_2COCH_3$ $C_5H_8O_2$ (Hill)

Molar mass 100.12 g/mol

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

Acetylacetone (>= 90 % - <= 100 %)

123-54-6

Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Consult doctor if feeling unwell.

Skin contact

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

shower.

Eye contact

After eye contact: rinse out with plenty of water.

Ingestion

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

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

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Cough, Nausea, Dizziness, irritant effects, Vomiting, Headache, Shortness of breath, respiratory arrest, Unconsciousness

Indication of any immediate medical attention and special treatment needed

Laxative: Sodium sulfate (1 tablespoon/1/4 I water).

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Water, Foam, Carbon dioxide (CO2), Dry powder

Unsuitable extinguishing media

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

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 vapors possible in the event of fire.

Advice for firefighters

Special protective equipment for fire-fighters

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

Further information

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

SECTION 6. Accidental release measures

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.

Advice for emergency responders:

Protective equipment see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

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Advice on protection against fire and explosion

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

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis Value Threshold Remarks

limits

Acetylacetone 123-54-6

ACGIH Time Weighted Average 25 ppm

(TWA):

Skin designation: Can be absorbed through the skin.

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Change contaminated clothing. Application of skin- protective barrier cream recommended. Wash hands after working with substance.

Eye/face protection
Safety glasses

Hand protection

full contact:

Glove material: butyl-rubber
Glove thickness: 0.7 mm
Break through time: > 480 min

splash contact:

Glove material: Nitrile rubber Glove thickness: 0.40 mm Preak through time: > 30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 730 Camatril® - Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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This recommendation applies only to the product stated in the safety data sheet and supplied by us as well as to the purpose specified by us. 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).

Other protective equipment:

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapors/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapors of organic compounds The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are performed according to the instructions of the producer. These measures have to be properly documented.

SECTION 9. Physical and chemical properties

Physical state liquid

Color colorless

malodorous Odor

Odor Threshold No information available.

6 pН

> at 200 g/l 68 °F (20 °C)

Melting point -23 °C

Boiling point/boiling range 280 - 284 °F (138 - 140 °C)

at 1,013 hPa

Flash point 93 °F (34 °C)

Method: c.c.

No information available. Evaporation rate

No information available. Flammability (solid, gas)

Lower explosion limit 2.4 %(V)

Upper explosion limit 11.4 %(V)

Vapor pressure 9 hPa

at 68 °F (20 °C)

Relative vapor density 3.5

Density 0.97 g/cm³

at 68 °F (20 °C)

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Relative density No information available.

Water solubility 200 g/l

at 68 °F (20 °C)

Partition coefficient: n-

octanol/water

log Pow: 0.40 (experimental)

(Lit.) Bioaccumulation is not expected.

Autoignition temperature No information available.

Decomposition temperature No information available.

Viscosity, dynamic 0.6 mPa.s

at 68 °F (20 °C)

Explosive properties Not classified as explosive.

Oxidizing properties none

Ignition temperature 644 °F (340 °C)

SECTION 10. Stability and reactivity

Reactivity

Vapor/air-mixtures are explosive at intense warming.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:

Acids, Bases, Amines, Aldehydes, anhydrides, Oxidizing agents, Peroxides, peroxi compounds, Hydrogen fluoride, Halogenated compounds, Cyanides

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

hydrides, nitrides, Alkali metals

Conditions to avoid

Heating.

Incompatible materials

Mild steel, Zinc, Copper, Nickel, various plastics

Hazardous decomposition products

no information available

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

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SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Acute oral toxicity

LD50 Rat: 575 mg/kg (External MSDS)

absorption

Symptoms: Irritations, Nausea, Vomiting, Unconsciousness

Acute inhalation toxicity

Symptoms: Dizziness, Headache, Nausea, Unconsciousness, Symptoms may be delayed.

Skin irritation Rabbit

Result: No irritation (External MSDS)

Eye irritation

Rabbit

Result: No eye irritation

(External MSDS)

Genotoxicity in vivo

Micronucleus test

Result: positive

(National Toxicology Program)

Specific target organ systemic toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

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.

OSHA No ingredient of this product present at levels greater than or

equal to 0.1% is identified as a carcinogen or potential

carcinogen by OSHA.

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.

ACGIH No ingredient of this product present at levels greater than or

equal to 0.1% is identified as a carcinogen or potential

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carcinogen by ACGIH.

Further information

Systemic effects:

After absorption:

Irritations, Cough, Nausea, Vomiting, Dizziness, Headache, Shortness of breath, respiratory

arrest, Unconsciousness

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 Lepomis macrochirus (Bluegill sunfish): 60.1 mg/l; 96 h (ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 75 mg/l; 48 h (ECOTOX Database)

EC5 E.sulcatum: 11 mg/l; 72 h (maximum permissible toxic concentration) (IUCLID)

Toxicity to algae

IC5 Scenedesmus quadricauda (Green algae): 2.7 mg/l; 8 d (maximum permissible toxic concentration) (IUCLID)

IC5 M.aeruginosa: 8.5 mg/l; 8 d (IUCLID)

Toxicity to bacteria

EC5 Pseudomonas putida: 67 mg/l; 16 h (maximum permissible toxic concentration) (IUCLID)

Persistence and degradability

Biodegradability

79 - 88 %; 28 d

OECD Test Guideline 301C

Readily biodegradable.

Ratio BOD/ThBOD

BOD5 5.6 %

(Lit.)

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0.40

(experimental)

(Lit.) Bioaccumulation is not expected.

Mobility in soil

No information available.

Additional ecological information

Discharge into the environment must be avoided.

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

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SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number UN 2310

Proper shipping name PENTANE-2,4-DIONE

Class 3 (6.1)
Packing group III
Environmentally hazardous --

Air transport (IATA)

UN number UN 2310

Proper shipping name PENTANE-2,4-DIONE

Class 3 (6.1)
Packing group III
Environmentally hazardous -Special precautions for user no

Sea transport (IMDG)

UN number UN 2310

Proper shipping name PENTANE-2,4-DIONE

Class 3 (6.1)

Packing group III

Environmentally hazardous -
Special precautions for user yes

EmS F-E S-D

SECTION 15. Regulatory information

United States of America

SARA 313

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.

SARA 302

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311,

Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311,

Table 117.3.

DEA List I

Not listed

DEA List II

Not listed

TSCA 12b

Ingredients

Acetylacetone 123-54-6

US State Regulations

Massachusetts Right To Know

Ingredients
Acetylacetone

Pennsylvania Right To Know

Ingredients

Acetylacetone

New Jersey Right To Know

Ingredients

Acetylacetone

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA: All components of the product are listed in the TSCA-inventory.

DSL: All components of this product are on the Canadian DSL.

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

Labeling

Hazard pictograms





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Signal Word Warning

Hazard Statements

H226 Flammable liquid and vapor.

H302 Harmful if swallowed.

Precautionary Statements

Prevention

P210 Keep away from heat.

Full text of H-Statements referred to under sections 2 and 3.

H226 Flammable liquid and vapor.

H302 Harmful if swallowed.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Revision Date 07/22/2015

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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