

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.7

Revision Date 21.03.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Acetylacetone for synthesis

Product Number : 8.00023

Catalogue No. : 800023

Brand : Millipore

Index-No. : 606-029-00-0

REACH No. : 01-2119458968-15-XXXX

CAS-No. : 123-54-6

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

Identified uses : Chemical for synthesis

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Chemie GmbH
Eschenstrasse 5
D-82024 TAUFKIRCHEN

Telephone : +49 (0)89 6513-1130

Fax : +49 (0)89 6513-1161

E-mail address : technischerservice@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : 0800 181 7059 (CHEMTREC Deutschland)
+49 (0)696 43508409 (CHEMTREC
weltweit)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008



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.

Precautionary statement(s)

P210

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233

Keep container tightly closed.

P280

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

P301 + P312

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.

P304 + P340 + P311

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.

Supplemental Hazard Statements

none

Reduced Labeling (<= 125 ml)

Pictogram



Signal Word

Danger

Hazard statement(s)

H311 + H331

Toxic in contact with skin or if inhaled.

Precautionary statement(s)

P304 + P340 + P311

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.

Supplemental Hazard Statements

none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	:	C5H8O2
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
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Acetylacetone			
CAS-No.	123-54-6	Flam. Liq. 3; Acute Tox. 4;	<= 100 %
EC-No.	204-634-0	Acute Tox. 3; H226, H302,	
Index-No.	606-029-00-0	H331, H311	

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

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) 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.

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.

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



SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Derived No Effect Level (DNEL)

Application Area	Routes of exposure	Health effect	Value
Workers	Skin contact	Long-term systemic effects	12mg/kg BW/d
Workers	Inhalation	Long-term systemic effects	84 mg/m ³

Predicted No Effect Concentration (PNEC)

Compartment	Value
Soil	0,01582 mg/kg
Sea water	0,0026 mg/l
Fresh water	0,026 mg/l
Sewage treatment plant	1,32 mg/l
Fresh water sediment	0,155 mg/kg
Sea sediment	0,0155 mg/kg

8.2 Exposure controls

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).

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).

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

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Physical state	liquid
b) Color	colorless
c) Odor	ester-like
d) Melting point/freezing point	Melting point/range: ca.-47,5 - -17,6 °C at 1.013 hPa - OECD Test Guideline 102
e) Initial boiling point and boiling range	139,5 °C at 1.013 hPa - OECD Test Guideline 103
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 11,4 %(V) Lower explosion limit: 1,7 %(V)
h) Flash point	35 °C - closed cup - Regulation (EC) No. 440/2008, Annex, A.9
i) Autoignition temperature	No data available
j) Decomposition temperature	Distillable in an undecomposed state at normal pressure.
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: ca.0,76 mPa.s at 20 °Cca.0,63 mPa.s at 40 °C
m) Water solubility	ca.153,8 g/l at 20 °C - Regulation (EC) No. 440/2008, Annex, A.6- completely soluble
n) Partition coefficient: n-octanol/water	log Pow: ca.0,68 at 40 °C - OECD Test Guideline 117 - Bioaccumulation is not expected.
o) Vapor pressure	7,9 hPa at 20 °C - OECD Test Guideline 104
p) Density	0,972 g/cm ³ at 25 °C
Relative density	0,97 at 20 °C - Regulation (EC) No. 440/2008, Annex, A.3
q) Relative vapor density	
r) Particle	No data available



characteristics

- 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
- Regulation (EC) No. 440/2008, Annex, A.5

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

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

Strong oxidizing agents, Reducing agents, Strong bases, Metals

10.6 Hazardous decomposition products

Peroxides

In the event of fire: see section 5

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 - vapor

(OECD Test Guideline 403)

Symptoms: mucosal irritations, Cough

LD50 Dermal - Rabbit - female - 790 mg/kg

Remarks: (ECHA)

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

No data available

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



Toxicity to bacteria	static test EC50 - activated sludge - 107,6 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - 10 mg/l - 34 d (OECD Test Guideline 210)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 18 mg/l - 21 d (OECD Test Guideline 211)

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2310

IMDG: 2310

IATA: 2310

14.2 UN proper shipping name

ADR/RID: PENTANE-2,4-DIONE

Millipore- 8.00023

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The life science business of Merck operates as MilliporeSigma in the US and Canada



IMDG: PENTANE-2,4-DIONE
IATA: Pentane-2,4-dione

14.3 Transport hazard class(es)

ADR/RID: 3 (6.1) IMDG: 3 (6.1) IATA: 3 (6.1)

14.4 Packaging group

ADR/RID: III IMDG: III IATA: III

14.5 Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

14.6 Special precautions for user

Tunnel restriction code : (D/E)
Further information : No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

: FLAMMABLE LIQUIDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

A Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

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

H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H311 + H331	Flammable liquid and vapor.
H331	Harmful if swallowed.



Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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