SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.7
Revision Date 07.06.2023
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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	:	Diacetyl for synthesis
Product Number	:	8.03528
Catalogue No.	:	803528
Brand	:	Millipore
REACH No.	:	A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	:	431-03-8

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	:	Merck Life Science S.r.l. Via Monte Rosa 93 I-20149 MILANO
Telephone	:	+39 02 3341 7340
Fax	:	+39 02 3801 0737
E-mail address	:	serviziotecnico@merckgroup.com

1.4 Emergency telephone

Emergency Phone #	:	800-789-767 (CHEMTREC Italia) +39-02-4555-7031 (CHEMTREC chiamate internazionali) +39 02-6610-1029 (Centro Antiveleni Niguarda Ca' Granda - Milano)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008
Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 3), H331

Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318
Skin sensitization (Category 1), H317
Specific target organ toxicity - repeated exposure, Inhalation (Category 2), Respiratory system, H373

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)	
H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H373	May cause damage to organs (Respiratory system) through prolonged or repeated exposure if inhaled.
Precautionary statement(s)	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P314	Get medical advice/ attention if you feel unwell.
Supplemental Hazard Statements	none

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word	Danger
Hazard statement(s)	
H331	Toxic if inhaled.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.

Precautionary statement(s)

P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
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	:	C4H6O2
Molecular weight	:	86,09 g/mol
CAS-No.	:	431-03-8
EC-No.	:	207-069-8

Component		Classification	Concentration
butanedione			
CAS-No. EC-No.	431-03-8 207-069-8	Flam. Liq. 2; Acute Tox. 4; Acute Tox. 3; Skin Irrit. 2; Eye Dam. 1; Skin Sens. 1; STOT RE 2; H225, H302, H331, H315, H318, H317, H373	<= 100 %

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. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. 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
Carbon oxides
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

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

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). Tightly fitting safety goggles

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).
Splash contact
Material: butyl-rubber
Minimum layer thickness: 0,7 mm
Break through time: 240 min

Material tested:Butoject® (KCL 898)

Body Protection
Flame retardant antistatic protective clothing.

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

The entrepeneur 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	yellow
c)	Odor	strongStench.
d)	Melting point/freezing point	Melting point: -2 °C
e)	Initial boiling point and boiling range	88 - 89 °C at 1.013,25 hPa
f)	Flammability (solid, gas)	No data available
g)	Upper/lower flammability or explosive limits	Upper explosion limit: 13,0 %(V) Lower explosion limit: 2,4 %(V)
h)	Flash point	7 °C - closed cup
i)	Autoignition temperature	345 °C
j)	Decomposition temperature	No data available
k)	pH	3,2
l)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m)	Water solubility	200 g/l at 25 °C - soluble
n)	Partition coefficient: n-octanol/water	log Pow: -1,34 - (Lit.), Bioaccumulation is not expected.
o)	Vapor pressure	69,6 hPa at 20 °C
p)	Density	0,99 g/cm3 at 15 °C
	Relative density	No data available

q)	Relative vapor density	No data available
r)	Particle characteristics	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	none

9.2 Other safety information

Relative vapor density	3,45

SECTION 10: Stability and reactivity

10.1 Reactivity
Vapors may form explosive mixture with air.

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:
alkalines
Acids
various plastics
Risk of ignition or formation of inflammable gases or vapours with:
strong oxidising agents

10.4 Conditions to avoid
Warming.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 1.580 mg/kg
Remarks: Behavioral:Somnolence (general depressed activity).
Behavioral:Convulsions or effect on seizure threshold.
(RTECS)
Acute toxicity estimate Oral - 1.580 mg/kg
(Calculation method)
LC50 Inhalation - Rat - 4 h - 2,25 - 5,2 mg/l - vapor

Remarks: (External MSDS)
Symptoms: Possible damages:, Irritation symptoms in the respiratory tract.
Acute toxicity estimate Inhalation - 2,25 mg/l - vapor

(Calculation method)
LD50 Dermal - Rabbit - > 5.000 mg/kg
Remarks: (RTECS)

Skin corrosion/irritation
Skin - Rabbit
Result: Irritations
Remarks: (External MSDS)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe eye irritation
Remarks: (External MSDS)

Respiratory or skin sensitization
May cause allergic skin reaction.

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
Inhalation - May cause damage to organs through prolonged or repeated exposure.
- Respiratory system

Aspiration hazard
No data available

11.2 Additional Information

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.

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

After absorption of toxic quantities:

Headache

Nausea

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - Leuciscus idus (Golden orfe) - 46 - 100 mg/l - 96 h Remarks: (External MSDS)
Toxicity to bacteria	Remarks: (Hommel) (butanedione)

12.2 Persistence and degradability

Biodegradability Result: - Readily biodegradable.

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

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2346 IMDG: 2346 IATA: 2346

14.2 UN proper shipping name

ADR/RID: BUTANEDIONE
IMDG: BUTANEDIONE
IATA: Butanedione

14.3 Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

14.4 Packaging group

ADR/RID: II IMDG: II IATA: II

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.	H2	ACUTE TOXIC
	P5c	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

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

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

H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H315	Causes skin irritation.

H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H331	Highly flammable liquid and vapor.
H373	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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