

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.8

Revision Date 20.10.2022

Print Date 09.11.2022

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 : Diisobutyl ketone for synthesis

Product Number : 8.18831

Catalogue No. : 818831

Brand : Millipore

Index-No. : 606-005-00-X

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. : 108-83-8

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 KGaA
Frankfurter Str. 250
D-64271 DARMSTADT

Telephone : +49 (0)6151 72-0

Fax : +49 6151 727780

E-mail address : TechnicalService@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : +(44)-870-8200418 (CHEMTREC (GB))
+(353)-19014670 (CHEMTREC Ireland)
001-803-017-9114 (CHEMTREC India)

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

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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

Warning

Hazard statement(s)

H226

Flammable liquid and vapor.

H335

May cause respiratory irritation.

Precautionary statement(s)

P210

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

P233

Keep container tightly closed.

P240

Ground and bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P242

Use non-sparking tools.

P243

Take action to prevent static discharges.

Supplemental Hazard Statements

none

Reduced Labeling (<= 125 ml)

Pictogram



Signal Word

Warning

Hazard statement(s)

none

Precautionary statement(s)

none

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 : C₉H₁₈O
Molecular weight : 142,24 g/mol
CAS-No. : 108-83-8
EC-No. : 203-620-1
Index-No. : 606-005-00-X

Component		Classification	Concentration
2,6-Dimethylheptan-4-one			
CAS-No.	108-83-8	Flam. Liq. 3; STOT SE 3; H226, H335 Concentration limits: >= 10 %: STOT SE 3, H335;	<= 100 %
EC-No.	203-620-1		
Index-No.	606-005-00-X		



SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

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

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

Foam Carbon dioxide (CO₂) 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.

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

In the event of fire, wear self-contained breathing apparatus.

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 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 protection against fire and explosion

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

Hygiene measures

Change contaminated clothing. Wash hands 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.

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). Safety glasses

Skin protection

required



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.

Recommended Filter type: Filter type ABEK

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	No data available
d) Melting point/freezing point	Melting point/freezing point: -45,98 °C at ca.1013,0 hPa
e) Initial boiling point and boiling range	165 - 170 °C at 1.013 hPa
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 6,2 %(V) Lower explosion limit: 0,8 %(V)
h) Flash point	49 °C - closed cup
i) Autoignition temperature	345 °C at 1013,0 hPa
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 0,869 mPa.s at 25 °C
m) Water solubility	0,43 g/l at 25 °C - partly soluble
n) Partition coefficient: n-octanol/water	log Pow: 3,71 at 25 °C
o) Vapor pressure	2,3 hPa at 20 °C
p) Density	0,809 g/cm ³
Relative density	No data available



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|-----------------------------|-------------------|
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| | |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

Surface tension	22,8 mN/m at 25 °C
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Relative vapor density	4,91 - (Air = 1.0)
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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

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

Strong oxidizing agents, Strong reducing agents, Strong bases

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 - male and female - > 2.000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - > 14,5 mg/l

(OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - > 2.000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h



(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

Germ cell mutagenicity

No data available

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Carcinogenicity

No data available

Reproductive 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

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.

Repeated dose toxicity - Rat - male - Oral - NOAEL (No observed adverse effect level) - 2.000 mg/kg

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish

flow-through test LC50 - *Oncorhynchus mykiss* (rainbow trout) - 30 mg/l - 96 h



	(OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - 37,2 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	Growth inhibition EC50 - Pseudokirchneriella subcapitata (green algae) - 46,9 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 20 d
Result: 88 % - Readily biodegradable.
(OECD Test Guideline 301D)

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

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1157	IMDG: 1157	IATA: 1157
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14.2 UN proper shipping name

ADR/RID: DIISOBUTYL KETONE
IMDG: DIISOBUTYL KETONE
IATA: Diisobutyl ketone

14.3 Transport hazard class(es)

ADR/RID: 3	IMDG: 3	IATA: 3
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14.4 Packaging group

ADR/RID: III	IMDG: III	IATA: III
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14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

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.

Other regulations

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.

H226	Flammable liquid and vapor.
H335	May cause respiratory irritation.



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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