

SAFETY DATA SHEET

Version 8.6
Revision Date 01.07.2021
Print Date 27.01.2022**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

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 sheetCompany : MilliporeSigma Canada Ltd
2149 WINSTON PARK DRIVE
OAKVILLE ON L6H 6J8
CANADA

Telephone : +1 905 829-9500

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1.4 Emergency telephoneEmergency 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 Hazardous Products Regulations (HPR) (SOR/2015-17)**

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 GHS Label elements, including precautionary statements

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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
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

Molecular weight : 142.24 g/mol

Component	Classification	Concentration *
2,6-Dimethylheptan-4-one		
	Flam. Liq. 3; STOT SE 3; H226, H335 Concentration limits: >= 10 %: STOT SE 3, H335;	<= 100 %
* Weight %		

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

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

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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

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. Chemisorb®). 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 (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

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
2,6-Dimethylheptan-4-one	108-83-8	TWA	25 ppm 145 mg/m ³	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
Remarks	Occupational exposure limit is based on irritation effects and its adjustment to compensate for unusual work schedules is not required			
		TWA	25 ppm	Canada. British Columbia OEL
		TWAEV	25 ppm 145 mg/m ³	Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants
		TWA	25 ppm	USA. ACGIH Threshold Limit Values (TLV)

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Wash hands 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

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.

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) Appearance | Form: liquid
Color: colorless |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/freezing point: -45.98 °C (-50.76 °F) at ca.1013.0 hPa |
| f) Initial boiling point and boiling range | 165 - 170 °C 329 - 338 °F at 1,013 hPa |
| g) Flash point | 49 °C (120 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 6.2 %(V)
Lower explosion limit: 0.8 %(V) |
| k) Vapor pressure | 2.3 hPa at 20 °C (68 °F) |
| l) Vapor density | 4.91 - (Air = 1.0) |
| m) Relative density | No data available |
| n) Water solubility | 0.43 g/l at 25 °C (77 °F) - partly soluble |

- o) Partition coefficient: log Pow: 3.71 at 25 °C (77 °F)
n-octanol/water
- p) Autoignition temperature 345 °C (653 °F) at 1013.0 hPa
- q) Decomposition temperature No data available
- r) Viscosity 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 (77 °F)
Relative vapor density	4.91 - (Air = 1.0)

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)

No data available

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

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 - 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.

Stomach - Irregularities - Based on Human Evidence

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

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

12.6 Other adverse effects

No data available

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

SECTION 14: Transport information

TDG

UN number: 1157 Class: 3 Packing group: III
Proper shipping name: DIISOBUTYL KETONE
Labels: 3
ERG Code: 128
Marine pollutant: no

IMDG

UN number: 1157 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: DIISOBUTYL KETONE

IATA

UN number: 1157 Class: 3 Packing group: III
Proper shipping name: Diisobutyl ketone

SECTION 15: Regulatory information

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

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

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