# SAFETY DATA SHEET

Version 8.4
Revision Date 02.07.2024
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## SECTION 1: Identification of the hazardous chemical and of the supplier

### 1.1 Product identifiers

Product name : Isopropyl methyl ketone for synthesis

Product Number : 8.05966
Catalogue No. : 805966
Brand : Millipore
CAS-No. : 563-80-4

### 1.2 Other means of identification

No data available

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

Identified uses : Chemical for synthesis

### 1.4 Details of the supplier of the safety data sheet

Company : Merck Sdn. Bhd.
Co. No: 178145
No. 4, Jalan U1/26, Section U1,
40150 HICOM GLENMARIE INDUSTRIAL PARK,SHAH ALA
MALAYSIA

Telephone : +60 (0)3-74943688
Fax : +60 (0)3-74910850

### 1.5 Emergency telephone

Emergency Phone # : 1-800-815-308 (CHEMTREC) * +60 3-
9212 5794 (CHEMTREC Intl.)

## Section 2: Hazard identification

### 2.1 GHS Classification

Classification according to CLASS regulations 2013
Flammable liquids (Category 2), H225

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

### 2.2 GHS Label elements, including precautionary statements

Labelling according to CLASS regulations 2013
Pictogram

Signal Word Danger



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Hazard Statements
H225 Highly flammable liquid and vapor.

Precautionary Statements

Prevention
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233 Keep container tightly closed.

Response
P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.

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

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

**Reduced Labeling (<= 125 ml)**
Pictogram

Signal Word Danger

Hazard Statements none

Precautionary Statements none
Refer to the Safety Data Sheet before use.

**2.3 Other hazards** - none

## SECTION 3: Composition and information of the ingredients of the hazardous chemical

Substance / Mixture : Substance

**3.1 Substances**

Formula : C5H10O
Molecular weight : 86.13 g/mol
CAS-No. : 563-80-4
EC-No. : 209-264-3
Index-No. : 606-007-00-0

**Hazardous ingredients**

| Component | Classification | Concentration |
|---|---|---|
| **3-methylbutanone** | | |
| | Flam. Liq. 2; H225 | <= 100 % |

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



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## 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: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

### 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

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.



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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. 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 and personal protection

### 8.1 Control parameters

**Ingredients with workplace control parameters**

| Component | CAS-No. | Value | Control parameters | Basis |
|---|---|---|---|---|



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| | | | | |
|---|---|---|---|---|
| 3-methylbutanone | 563-80-4 | TWA | 200 ppm 705 mg/m3 | Malaysia. Occupational Safety and Health (Use and Standards of Exposure of Chemicals Hazardous to Health) Regulations 2000. |

### 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**
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 EN 16523-1 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: 120 min
Material tested:Butoject® (KCL 898)

**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) | Physical state | liquid |
| b) | Color | colorless |
| c) | Odor | fruity |
| d) | Melting point/freezing point | Melting point: -92 °C at 1,013 hPa |
| e) | Initial boiling point and boiling range | 93 - 95 °C at 1,013 hPa |



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| | | |
|---|---|---|
| f) | Flammability (solid, gas) | No data available |
| g) | Upper/lower flammability or explosive limits | Upper explosion limit: 9 %(V)<br>Lower explosion limit: 1.5 %(V) |
| h) | Flash point | -1 °C |
| i) | Autoignition temperature | No data available |
| j) | Decomposition temperature | No data available |
| k) | pH | No data available |
| l) | Viscosity | Viscosity, kinematic: No data available<br>Viscosity, dynamic: 0.5 mPa.s at 25 °C - OECD Test Guideline 114 |
| m) | Water solubility | 8.21 g/l at 20 °C - OECD Test Guideline 105 |
| n) | Partition coefficient: n-octanol/water | log Pow: 2.29 at 20 °C - Bioaccumulation is not expected. |
| o) | Vapor pressure | 53.33 hPa at 19.9 °C |
| p) | Density | 0.80 g/cm3 at 20 °C0.80 g/cm3 at 20 °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 | No data available |

### 9.2 Other safety information

| | |
|---|---|
| Surface tension | 24.3 mN/m at 22 °C<br>- Surface tension |

## 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:
Strong oxidizing agents
strong reducing agents
alkaline substances



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sodium

### 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 - > 2,000 mg/kg
(OECD Test Guideline 401)
Symptoms: Nausea, Vomiting, Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract., Aspiration may cause pulmonary edema and pneumonitis.
LC50 Inhalation - Rat - male and female - 4 h - 34.25 mg/l - vapor

(OECD Test Guideline 403)
LCLo Inhalation - Rat - 4 h - 20.4 mg/l

Remarks: (RTECS)
LD50 Dermal - Rabbit - 6,350 mg/kg
Remarks: (RTECS)
Dermal: absorption

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

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

**Respiratory or skin sensitization**
Sensitisation test: - Guinea pig
Result: Does not cause skin sensitization.
Remarks: (ECHA)

**Germ cell mutagenicity**
Test Type: In vitro mammalian cell gene mutation test
Test system: Mouse lymphoma test
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Metabolic activation: with and without metabolic activation



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Method: OECD Test Guideline 473
Result: negative
Test Type: Ames test
Test system: Escherichia coli/Salmonella 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

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

After absorption:

We have no description of any toxic symptoms.

Other information

The following applies to ketones in general: when vapours/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

Further data:

Handle in accordance with good industrial hygiene and safety practice.

## SECTION 12: Ecological information

### 12.1 Toxicity

| | |
|---|---|
| Toxicity to fish | flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - > 68 mg/l - 96 h<br>(OECD Test Guideline 203) |
| Toxicity to daphnia | semi-static test EC50 - Daphnia magna (Water flea) - > 81 mg/l - |



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| | |
|---|---|
| and other aquatic invertebrates | 48 h<br>(OECD Test Guideline 202) |
| Toxicity to algae | static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 44.23 mg/l - 72 h<br>(OECD Test Guideline 201) |

**12.2 Persistence and degradability**

| | |
|---|---|
| Biodegradability | aerobic - Exposure time 28 d<br>Result: 84 % - Readily biodegradable.<br>(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 Endocrine disrupting properties**

No data available

**12.7 Other adverse effects**

Discharge into the environment must be avoided.

## SECTION 13: Disposal information

**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. According to Quality Environment Regulation (Scheduled Waste) 2005, waste need to be sent to designated premise for recycle, treatment or disposal. Please contact Kualiti Alam for waste classification and correct disposal method.

## SECTION 14: Transportation information

**14.1 UN number**

ADR/RID: 2397 IMDG: 2397 IATA-DGR: 2397

**14.2 UN proper shipping name**

| | |
|---|---|
| ADR/RID: | 3-METHYLBUTAN-2-ONE |
| IMDG: | 3-METHYLBUTAN-2-ONE |
| IATA-DGR: | 3-Methylbutan-2-one |

**14.3 Transport hazard class(es)**

ADR/RID: 3 IMDG: 3 IATA-DGR: 3



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**14.4 Packaging group**
ADR/RID: II IMDG: II IATA-DGR: II

**14.5 Environmental hazards**
ADR/RID: no IMDG Marine pollutant: no IATA-DGR: no

**14.6 Special precautions for user**
None

**14.7 Incompatible materials**

**Other regulations**
Hazchem Code : •3YE

## SECTION 15: Regulatory information

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

No data available

## SECTION 16: Other information

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

H225 Highly flammable liquid and vapor.

**Further information**
The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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