SAFETY DATA SHEET

Version 8.2
Revision Date 23.06.2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

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 : Sigma-Aldrich Pty. Ltd.
Suite 1, Level 1, Building B
11 Talavera Road
MACQUARIE PARK NSW 2113
AUSTRALIA

Telephone : +61 1800 800 097

1.5 Emergency telephone

Emergency Phone # : Free call (24/7): 1800 448 465
Int'l (24/7): +61 2 9037 2994
(CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

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

Pictogram

Signal word Danger

Hazard statement(s)
H225 Highly flammable liquid and vapor.

Precautionary statement(s)

Prevention
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No

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	smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
Response	
P303 + P361 + P353	IF ON SKIN (or hair): 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 to extinguish.
Storage	
P403 + P235	Store in a well-ventilated place. Keep cool.
Disposal	
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

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.

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.

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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.

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

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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.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.3 no other specific uses are stipulated.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
3-methylbutanone	563-80-4	TWA	200 ppm 705 mg/m3	Australia. Workplace Exposure Standards for Airborne Contaminants.

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 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: 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.

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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	fruity
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point: -92 °C at 1,013 hPa
f)	Initial boiling point and boiling range	93 - 95 °C at 1,013 hPa
g)	Flash point	-1 °C
h)	Evaporation rate	5.6
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 9 %(V) Lower explosion limit: 1.5 %(V)
k)	Vapor pressure	53.33 hPa at 19.9 °C
l)	Vapor density	No data available
m)	Relative density	No data available
n)	Water solubility	8.21 g/l at 20 °C - OECD Test Guideline 105
o)	Partition coefficient: n-octanol/water	log Pow: 2.29 at 20 °C - Bioaccumulation is not expected.
p)	Autoignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 0.5 mPa.s at 25 °C - OECD Test Guideline 114
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 - Surface tension

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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
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
(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

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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
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) - >

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	68 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - > 81 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 44.23 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 84 % - 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

Discharge into the environment must be avoided.

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

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

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

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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

Notification status

AICS:	On the inventory, or in compliance with the inventory
DSL:	All components of this product are on the Canadian DSL
ENCS:	On the inventory, or in compliance with the inventory
ISHL:	On the inventory, or in compliance with the inventory
KECI:	On the inventory, or in compliance with the inventory
NZIoC:	On the inventory, or in compliance with the inventory
PICCS:	On the inventory, or in compliance with the inventory

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 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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