SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 8.4
Revision Date 19.02.2023
Print Date 19.02.2023

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
Index-No.	:	606-007-00-0
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.	:	563-80-4

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	:	Sigma-Aldrich Ireland Limited Vale Road Arklow CO WICKLOW CO WICKLOW IRELAND
Telephone	:	+353 402-20300
E-mail address	:	TechnicalService@merckgroup.com

1.4 Emergency telephone

Emergency Phone #	:	+(353)-19014670 (CHEMTREC)

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

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

The life science business of Merck operates as MilliporeSigma in the US and Canada

Signal Word	Danger
Hazard statement(s)	
H225	Highly flammable liquid and vapor.
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	Danger
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	:	C5H10O
Molecular weight	:	86.13 g/mol
CAS-No.	:	563-80-4
EC-No.	:	209-264-3
Index-No.	:	606-007-00-0

No components need to be disclosed according to the applicable regulations.

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.

The life science business of Merck operates as MilliporeSigma in the US and Canada

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.

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.

The life science business of Merck operates as MilliporeSigma in the US and Canada

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

Component	CAS-No.	Control parameters	Value	Basis
3-methylbutanone	563-80-4	OELV - 8 hrs (TWA)	20 ppm 70.5 mg/m3	Ireland. List of Chemical Agents and Occupational Exposure Limit Values - Schedule 1

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
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)

The life science business of Merck operates as MilliporeSigma in the US and Canada

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	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
f)	Flammability (solid, gas)	No data available
g)	Upper/lower flammability or explosive limits	Upper explosion limit: 9 %(V) 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 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	No data available

The life science business of Merck operates as MilliporeSigma in the US and Canada

characteristics

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

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 - 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

The life science business of Merck operates as MilliporeSigma in the US and Canada

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
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

The life science business of Merck operates as MilliporeSigma in the US and Canada

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 (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

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

No data available

12.7 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. Notice Directive on waste 2008/98/EC.

The life science business of Merck operates as MilliporeSigma in the US and Canada

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2397 IMDG: 2397 IATA: 2397

14.2 UN proper shipping name

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

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. : FLAMMABLE LIQUIDS

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.

H225 Highly flammable liquid and vapor.

The life science business of Merck operates as MilliporeSigma in the US and Canada

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

The life science business of Merck operates as MilliporeSigma in the US and Canada

The life science business of Merck operates as MilliporeSigma in the US and Canada