ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

Isophorone

Revision Date:2026-06-06 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name	: Isophorone
CBnumber	: CB7743348
CAS	: 78-59-1
EINECS Number	: 201-126-0
Synonyms	: Isophorone,3,5,5-trimethylcyclohex-2-en-1-one

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word Warning

Precautionary statements

P201 Obtain special instructions before use.

P202 Do not handle until all safety precautions have been read and understood.

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P264 Wash hands thoroughly after handling.

P264 Wash skin thouroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P271 Use only outdoors or in a well-ventilated area.

P273 Avoid release to the environment.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P308+P313 IF exposed or concerned: Get medical advice/attention.

P370+P378 In case of fire: Use … for extinction.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

P501 Dispose of contents/container to.....

Hazard statements

H227 Combustible liquid

H302 Harmful if swallowed

H312 Harmful in contact with skin

H319 Causes serious eye irritation

H335 May cause respiratory irritation

H336 May cause drowsiness or dizziness

H351 Suspected of causing cancer

H402 Harmful to aquatic life

SECTION 3: Composition/information on ingredients

Substance

Product name	: Isophorone
Synonyms	: Isophorone,3,5,5-trimethylcyclohex-2-en-1-one
CAS	: 78-59-1
EC number	: 201-126-0
MF	: C9H14O
MW	: 138.21

SECTION 4: First aid measures

Description of first aid measures

General advice

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

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

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

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

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.

Special hazards arising from the substance or mixture

Nature of decomposition products not known. Combustible.

Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

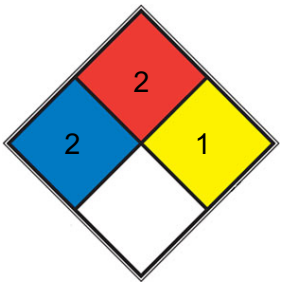
Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

NFPA 704



■	HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. diethyl ether, ammonium phosphate, iodine)
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
■	REACT	1	Normally stable, but can become unstable at elevated temperatures and pressures (e.g. propene)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

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.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,7 mm Break through time: 480 min Material tested:Butoject? (KCL 898)

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: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 120 min

Material tested:Camatril? (KCL 730 / Aldrich Z677442, Size M)

Body Protection

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.

Exposure limits

TLV-TWA 25 mg/m^3 (5 ppm); IDLH 800 ppm.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	light yellow liquid, clear
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: -8 °C - lit.
Initial boiling point and boiling range	213 - 214 °C - lit.
Flash point	96,0 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	Upper explosion limit: 3,8 %(V) Lower explosion limit: 0,8 %(V)

limits	
Vapour pressure	1,3 hPa at 38,0 °C 0,3 hPa at 20,0 °C
Vapour density	4.77 (vs air)
Relative density	No data available
Water solubility	14,5 g/l - completely soluble
Partition coefficient: n-octanol/water	log Pow: 1,67 at 20 °C - Bioaccumulation is not expected.
Autoignition temperature	462,0 °C
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: 2,83 mm2/s at 20 °C - OECD Test Guideline 114 Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	(x 10^{-6} atm?m^3/mol): 5.8 (calculated, U.S. EPA, 1980a)

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents

Conditions to avoid

Strong heating.

Incompatible materials

No data available

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 1.500 mg/kg

Remarks:

(ECHA)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

LC50 Inhalation - Rat - male - 4 h - 7 mg/l Remarks:

(ECHA)

LD50 Dermal - Rabbit - male and female - 1.200 mg/kg Remarks:

(ECHA)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation. (Draize Test)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

Salmonella typhimurium Result: negative Remarks:

(National Toxicology Program)

In vitro mammalian cell gene mutation test mouse lymphoma cells

Result: Positive results were obtained in some in vitro tests. Remarks:

(ECHA)

Chromosome aberration test in vitro

Chinese hamster ovary cells Result: negative

Remarks:

(ECHA)

Chromosome aberration test in vitro Chinese hamster lung cells

Result: Positive results were obtained in some in vitro tests. Remarks:

(ECHA)

sister chromatid exchange assay Chinese hamster ovary cells Result: negative

Remarks:

(ECHA)

unscheduled DNA synthesis assay rat hepatocytes

Result: negative Remarks:

(ECHA)

Drosophila melanogaster (vinegar fly) - male Result: negative

Remarks:

(ECHA)

Mouse - male and female Result: negative Remarks:

(ECHA)

Result: negative Remarks:

(National Toxicology Program)

Carcinogenicity

Suspected of causing cancer.

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory Tract Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) Acute inhalation toxicity - mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Toxicity

LD50 in male, female rats and male mice (mg/kg): 2700 ±200, 2100 ±200, 2200 ±200 orally (PB90-180225)

SECTION 12: Ecological information

Toxicity

Toxicity to fish

flow-through test LC50 - Pimephales promelas (fathead minnow) - 228 mg/l - 96 h

Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates

static test LC50 - Daphnia magna (Water flea) - 120 mg/l - 48 h (US-EPA)

Toxicity to algae

static test EC50 - Desmodesmus subspicatus (green algae) - 475 mg/l - 72 h

Remarks: (ECHA)

Toxicity to bacteria

EC10 - Pseudomonas putida - 435 mg/l - 18 h

Remarks: (External MSDS)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 95 % - Readily biodegradable. (Directive 67/548/EEC Annex V, C.4.A.)

Bioaccumulative potential

Bioaccumulation Cyprinus carpio (Carp) - 42 Days

at 25 °C - 0,5 mg/l(isophorone)

Bioconcentration factor (BCF): 1,1 - 1,8 (OECD Test Guideline 305)

Mobility in soil

No data available

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.

Toxics Screening Level

The initial threshold screening level (ITSL) for isophorone is 280 µg/m3 (1-hour average).

Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

Waste Disposal

Incineration.

SECTION 14: Transport information

UN number

ADR/RID: - IMDG: - IATA: -

UN proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

Packaging group

ADR/RID: - IMDG: - IATA: -

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: https://www.mee.gov.cn/

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

Korea Existing Chemicals List (KECL):Listed. website: http://ncis.nier.go.kr

New Zealand Inventory of Chemicals (NZIoC):Listed. website: https://www.epa.govt.nz/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

【1】CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

【2】ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

【3】ECHA - European Chemicals Agency, website: https://echa.europa.eu/

【4】eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

【5】ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

【6】Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

【7】HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

【8】IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

【9】IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

【10】Sigma-Aldrich, website: https://www.sigmaaldrich.com/

Other Information

The occupational exposure limit value should not be exceeded during any part of the working exposure.