

1 Identification

Product identifier

Product name: Isophorone

Stock number: L04130

CAS Number:

78-59-1

EC number:

201-126-0

Index number:

606-012-00-8

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

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS08 Health hazard

Carc. 2 H351 Suspected of causing cancer.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Eye Irrit. 2 H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

H227 Combustible liquid.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS07 GHS08

Signal word

Warning

Hazard statements

H227 Combustible liquid.

H302+H312 Harmful if swallowed or in contact with skin.

H319 Causes serious eye irritation.

H351 Suspected of causing cancer.

H335 May cause respiratory irritation.

Precautionary statements

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

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

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. Continue rinsing.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

B3 - Combustible liquid

D2B - Toxic material causing other toxic effects



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 2 Health (acute effects) = 2

FIRE 2 Flammability = 2

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

Product name: **Isophorone**

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3 Composition/information on ingredients

Chemical characterization: Substances
CAS# Description:
78-59-1 3,5,5-Trimethylcyclohex-2-enone
Identification number(s):
EC number: 201-126-0
Index number: 606-012-00-8

4 First-aid measures

Description of first aid measures
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Seek medical treatment.
Information for doctor
Most important symptoms and effects, both acute and delayed No further relevant information available.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media
Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
Special hazards arising from the substance or mixture
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.
Methods and material for containment and cleaning up:
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose of contaminated material as waste according to section 13.
Ensure adequate ventilation.
Prevention of secondary hazards: Keep away from ignition sources.
Reference to other sections
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage

Handling
Precautions for safe handling
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Information about protection against explosions and fires: Keep ignition sources away.
Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: No special requirements.
Information about storage in one common storage facility:
Do not store together with acids.
Store away from strong bases.
Store away from oxidizing agents.
Further information about storage conditions:
Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.
Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:

78-59-1 3,5,5-Trimethylcyclohex-2-enone (100.0%)

PEL (USA)	Long-term value: 140 mg/m³, 25 ppm
REL (USA)	Long-term value: 23 mg/m³, 4 ppm
TLV (USA)	Ceiling limit value: 28 mg/m³, 5 ppm
EL (Canada)	Short-term value: C 5 ppm

Additional information: No data

Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Do not inhale dust / smoke / mist.

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USA

Product name: Isophorone	
<div>Avoid contact with the eyes. Avoid contact with the eyes and skin. Maintain an ergonomically appropriate working environment. Breathing equipment: Use suitable respirator when high concentrations are present. Recommended filter device for short term use: Use a respirator with organic vapor/acid gas cartridges as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards such as NIOSH (USA) or CEN (EU). Protection of hands: Impervious gloves Check protective gloves prior to each use for their proper condition. The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer. Penetration time of glove material (in minutes) Not determined Eye protection: Safety glasses Body protection: Protective work clothing.</div>	

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9 Physical and chemical properties

Information on basic physical and chemical properties	
General Information	
Appearance:	
Form:	Liquid
Color:	Colorless
Odor:	Not determined
Odor threshold:	Not determined.
pH-value:	Not determined.
Change in condition	
Melting point/Melting range:	-8 °C (18 °F)
Boiling point/Boiling range:	99 °C (210 °F) (18mm Hg)
Sublimation temperature / start:	Not determined
Flash point:	
Flash point:	84 °C (183 °F)
Flammability (solid, gaseous)	Not applicable.
Ignition temperature:	460 °C (860 °F)
Decomposition temperature:	Not determined
Auto igniting:	Not determined.
Danger of explosion:	
Explosion limits:	Not determined.
Lower:	0.8 Vol %
Upper:	3.8 Vol %
Vapor pressure at 20 °C (68 °F):	0.33 hPa
Density at 20 °C (68 °F):	0.922 g/cm³ (7.694 lbs/gal)
Relative density	Not determined.
Vapor density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water at 20 °C (68 °F):	12 g/l
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not determined.
kinematic:	Not determined.
Other information	No further relevant information available.

10 Stability and reactivity

Reactivity No information known.	
Chemical stability Stable under recommended storage conditions.	
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.	
Possibility of hazardous reactions Reacts with strong oxidizing agents	
Conditions to avoid No further relevant information available.	
Incompatible materials:	
Acids	
Oxidizing agents	
Bases	
Hazardous decomposition products: Carbon monoxide and carbon dioxide	

11 Toxicological information

Information on toxicological effects	
Acute toxicity:	
Harmful in contact with skin.	
Harmful if swallowed.	
Danger through skin absorption.	
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for this substance.	
LD/LC50 values that are relevant for classification:	
Oral	LD50 700 mg/kg (guinea pig) 2690 mg/kg (mouse) 1870 mg/kg (rat) 1420 mg/kg (rabbit)
Dermal	LD50 1200 mg/kg (mam) 1390 mg/kg (rat) 1500 µL/kg (rabbit)
Inhalative	LC50 7000 mg/m3 (rat) LC50/8H 4600 ppm/8H (guinea pig)
Skin irritation or corrosion: May cause irritation	
Eye irritation or corrosion: Causes serious eye irritation.	
Sensitization: No sensitizing effects known.	
Germ cell mutagenicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains mutation data for this substance.	

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USA

Product name: **Isophorone**

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Carcinogenicity:
Suspected of causing cancer.
ACGIH A3: Animal carcinogen: Agent is carcinogenic in experimental animals at a relatively high dose, by route(s) of administration, at site(s), of histologic type(s), or by mechanism(s) not considered relevant to worker exposure. Available epidemiologic studies do not confirm an increased risk of cancer in exposed humans. Available evidence suggests that the agent is not likely to cause cancer in humans except under uncommon or unlikely routes or levels of exposure.
EPA-C: Possible human carcinogen: limited evidence of carcinogenicity in animals in the absence of human data.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains tumorigenic and/or carcinogenic and/or neoplastic data for this substance.
Reproductive toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains reproductive data for this substance.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: May cause respiratory irritation.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for this substance.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Additional ecological information:
General notes:
Do not allow product to reach ground water, water course or sewage system.
Do not allow material to be released to the environment without proper governmental permits.
Danger to drinking water if even small quantities leak into the ground.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, ADN, IMDG, IATA	Not applicable
UN proper shipping name DOT, ADN, IMDG, IATA	Not applicable
Transport hazard class(es) DOT, ADR, ADN, IMDG, IATA Class	Not applicable
Packing group DOT, IMDG, IATA	Not applicable
Environmental hazards:	Not applicable.
Special precautions for user	Not applicable.
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT Hazardous substance:	5000 lbs, 2270 kg
Marine Pollutant (DOT):	No
UN "Model Regulation":	-

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms



GHS07 GHS08

Signal word Warning

Hazard statements

H227 Combustible liquid.
H302+H312 Harmful if swallowed or in contact with skin.
H319 Causes serious eye irritation.
H351 Suspected of causing cancer.
H335 May cause respiratory irritation.

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
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. Continue rinsing.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

National regulations

All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.
All components of this product are listed on the Canadian Domestic Substances List (DSL).

SARA Section 313 (specific toxic chemical listings) Substance is not listed.

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USA

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California Proposition 65
Prop 65 - Chemicals known to cause cancer Substance is not listed.
Prop 65 - Developmental toxicity Substance is not listed.
Prop 65 - Developmental toxicity, female Substance is not listed.
Prop 65 - Developmental toxicity, male Substance is not listed.
Information about limitation of use: For use only by technically qualified individuals.
Other regulations, limitations and prohibitive regulations
Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.
Substance is not listed.
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information
Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department
Date of preparation / last revision 11/23/2015 / -
Abbreviations and acronyms:
RID: Règlement International concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
ICAO: International Civil Aviation Organization
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
DOT: US Department of Transportation
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)

USA