

SAFETY DATA SHEET

Creation Date 19-Apr-2012

Revision Date 18-Dec-2025

Revision Number 7

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name Isophorone

Cat No. : AC122640000; AC122640010; AC122640025; AC122640050; AC122645000

CAS No 78-59-1
Synonyms 3,5,5-Trimethyl-2-cyclohexen-1-one

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11

Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99

CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 4
Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Serious Eye Damage/Eye Irritation	Category 2
Carcinogenicity	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Warning

Hazard Statements

Combustible liquid
Causes serious eye irritation
May cause respiratory irritation
Suspected of causing cancer
Harmful if swallowed or in contact with skin

**Precautionary Statements****Prevention**

Obtain special instructions before use
Do not handle until all safety precautions have been read and understood
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear eye/face protection
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
Keep cool
Wear protective gloves/protective clothing/eye protection/face protection

Response

IF exposed or concerned: Get medical attention/advice

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing

Skin

IF ON SKIN: Wash with plenty of soap and water
Call a POISON CENTER or doctor if you feel unwell
Take off contaminated clothing and wash before reuse

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam to extinguish

Storage

Store locked up
Store in a well-ventilated place. Keep container tightly closed

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
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Isophorone	78-59-1	>95
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4. First-aid measures

General Advice	If symptoms persist, call a physician.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Get medical attention. Wash off immediately with plenty of water for at least 15 minutes.
Inhalation	Remove to fresh air. If breathing is difficult, give oxygen. Get medical attention.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	None reasonably foreseeable. . Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	84 °C / 183.2 °F
Method -	No information available
Autoignition Temperature	460 °C / 860 °F
Explosion Limits	
Upper	3.8%
Lower	0.8%
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Combustible material. Containers may explode when heated. Keep product and empty container away from heat and sources of ignition. Risk of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health
2

Flammability
2

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition.

7. Handling and Storage

Handling Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition.

Storage. Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Isophorone	Ceiling: 5 ppm	(Vacated) TWA: 4 ppm (Vacated) TWA: 23 mg/m ³ TWA: 25 ppm TWA: 140 mg/m ³	IDLH: 200 ppm REL = 4 ppm (TWA) REL = 23 mg/m ³ (TWA)	Ceiling: 5 ppm

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Tight sealing safety goggles. Face protection shield.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended Filter type: Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State

Color

Odor

Odor Threshold

Property

Melting Point/Range

Softening Point

Boiling Point/Range

Flash Point

Liquid

Light yellow

Mint-like

No information available

Values

-8 °C / 17.6 °F

No data available

213 - 214 °C / 415.4 - 417.2 °F

84 °C / 183.2 °F

Remarks

Method

Method - No information available

Flammability (liquid)	Combustible liquid	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 0.8 Upper 3.8	
Autoignition Temperature	460 - °C / 860 - °F	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	2.6 mPa at 20 °C	
Water Solubility	12 g/L (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Isophorone	1.67	
Vapor Pressure	0.4 hPa @ 20 °C	
Density / Specific Gravity	0.920	
Bulk Density	Not applicable	Liquid
Vapor Density	4.8 (Air = 1.0)	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	
Other Information		
Molecular Formula	C9 H14 O	
Molecular Weight	138.21	
Explosive Properties	explosive air/vapour mixtures possible	

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents, Strong acids, Strong bases
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	May cause irritation of respiratory tract.
Ingestion	Ingestion may cause irritation to mucous membranes.
Eyes	Irritating to eyes. Contact with eyes may cause irritation.
Skin	Irritating to skin. May cause eye/skin irritation.

Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isophorone	LD50 = 1870 mg/kg (Rat)	LD50 = 1700 mg/kg (Rat)	LC50 = 7 mg/L (Rat) 4 h

Toxicologically Synergistic Products	No information available
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(b) skin corrosion/irritation; Based on available data, the classification criteria are not met

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory

Based on available data, the classification criteria are not met

Skin

Based on available data, the classification criteria are not met

(e) germ cell mutagenicity; Based on available data, the classification criteria are not met

(f) carcinogenicity; Category 2

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Isophorone	78-59-1	Group 2B	Not listed	A3	X	A3

ACGIH: (American Conference of Governmental Industrial Hygienists)

A1 - Known Human Carcinogen

A2 - Suspected Human Carcinogen

A3 - Animal Carcinogen

ACGIH: (American Conference of Governmental Industrial Hygienists)

Mexico - Occupational Exposure Limits - Carcinogens

Mexico - Occupational Exposure Limits - Carcinogens

A1 - Confirmed Human Carcinogen

A2 - Suspected Human Carcinogen

A3 - Confirmed Animal Carcinogen

A4 - Not Classifiable as a Human Carcinogen

A5 - Not Suspected as a Human Carcinogen

(g) reproductive toxicity; Based on available data, the classification criteria are not met

(h) STOT-single exposure; Category 3

Results / Target organs

Respiratory system.

(i) STOT-repeated exposure; Based on available data, the classification criteria are not met

Target Organs

None known.

(j) aspiration hazard; Based on available data, the classification criteria are not met

Other Adverse Effects

The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

Other Adverse Effects

The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties

This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Isophorone	EC50: 51.1 - 342 mg/L, 96h (Pseudokirchneriella)	LC50: 132 - 159 mg/L, 96h flow-through (Pimephales)	Not listed	EC50: = 117 mg/L, 48h (Daphnia magna)

	subcapitata) EC50: = 475.4 mg/L, 72h (Desmodesmus subspicatus)	promelas) LC50: 213 - 271 mg/L, 96h static (Pimephales promelas) LC50: 180 - 250 mg/L, 96h static (Lepomis macrochirus)		
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Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility . Will likely be mobile in the environment due to its water solubility.

Component	log Pow
Isophorone	1.67

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT COMBUSTIBLE LIQUID, NOT REGULATED FOR TRANSPORT IN THIS QUANTITY
According to 49 CFR §173.150(f)(1), this material should be reclassified as NA1993, Combustible Liquid, NOS if it is shipped in bulk

UN-No NA1993
Proper Shipping Name Combustible liquid, n.o.s.
Packing Group III

TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Isophorone	78-59-1	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

-/- - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Isophorone	78-59-1	X	-	201-126-0	X	X	X	X	X	KE-34467

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations**SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act)

Component	CWA - Hazardous Substances	CWA - Reportable Quantities	CWA - Toxic Pollutants	CWA - Priority Pollutants
Isophorone	-	-	X	X

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Isophorone	X		-

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355).

Component	Hazardous Substances RQs	CERCLA Extremely Hazardous Substances RQs	SARA Reportable Quantity (RQ)
Isophorone	5000 lb	-	5000 lb 2270 kg

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Isophorone	X	X	X	X	X

U.S. Department of Transportation

Reportable Quantity (RQ): Y
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade Slight risk, Grade 1

Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous	REACH Regulation (EC 1907/2006) article 59 - Candidate List of

			Substances	Substances of Very High Concern (SVHC)
Isophorone	78-59-1	-	Use restricted. See entry 75. (see link for restriction details)	-

REACH links

<https://echa.europa.eu/substances-restricted-under-reach>

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Isophorone	78-59-1	Listed	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Isophorone	78-59-1	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information**Prepared By**

Product stewardship (Regulatory Affairs)
Thermo Fisher Scientific
email - begel.sdsdesk@thermofisher.com

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Revision Summary

Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS