

SAFETY DATA SHEET

Creation Date 19-Apr-2012

Revision Date 26-Jan-2018

Revision Number 4

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 Not for food, drug, pesticide or biocidal product use

Details of the supplier of the safety data sheet

Company

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

Emergency Telephone Number

For information **US** call: 001-800-ACROS-01 / **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 by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

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

**Precautionary Statements****Prevention**

Obtain special instructions before use
 Do not handle until all safety precautions have been read and understood
 Use personal protective equipment as required
 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/sparks/open flames/hot surfaces. - No smoking
 Keep cool

Response

IF exposed or concerned: Get medical attention/advice

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Skin

IF ON SKIN: Wash with plenty of soap and water
 Call a POISON CENTER or doctor/physician if you feel unwell
 Wash contaminated clothing 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 for extinction

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

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Isophorone	78-59-1	>95

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	Obtain medical attention. Wash off immediately with plenty of water for at least 15 minutes.
Inhalation	Move to fresh air. If breathing is difficult, give oxygen. Obtain medical attention.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	None reasonably foreseeable. . Breathing difficulties. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray.
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. 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. 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 and sources of ignition.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	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 TWA: 4 ppm TWA: 23 mg/m ³	Ceiling: 5 ppm Ceiling: 25 mg/m ³

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH IDLH: The National Institute for Occupational Safety and Health Immediately Dangerous to Life or 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 Tightly fitting safety goggles. Face-shield.

Skin and body protection Long sleeved clothing.

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.

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

9. Physical and chemical properties

Physical State	Liquid
Appearance	Light yellow
Odor	mint-like
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-8 °C / 17.6 °F
Boiling Point/Range	213 - 214 °C / 415.4 - 417.2 °F
Flash Point	84 °C / 183.2 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	3.8%
Lower	0.8%
Vapor Pressure	0.4 hPa @ 20 °C
Vapor Density	4.8 (Air = 1.0)
Specific Gravity	0.920
Solubility	soluble
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	460 °C / 860 °F
Decomposition Temperature	No information available
Viscosity	2.6 mPa at 20 °C
Molecular Formula	C ₉ H ₁₄ O
Molecular Weight	138.21

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

Acute Toxicity

Product Information

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isophorone	LD50 = 1870 mg/kg (Rat)	LD50 = 1700 mg/kg (Rat) LD50 = 1390 mg/kg (Rat)	LC50 = 7 mg/L (Rat) 4 h

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity 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	Not listed	Not listed	A3	Not listed	A3

ACGIH: (American Conference of Governmental Industrial Hygienists)

*A1 - Known Human Carcinogen
A2 - Suspected Human Carcinogen
A3 - Animal Carcinogen*

Mexico - Occupational Exposure Limits - Carcinogens

*ACGIH: (American Conference of Governmental Industrial Hygienists)
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*

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

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 subcapitata) EC50: = 475.4 mg/L, 72h (Desmodesmus subspicatus)	LC50: 132 - 159 mg/L, 96h flow-through (Pimephales promelas) LC50: 213 - 271 mg/L, 96h static (Pimephales promelas) LC50: 180 - 250 mg/L, 96h static (Lepomis macrochirus)	Not listed	EC50: = 117 mg/L, 48h (Daphnia magna)

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	1.66

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	Not regulated
TDG	Not regulated
IATA	Not regulated
IMDG/IMO	Not regulated

15. Regulatory information

All of the components in the product are on the following Inventory lists: X = listed

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
Isophorone	X	X	-	201-126-0	-		X	X	X	X	X

Legend:

X - Listed

E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.

F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.

N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.

P - Indicates a commenced PMN substance

R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.

S - Indicates a substance that is identified in a proposed or final Significant New Use Rule

T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.

XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B)).

Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.

Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations**TSCA 12(b)**

SARA 313 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

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)

Component	Hazardous Substances RQs	CERCLA EHS RQs
Isophorone	5000 lb	-

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): N
 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

16. Other information

Prepared By Regulatory Affairs
 Thermo Fisher Scientific
 Email: EMSDS.RA@thermofisher.com

Creation Date 19-Apr-2012
Revision Date 26-Jan-2018
Print Date 26-Jan-2018
Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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