

Creation Date 19-Apr-2012

Revision Date 13-Dec-2020

Revision Number 7

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: Isophorone
Cat No. : 122640000; 122640010; 122640025; 122640050; 122645000
Synonyms 3,5,5-Trimethyl-2-cyclohexen-1-one
CAS-No 78-59-1
EC-No. 201-126-0
Molecular Formula C9 H14 O
Reach Registration Number 01-2119497282-32

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

Recommended Use Laboratory chemicals.
Sector of use SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites
Product category PC21 - Laboratory chemicals
Process categories PROC15 - Use as a laboratory reagent
Environmental release category ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)
Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company **UK entity/business name**
 Fisher Scientific UK
 Bishop Meadow Road, Loughborough,
 Leicestershire LE11 5RG, United Kingdom

EU entity/business name
 Acros Organics BVBA
 Janssen Pharmaceuticaaan 3a
 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. 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

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

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Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity	Category 4 (H302)
Acute dermal toxicity	Category 4 (H312)
Serious Eye Damage/Eye Irritation	Category 2 (H319)
Carcinogenicity	Category 2 (H351)
Specific target organ toxicity - (single exposure)	Category 3 (H335)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

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

Precautionary Statements

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P312 - Call a POISON CENTER or doctor/physician if you feel unwell
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
P280 - Wear protective gloves/protective clothing/eye protection/face protection

2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

Toxicity to Soil Dwelling Organisms
Toxic to terrestrial vertebrates

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008
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Isophorone	78-59-1	EEC No. 201-126-0	>95	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Eye Irrit. 2 (H319) Carc. 2 (H351) STOT SE 3 (H335)
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Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Isophorone	STOT SE 3 :: C>=10%	-	-

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Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of 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.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Inhalation	Remove to fresh air. If breathing is difficult, give oxygen. Get medical attention.
Self-Protection of the First Aider	Use personal protective equipment as required.

4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable. . Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician	Treat symptomatically.
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SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

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).

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5.3. Advice for firefighters

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

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

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

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe 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.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK)
(Germany)

Class 10

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s): **UK** - EH40/2005 Work Exposure Limits, Third edition. Published 2018. **IRE** - 2018 Code of Practice for the Chemical Agents Regulations, Schedule 1. Published by the Health and Safety Authority

Component	The United Kingdom	European Union	Ireland
Isophorone	STEL: 5 ppm 15 min STEL: 29 mg/m ³ 15 min		STEL: 5 ppm 15 min STEL: 25 mg/m ³ 15 min

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Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

Derived No Effect Level (DNEL) No information available

<u>Route of exposure</u>	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral Dermal Inhalation				

Predicted No Effect Concentration (PNEC) No information available.

8.2. Exposure controls

Engineering Measures

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

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments (minimum requirement)
Natural rubber	See manufacturers	-	EN 374	
Nitrile rubber	recommendations			
Neoprene				
PVC				

Skin and body protection Long sleeved clothing

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 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

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EN14387

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141
When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Light yellow	
Odor	Mint-like	
Odor Threshold	No data available	
Melting Point/Range	-8 °C / 17.6 °F	
Softening Point	No data available	
Boiling Point/Range	213 - 214 °C / 415.4 - 417.2 °F	
Flammability (liquid)	Combustible liquid	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 0.8 Upper 3.8	
Flash Point	84 °C / 183.2 °F	Method - No information available
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	1.66	
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)	

9.2. Other information

Molecular Formula	C9 H14 O
Molecular Weight	138.21
Explosive Properties	explosive air/vapour mixtures possible

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Stable under normal conditions.

10.3. Possibility of hazardous reactions

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Hazardous Polymerization Hazardous Reactions

Hazardous polymerization does not occur.
None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases.

10.6. Hazardous decomposition products

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

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

Oral Category 4
Dermal Category 4
Inhalation Based on available data, the classification criteria are not met

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

(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

(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

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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.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects Do not empty into drains.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Isophorone	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)	EC50: = 117 mg/L, 48h (Daphnia magna)	EC50: 51.1 - 342 mg/L, 96h (Pseudokirchneriella subcapitata) EC50: = 475.4 mg/L, 72h (Desmodesmus subspicatus)

12.2. Persistence and degradability

Persistence Soluble in water, Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Isophorone	1.66	7

12.4. Mobility in soil

The product is water soluble, and may spread in water systems. Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB assessment

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB).

12.6. Endocrine disrupting properties

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects Persistent Organic Pollutant Ozone Depletion Potential

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

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Contaminated Packaging	Dispose of this container to hazardous or special waste collection point.
European Waste Catalogue (EWC)	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
Other Information	Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
14.4. Packing group

ADR Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
14.4. Packing group

IATA Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
14.4. Packing group

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

X = listed, Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), China (IECSC), Japan (ENCS), Australia (AICS), Korea (ECL).

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	IECSC	AICS	KECL
Isophorone	201-126-0	-		X	X	-	X	X	X	X	KE-3446 7

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals
Not applicable

National Regulations

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WGK Classification See table for values

Component	Germany - Water Classification (VwVwS)	Germany - TA-Luft Class
Isophorone	WGK1	Class I : 20 mg/m ³ (Massenkonzentration)

Component	France - INRS (Tables of occupational diseases)
Isophorone	Tableaux des maladies professionnelles (TMP) - RG 84

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed
H312 - Harmful in contact with skin
H319 - Causes serious eye irritation
H351 - Suspected of causing cancer
H335 - May cause respiratory irritation

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC (volatile organic compound)

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

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Revision Summary

Update to CLP Format.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006
COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No
1907/2006**

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 Safety Data Sheet