

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

### 1.1. Product identifier

<b>Product Description:</b>	<b>Isophorone</b>
<b>Cat No. :</b>	<b>122640000; 122640010; 122640025; 122640050; 122645000</b>
<b>Synonyms</b>	3,5,5-Trimethyl-2-cyclohexen-1-one
<b>Index No</b>	606-012-00-8
<b>CAS No</b>	78-59-1
<b>EC No</b>	201-126-0
<b>Molecular Formula</b>	C9 H14 O
<b>REACH registration number</b>	01-2119497282-32

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

<b>Recommended Use</b>	Laboratory chemicals.
<b>Sector of use</b>	SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites
<b>Product category</b>	PC21 - Laboratory chemicals
<b>Process categories</b>	PROC15 - Use as a laboratory reagent
<b>Environmental release category</b>	ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)
<b>Uses advised against</b>	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**  
Thermo Fisher Scientific  
Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

**E-mail address** begel.sdsdesk@thermofisher.com

### 1.4. 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

**CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567**

**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 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 person to fresh air and keep 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  
This product does not contain any known or suspected endocrine disruptors

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

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## 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
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)

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Isophorone	STOT SE 3 (H335) :: 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

<b>General Advice</b>	If symptoms persist, call a physician.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Get medical attention. Wash off immediately with plenty of water for at least 15 minutes.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water.
<b>Inhalation</b>	Remove to fresh air. If breathing is difficult, give oxygen. Get medical attention.
<b>Self-Protection of the First Aider</b>	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

<b>Notes to Physician</b>	Treat symptomatically.
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## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### Suitable Extinguishing Media

Water spray, carbon dioxide (CO<sub>2</sub>), 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

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ignition. Risk of ignition.

## **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

### **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**      Class 10  
**Storage Class (LGK) (Germany)**

### **7.3. Specific end use(s)**

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1. Control parameters**

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## Exposure limits

List source(s): **UK** - EH40/2005 Work Exposure Limits, Fourth edition. Published 2020. **IRE** - 2021 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 <sup>3</sup> 15 min		STEL: 5 ppm 15 min STEL: 25 mg/m <sup>3</sup> 15 min

## Biological limit values

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

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

See table for values

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Isophorone 78-59-1 (>95)		DNEL = 41mg/kg bw/day		DNEL = 20.5mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Isophorone 78-59-1 (>95)	DNEL = 22mg/m <sup>3</sup>	DNEL = 22mg/m <sup>3</sup>	DNEL = 11mg/m <sup>3</sup>	DNEL = 11mg/m <sup>3</sup>

## Predicted No Effect Concentration (PNEC)

See values below.

## 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
Natural rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Nitrile rubber				
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

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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 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

<b>Physical State</b>	Liquid	
<b>Appearance</b>	Light yellow	
<b>Odor</b>	Mint-like	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	-8 °C / 17.6 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	213 - 214 °C / 415.4 - 417.2 °F	
<b>Flammability (liquid)</b>	Combustible liquid	On basis of test data
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	<b>Lower</b> 0.8 <b>Upper</b> 3.8	
<b>Flash Point</b>	84 °C / 183.2 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	460 - °C / 860 - °F	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	2.6 mPa at 20 °C	
<b>Water Solubility</b>	12 g/L (20°C)	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Component</b>	<b>log Pow</b>	
Isophorone	1.67	
<b>Vapor Pressure</b>	0.4 hPa @ 20 °C	
<b>Density / Specific Gravity</b>	0.920	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	4.8 (Air = 1.0)	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

### 9.2. Other information

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

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## 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

#### 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 (CO<sub>2</sub>).

## 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

Component	EU	UK	Germany	IARC
Isophorone				Group 2B

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- (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.

## 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	1.67	7 dimensionless

### 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

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

**12.7. Other adverse effects**

**Persistent Organic Pollutant**

This product does not contain any known or suspected substance

**Ozone Depletion Potential**

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.

**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

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

### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Isophorone	78-59-1	201-126-0	-	-	X	X	KE-34467	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Isophorone	78-59-1	X	ACTIVE	X	-	X	X	X

**Legend:** X - Listed '-' - Not Listed

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

### 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 Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isophorone	78-59-1	-	Use restricted. See item 75. (see link for restriction details)	-

### REACH links

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

### Seveso III Directive (2012/18/EC)

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
Isophorone	78-59-1	Not applicable	Not applicable

### 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

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

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

### National Regulations

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

### WGK Classification

See table for values

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

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

## 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/NDSL** - 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.

**Creation Date** 19-Apr-2012  
**Revision Date** 25-Sep-2023  
**Revision Summary** Not applicable.

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**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

## 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**