

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

### 1.1. Product identifier

**Product Description:** Lead in Isooctane standard solution, Specpure®, 0µg/g(0.000g/gal)  
**Cat No. :** 45330  
**Molecular Formula** Matrix: Isooctane

### 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** Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

**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

Flammable liquids

Category 2 (H225)

#### Health hazards

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Aspiration Toxicity  
Skin Corrosion/Irritation  
Specific target organ toxicity - (single exposure)

Category 1 (H304)  
Category 2 (H315)  
Category 3 (H336)

## **Environmental hazards**

Acute aquatic toxicity  
Chronic aquatic toxicity

Category 1 (H400)  
Category 1 (H410)

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



Signal Word

Danger

## **Hazard Statements**

H225 - Highly flammable liquid and vapor  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H336 - May cause drowsiness or dizziness  
H410 - Very toxic to aquatic life with long lasting effects

## **Precautionary Statements**

P264 - Wash face, hands and any exposed skin thoroughly after handling  
P280 - Wear protective gloves/protective clothing  
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
P331 - Do NOT induce vomiting  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower  
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

## **2.3. Other hazards**

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

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### **3.2. Mixtures**

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Isooctane	540-84-1	EEC No. 208-759-1	100	Flam. Liq. 2 (H225) Asp. Tox. 1 (H304) Skin Irrit. 2 (H315) STOT SE 3 (H336) Aquatic Acute 1 (H400)

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				Aquatic Chronic 1 (H410)
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Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Isooctane	-	1	-

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>	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water. Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs (by aspiration).
<b>Self-Protection of the First Aider</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

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

**Notes to Physician** Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Carbon dioxide (CO<sub>2</sub>). Powder. Foam. Water may be ineffective. 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

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Do not allow run-off from fire-fighting to enter drains or water courses.

#### **Hazardous Combustion Products**

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

### 5.3. Advice for firefighters

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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

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

### 6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

### 6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

### 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. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

### 7.2. Conditions for safe storage, including any incompatibilities

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

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 3  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

List source(s):

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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

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

See table for values

Component	Acute effects local (Oral)	Acute effects systemic (Oral)	Chronic effects local (Oral)	Chronic effects systemic (Oral)
Isooctane 540-84-1 ( 100 )				699 mg/kg bw/day

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Isooctane 540-84-1 ( 100 )				DNEL = 773mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Isooctane 540-84-1 ( 100 )				DNEL = 2035mg/m <sup>3</sup>

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. 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** Wear safety glasses with side shields (or goggles) (European standard - EN 166)

**Hand Protection** Protective gloves

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

**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 compatability, 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** In case of insufficient ventilation, wear suitable respiratory equipment  
**Recommended Filter type:** Organic gases and vapours filter

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**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.  
When RPE is used a face piece Fit Test should be conducted

**Environmental exposure controls** Prevent product from entering drains. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

<b>Physical State</b>	Liquid	
<b>Appearance</b>	Colorless	
<b>Odor</b>	Practically odorless	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flammability (liquid)</b>	Highly flammable	On basis of test data
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	-7 °C / 19.4 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	No data available	
<b>Water Solubility</b>	Immiscible	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	23 hPa @ 20 °C	
<b>Density / Specific Gravity</b>	0.692 g/cm <sup>3</sup>	@ 20 °C
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

### 9.2. Other information

**Molecular Formula** Matrix: Isooctane  
**Explosive Properties** Vapors may form explosive mixtures with air

## 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** No information available.  
**Hazardous Reactions** None under normal processing.

**10.4. Conditions to avoid** Keep away from open flames, hot surfaces and sources of ignition.

**10.5. Incompatible materials** Acids. Strong bases. Oxidizing agent.

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## 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

Based on available data, the classification criteria are not met

Dermal

Based on available data, the classification criteria are not met

Inhalation

Based on available data, the classification criteria are not met

#### Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isooctane	LD50 5000 mg/kg ( Rat )	2000 mg/kg (Rabbit)	LC50 = 33.52 mg/L ( Rat ) 4 h

##### (b) skin corrosion/irritation;

Category 2

##### (c) serious eye damage/irritation;

Based on available data, the classification criteria are not met

##### (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;

Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

##### (g) reproductive toxicity;

Based on available data, the classification criteria are not met

##### (h) STOT-single exposure;

Category 3

Results / Target organs

Central nervous system (CNS).

##### (i) STOT-repeated exposure;

Based on available data, the classification criteria are not met

Target Organs

None known.

##### (j) aspiration hazard;

Category 1

#### Symptoms / effects, both acute and delayed

Inhalation of high vapor concentrations may cause symptoms like 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.

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## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

#### Ecotoxicity effects

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Isooctane	LC50 = 0.11 mg/l, 96h, (Rainbow trout)	EC50= 0.4 mg/l, 48h (Daphnia magna)	EC50= 2.94 mg/l, 72h

Component	Microtox	M-Factor
Isooctane		1

### 12.2. Persistence and degradability

#### Persistence

May persist.

#### Degradation in sewage treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

### 12.3. Bioaccumulative potential

Product has a high potential to bioconcentrate

### 12.4. Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and floats on water Is not likely mobile in the environment due its low water solubility. Is not likely mobile in the environment due its low water solubility and propensity to bind to soil particles

### 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.

#### Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

#### European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

#### Other Information

Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Can be landfilled or incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains.

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## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

**14.1. UN number** UN1262  
**14.2. UN proper shipping name** OCTANES  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** II  
**Marine Pollutant** This product contains a chemical which is listed as a marine pollutant according to IMDG/IMO

### ADR

**14.1. UN number** UN1262  
**14.2. UN proper shipping name** OCTANES  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** II

### IATA

**14.1. UN number** UN1262  
**14.2. UN proper shipping name** OCTANES  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** II

**14.5. Environmental hazards** Dangerous for the environment  
Product is a marine pollutant according to the criteria set by IMDG/IMO

**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

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
Isooctane	540-84-1	208-759-1	-	-	X	X	KE-34634	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Isooctane	540-84-1	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)

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Isooctane	540-84-1	-	Use restricted. See item 75. (see link for restriction details)	-
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## 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
Isooctane	540-84-1	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

Water endangering class = 2 (self classification)

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Isooctane	WGK2	

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
Isooctane 540-84-1 ( 100 )	Prohibited and Restricted Substances		

## 15.2. Chemical safety assessment

Chemical Safety Assessment/Reports (CSA/CSR) are not required for mixtures

## SECTION 16: OTHER INFORMATION

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

H225 - Highly flammable liquid and vapor  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H336 - May cause drowsiness or dizziness  
H400 - Very toxic to aquatic life  
H410 - Very toxic to aquatic life with long lasting effects

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## 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/MDG** - 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)

### **Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]:**

**Physical hazards** On basis of test data

**Health Hazards** Calculation method

**Environmental hazards** Calculation method

### **Training Advice**

Chemical incident response training.

### **Prepared By**

Health, Safety and Environmental Department

### **Revision Date**

17-Mar-2024

### **Revision Summary**

New emergency telephone response service provider.

**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**