

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Revision Date 30-Nov-2024 **Revision Number 4**

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

1.1. Product identifier

Product Description: Sulfur in Isooctane standard solution, Specpure®, 500 µg/g (0.050%)

Cat No.: 45322

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

Recommended Use Laboratory chemicals.

SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites Sector of use

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

Poison Centre - Emergency

Ireland: National Poisons Information Centre (NPIC) information services **01 809 2166** (8am-10pm, 7 days a week)

Malta: +356 2395 2000 Cyprus: +357 2240 5611

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

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

Physical hazards

Flammable liquids Category 2 (H225)

Sulfur in Isooctane standard solution, Specpure®, 500 µg/g (0.050%)

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Health hazards

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

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician

P331 - Do NOT induce vomiting

P280 - Wear protective gloves/protective clothing

P264 - Wash face, hands and any exposed skin thoroughly after handling

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 %	GHS Classification - According to
Component	CAS NO	EC NO	weight %	GHS Classification - According to
				GB-CLP Regulations UK SI 2019/720 and
				UK SI 2020/1567

Sulfur in Isooctane standard solution, Specpure®, 500 µg/g (0.050%)

Isooctane	540-84-1	EEC No. 208-759-1	99.77	Flam. Liq. 2 (H225) Asp. Tox. 1 (H304) Skin Irrit. 2 (H315) STOT SE 3 (H336) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)
Butane, 1,1'-thiobis-	544-40-1	EEC No. 208-870-5	0.23	Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)

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

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 Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists,

call a physician.

Ingestion 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.

Inhalation 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).

Self-Protection of the First Aider 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

Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

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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

None under normal use conditions.

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

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)

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7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s):

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 (99.77)				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 (99.77)				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 (99.77)				DNEL = 2035mg/m ³	

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

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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

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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:** Particulates filter conforming to EN 143

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:- Particle filtering: EN149:2001 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

Physical State Liquid

Appearance Colorless

Odor Petroleum distillates
Odor Threshold No data available
Melting Point/Range -107 °C / -160.6 °F
Softening Point No data available

Boiling Point/Range 98 - 99 °C / 208.4 - 210.2 °F

Flammability (liquid) Highly flammable On basis of test data

Flammability (solid,gas) Not applicable Liquid

Explosion Limits Lower 1 Vol %

Upper 6 Vol %

Flash Point -7 °C / 19.4 °F Method - No information available

Autoignition Temperature

Decomposition Temperature
pH

415 °C / 779 °F
No data available
No information available

Viscosity

No data available

Water Solubility

Immiscible

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure 23 hPa @ 20 °C

Density / Specific Gravity0.692 g/cm3@ 20 °CBulk DensityNot applicableLiquidVapor DensityNo data available(Air = 1.0)

Particle characteristics Not applicable (liquid)

9.2. Other information

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 PolymerizationNo information available.Hazardous ReactionsNone under normal processing.

10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition.

10.5. Incompatible materials

None known.

10.6. Hazardous decomposition products

None under normal use conditions.

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		
Γ	Isooctane	LD50 5000 mg/kg (Rat)	2000 mg/kg (Rabbit)	LC50 = 33.52 mg/L (Rat) 4 h		
L						
Г	Butane, 1,1'-thiobis-	Butane, 1,1'-thiobis- LD50 = 2220 mg/kg (Rat)		-		

(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;

RespiratorySkin
Based on available data, the classification criteria are not met
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

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There are no known carcinogenic chemicals in this product

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

Category 3 (h) STOT-single exposure;

Results / Target organs Central nervous system (CNS).

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

Target Organs None known.

Category 1 (i) aspiration hazard;

delayed

Symptoms / effects.both acute and 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.

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	EC50= 0.4 mg/l, 48h (Daphnia	EC50= 2.94 mg/l, 72h
	trout)	magna)	
Butane, 1,1'-thiobis-	LC50: = 3.58 mg/L, 96h flow-through (Pimephales promelas)		

Component	Microtox	M-Factor
Isooctane		1

12.2. Persistence and degradability

Persistence Degradation in sewage Immiscible with water, Persistence is unlikely, based on information available.

treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste

water treatment plants.

May have some potential to bioaccumulate 12.3. Bioaccumulative potential

Spillage unlikely to penetrate soil The product is insoluble and floats on water The product 12.4. Mobility in soil

contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the

environment due to its volatility.

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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.

Dispose of this container to hazardous or special waste collection point. Empty containers **Contaminated Packaging**

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.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN1262 14.2. UN proper shipping name **OCTANES**

14.3. Transport hazard class(es) 14.4. Packing group II

Marine Pollutant This product contains a chemical which is listed as a marine pollutant according to

IMDG/IMO

ADR

UN1262 14.1. UN number **OCTANES**

14.2. UN proper shipping name 3

14.3. Transport hazard class(es) 14.4. Packing group

II

IATA

14.1. UN number UN1262 **OCTANES** 14.2. UN proper shipping name

14.3. Transport hazard class(es) 3 14.4. Packing group II

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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	ı	-	X	X	KE-34634	Χ	X
Butane, 1,1'-thiobis-	544-40-1	208-870-5	-	-	X	X	-	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Isooctane	540-84-1	Х	ACTIVE	X	-	X	Х	Х
Butane, 1,1'-thiobis-	544-40-1	Х	ACTIVE	X	-	X	Х	Х

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)
Isooctane	540-84-1	-	Use restricted. See entry 75. (see link for restriction details)	-
Butane, 1,1'-thiobis-	544-40-1	-	-	-

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
ı	Butane, 1,1'-thiobis-	544-40-1	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

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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	
Butane, 1,1'-thiobis-	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	Prohibited and Restricted		
540-84-1 (99.77)	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

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

H225 - Highly flammable liquid and vapor

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

Legend

CAS - Chemical Abstracts Service

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

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic

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

Inventory

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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%

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

Sulfur in Isooctane standard solution, Specpure®, 500 µg/g (0.050%)

NOEC - No Observed Effect Concentration POW - Partition coefficient Octanol:Water

PBT - Persistent, Bioaccumulative, Toxic 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

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

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MARPOL - International Convention for the Prevention of Pollution from Shins

ATE - Acute Toxicity Estimate VOC - (Volatile Organic Compound)

Key literature references and sources for data

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

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

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

Physical hazards On basis of test data Calculation method **Health Hazards Environmental hazards** Calculation method

Training Advice

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

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.

Chemical incident response training.

Health, Safety and Environmental Department **Prepared By**

Revision Date 30-Nov-2024 **Revision Summary** Not applicable.

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