

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

Creation Date 23-Mar-2012

Revision Date 08-Feb-2024

Revision Number 4

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

1.1. Product identifier

Product Description: Cat No. : Synonyms CAS No EC No Molecular Formula REACH registration number	Allyl isothiocyanate L02901 Allyl isorhodanide; Allyl isosulfocyanate; Isothiocyanic acid, allyl ester 57-06-7 200-309-2 C4 H5 N S -				
1.2. Relevant identified uses of the	substance or mixture and uses advised against				
Recommended Use Uses advised against	Laboratory chemicals. 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 3 (H226)

Health hazards

Allyl isothiocyanate

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Acute oral toxicity Acute dermal toxicity Acute Inhalation Toxicity - Vapors Skin Corrosion/Irritation Serious Eye Damage/Eye Irritation Specific target organ toxicity - (single exposure) <u>Environmental hazards</u>	Category 3 (H301) Category 2 (H310) Category 2 (H330) Category 2 (H315) Category 2 (H319) Category 3 (H335)
Acute aquatic toxicity	Category 1 (H400)
Chronic aquatic toxicity	Category 1 (H410)

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

- H226 Flammable liquid and vapor
- H301 Toxic if swallowed
- H315 Causes skin irritation
- H319 Causes serious eye irritation
- H335 May cause respiratory irritation
- H410 Very toxic to aquatic life with long lasting effects
- H310 + H330 Fatal in contact with skin or if inhaled

Precautionary Statements

P310 - Immediately call a POISON CENTER or doctor/physician

- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing
- P332 + P313 If skin irritation occurs: Get medical advice/attention
- P280 Wear protective gloves/protective clothing/eye protection/face protection
- P337 + P313 If eye irritation persists: Get medical advice/attention
- 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) Lachrymator (substance which increases the flow of tears)

Toxic to terrestrial vertebrates

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

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

Allyl isothiocyanate

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Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)	Allyl isothiocyanate	57-06-7	EEC No. 200-309-2	<100	Flam. Liq. 3 (H226) STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 3 (H301) Acute Tox. 2 (H310) Acute Tox. 2 (H330) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)
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Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Allyl isothiocyanate	-	10	-

REACH registration number

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.			
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.			
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.			
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.			
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.			
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				
	None reasonably foreseeable. 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.

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.

Allyl isothiocyanate

5.2. Special hazards arising from the substance or mixture

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

Hazardous Combustion Products

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulfur oxides, Hydrogen cyanide (hydrocyanic acid).

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. Thermal decomposition can lead to release of irritating gases and vapors.

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. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.

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

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. 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

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance.

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 away from heat, sparks and flame. Keep container tightly closed in a dry and well-ventilated place. To maintain product quality: Keep refrigerated.

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

7.3. Specific end use(s)

Allyl isothiocyanate

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	Acute effects	Chronic effects local	Chronic effects
	(Dermal)	systemic (Dermal)	(Dermal)	systemic (Dermal)
Allyl isothiocyanate 57-06-7 (<100)				DNEL = 96µg/kg bw/day

Component	Acute effects local	Acute effects	Chronic effects local	Chronic effects
	(Inhalation)	systemic (Inhalation)	(Inhalation)	systemic (Inhalation)
Allyl isothiocyanate 57-06-7 (<100)				DNEL = 0.335mg/m ³

Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Microorganisms in sewage treatment	Soil (Agriculture)
Allyl isothiocyanate 57-06-7 (<100)	PNEC = 0.13µg/L			

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Allyl isothiocyanate 57-06-7(<100)	PNEC = 0.013µg/L				

8.2. Exposure controls

Engineering Measures

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

Eye Protection		(European standard	I - EN 166)	
Hand Protection	Protectiv	e gloves		
	Breakthrough time See manufacturers recommendations	Glove thickness -	EU standard EN 374	Glove comments (minimum requirement)

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Molecular Weight

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	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	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 Odor Odor Threshold Melting Point/Range Softening Point Boiling Point/Range Flammability (liquid) Flammability (solid,gas) Explosion Limits	Light yellow pungent No data available -80 °C / -112 °F No data available 151 - 153 °C / 303.8 - 307.4 °F Flammable Not applicable No data available	@ 760 mmHg On basis of test data Liquid
Flash Point Autoignition Temperature Decomposition Temperature pH Viscosity Water Solubility Solubility in other solvents	46 °C / 114.8 °F No data available No data available No information available No data available 2 g/l @20°C No information available	Method - No information available
Partition Coefficient (n-octanol/wat		
Vapor Pressure Density / Specific Gravity Bulk Density Vapor Density Particle characteristics	5.3 mbar @ 20 °C 1.0175 Not applicable 3.41 Not applicable (liquid)	Liquid (Air = 1.0)
9.2. Other information		
Molecular Formula	C4 H5 N S	

99.15

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Explosive Properties Self-accelerating polymerisation temperature (SAPT) explosive air/vapour mixtures possible >50°C (packages up to 50kg)

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	None known, based on information available
10.2. Chemical stability	Moisture sensitive.
10.3. Possibility of hazardous react	ions
Hazardous Polymerization Hazardous Reactions	No information available. None under normal processing.
10.4. Conditions to avoid	Keep away from open flames, hot surfaces and sources of ignition. Exposure to air. Exposure to light. Incompatible products. Exposure to moist air or water.
10.5. Incompatible materials	Acids. Water. Strong oxidizing agents. Strong bases. Alcohols. Amines.
10.6 Hazardous decomposition pro	ducts

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides. Hydrogen cyanide (hydrocyanic acid).

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 3
Dermal	Category 2
Inhalation	Category 2

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Allyl isothiocyanate	LD50 = 112 mg/kg (Rat)	LD50 = 88 mg/kg (Rabbit)	LC50 0.206 - 0.508 mg/L (Rat) 4 h

(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization Respiratory Skin	No data available No data available
(e) germ cell mutagenicity;	No information available
(f) carcinogenicity;	No data available

Allyl isothiocyanate

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	Category 3
Results / Target organs	Respiratory system.
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	No data available
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

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

Component	Freshwater Fish	Water Flea	Freshwater Algae
Allyl isothiocyanate	LC50: 0.054 - 0.109 mg/L, 96h flow-through (Oryzias latipes) LC50: = 0.0856 mg/L, 96h		
	flow-through (Pimephales promelas)		

Component	Microtox	M-Factor
Allyl isothiocyanate	EC50 = 0.099 mg/L 15 min	10
	EC50 = 0.106 mg/L 30 min	
	EC50 = 0.11 mg/L 5 min	

12.2. Persistence and degradability Persistence Degradation in sewage treatment plant	Soluble in water, Persistence is unlikely, based on information available. Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.
12.3. Bioaccumulative potential	Bioaccumulation is unlikely
<u>12.4. Mobility in soil</u>	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	Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent

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assessment

and very bioaccumulative (vPvB).

<u>12.6. Endocrine disrupting</u> 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. Can be landfilled or incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains. Waste codes should be assigned by the user based on the application for which the product was used.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.4. Packing group

<u>14.1. UN number</u>	UN1545
<u>14.2. UN proper shipping name</u>	ALLYL ISOTHIOCYANATE, STABILIZED
<u>14.3. Transport hazard class(es)</u>	6.1
Subsidiary Hazard Class	3
<u>14.4. Packing group</u>	II
ADR	
<u>14.1. UN number</u>	UN1545
<u>14.2. UN proper shipping name</u>	ALLYL ISOTHIOCYANATE, STABILIZED
<u>14.3. Transport hazard class(es)</u>	6.1
Subsidiary Hazard Class	3
<u>14.4. Packing group</u>	II
IATA	
<u>14.1. UN number</u>	UN1545
<u>14.2. UN proper shipping name</u>	ALLYL ISOTHIOCYANATE, STABILIZED
<u>14.3. Transport hazard class(es)</u>	6.1
Subsidiary Hazard Class	3

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14.5. Environmental hazards Dangerous for the environment

Allyl isothiocyanate

Product is a marine pollutant according to the criteria set by IMDG/IMO

<u>14.6. Special precautions for user</u> Inhibitors have been added to stabilize this product. Inhibitor levels should be maintained. Hazardous polymerization may occur upon depletion of inhibitor.

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
Allyl isothiocyanate	57-06-7	200-309-2	-	-	Х	Х	-	Х	Х
•									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Allyl isothiocyanate	57-06-7	Х	ACTIVE	X	-	X	X	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 Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Allyl isothiocyanate	57-06-7	-	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)

ſ	Component	CAS No	Seveso III Directive (2012/18/EC) -	Seveso III Directive (2012/18/EC) -
			Qualifying Quantities for Major Accident	Qualifying Quantities for Safety Report
			Notification	Requirements
[Allyl isothiocyanate	57-06-7	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 = 3 (self classification)

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

H301 - Toxic if swallowed
H310 - Fatal in contact with skin
H330 - Fatal if inhaled
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
H400 - Very toxic to aquatic life
H410 - Very toxic to aquatic life with long lasting effects
H226 - Flammable liquid and vapor

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	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)

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

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

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. Chemical incident response training.

Allyl isothiocyanate

Prepared By Creation Date Revision Date Revision Summary Health, Safety and Environmental Department 23-Mar-2012 08-Feb-2024 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