

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

1.1. Product identifier

Product Description:	Thiophenol
Cat No. :	138870000; 138870010; 138870050; 138870250; 138875000
Synonyms	Phenyl mercaptan; Benzenethiol
CAS No	108-98-5
EC No	203-635-3
Molecular Formula	C6 H6 S
REACH registration number	01-2119480142-47

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

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

1.3. Details of the supplier of the safety data sheet

Company

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

EU entity/business name
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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Flammable liquids	Category 3 (H226)
Health hazards	
Acute oral toxicity	Category 2 (H300)
Acute dermal toxicity	Category 2 (H310)
Acute Inhalation Toxicity - Vapors	Category 1 (H330)
Skin Corrosion/Irritation	Category 2 (H315)
Serious Eye Damage/Eye Irritation	Category 2 (H319)
Reproductive Toxicity	Category 2 (H361)
Specific target organ toxicity - (single exposure)	Category 2 (H371)
	Category 3 (H335)
Specific target organ toxicity - (repeated exposure)	Category 1 (H372)
Environmental hazards	
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
- H315 - Causes skin irritation
- H319 - Causes serious eye irritation
- H371 - May cause damage to organs
- H335 - May cause respiratory irritation
- H361 - Suspected of damaging fertility or the unborn child
- H372 - Causes damage to organs through prolonged or repeated exposure
- H410 - Very toxic to aquatic life with long lasting effects
- H300 + H310 + H330 - Fatal if swallowed, in contact with skin or if inhaled

Precautionary Statements

- P264 - Wash face, hands and any exposed skin thoroughly after handling
- P330 - Rinse mouth
- P310 - Immediately call a POISON CENTER or doctor/physician
- P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
- P280 - Wear protective gloves/protective clothing/eye protection/face protection
- 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

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Stench

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
Benzenethiol	108-98-5	EEC No. 203-635-3	>95	Flam Liq. 3 (H226) STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 2 (H300) Acute Tox. 2 (H310) Acute Tox. 1 (H330) Repr. 2 (H361) STOT SE 2 (H371) STOT RE 1 (H372) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Benzenethiol	-	100	-

REACH registration number	01-2119480142-47
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Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice	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	Use personal protective equipment as required.

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

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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.

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 (CO₂), Sulfur oxides.

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

Use personal protective equipment as required. Ensure adequate ventilation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. 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. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

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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. Store under an inert atmosphere.

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): 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
Benzenethiol			TWA: 0.5 ppm 8 hr. : 2 mg/m ³ 8 hr. STEL: 1.5 ppm 15 min STEL: 6 mg/m ³ 15 min Skin

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)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

Engineering Measures

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. Ensure adequate ventilation, especially in confined areas.

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

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Personal protective equipment

Eye Protection 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)
Neoprene				
Natural rubber				
PVC				

Skin and body protection Long sleeved clothing.

Inspect gloves before use.

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

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

Remove gloves with care avoiding skin contamination.

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

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to 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	Clear	
Odor	Stench	
Odor Threshold	No data available	
Melting Point/Range	-15 °C / 5 °F	
Softening Point	No data available	
Boiling Point/Range	167 - 169 °C / 332.6 - 336.2 °F	@ 760 mmHg
Flammability (liquid)	Flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	50 °C / 122 °F	Method - No information available
Autoignition Temperature	450 °C / 842 °F	
Decomposition Temperature	> 200°C	
pH	5	saturated solution
Viscosity	0.981cSt at 30 °C	

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Water Solubility	Insoluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Benzenethiol	2.52	
Vapor Pressure	1.6 mmHg @ 25 °C	
Density / Specific Gravity	1.078	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C6 H6 S
Molecular Weight	110.17
Explosive Properties	explosive air/vapour mixtures possible

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Air sensitive.

10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous polymerization does not occur.
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid

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

10.5. Incompatible materials

Strong oxidizing agents. Acids.

10.6. Hazardous decomposition products

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

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 2
Dermal	Category 2
Inhalation	Category 1

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzenethiol	46 mg/kg (Rat)	134 mg/kg (Rabbit) 300 mg/kg (Rat)	LC50 = 33 ppm (Rat) 4 h

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- (b) skin corrosion/irritation; Category 2
- (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; Based on available data, the classification criteria are not met
There are no known carcinogenic chemicals in this product
- (g) reproductive toxicity; Category 2
- (h) STOT-single exposure; Category 2
Category 3
- Results / Target organs Central nervous system (CNS), Respiratory system.
- (i) STOT-repeated exposure; Category 1
- Route of exposure Oral
Target Organs Kidney.
- (j) aspiration hazard; Based on available data, the classification criteria are not met
- 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

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
Benzenethiol		EC50 = 0.0044 mg/L 48h	

Component	Microtox	M-Factor
Benzenethiol	EC50 = 0.875 mg/L 15 min EC50 = 0.875 mg/L 30 min EC50 = 0.875 mg/L 5 min	100

12.2. Persistence and degradability Not readily biodegradable

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Persistence
Degradation in sewage treatment plant Persistence is unlikely.
Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Benzenethiol	2.52	No data available

12.4. Mobility in soil Spillage unlikely to penetrate soil The product is insoluble and sinks in water The product evaporates slowly . Is not likely mobile in the environment due its low water solubility.
Spillage unlikely to penetrate soil

12.5. Results of PBT and vPvB assessment No data available for assessment.

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 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. 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.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN2337
14.2. UN proper shipping name Phenyl mercaptan
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group I

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ADR

14.1. UN number UN2337
14.2. UN proper shipping name Phenyl mercaptan
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group I

IATA

FORBIDDEN FOR IATA TRANSPORT

14.1. UN number UN2337
14.2. UN proper shipping name Phenyl mercaptan, FORBIDDEN FOR IATA TRANSPORT
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group I

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
Benzenethiol	108-98-5	203-635-3	-	-	X	X	KE-33799	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzenethiol	108-98-5	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

Not applicable

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)
Benzenethiol	108-98-5	-	-	-

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
Benzenethiol	108-98-5	Not applicable	Not applicable

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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 .

Take note of Directive 94/33/EC on the protection of young people at work

Take note of Dir 92/85/EC on the protection of pregnant and breastfeeding women 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
Benzenethiol	WGK3	

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
Benzenethiol 108-98-5 (>95)	Prohibited and Restricted Substances		

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

H300 - Fatal if swallowed

H310 - Fatal in contact with skin

H330 - Fatal if inhaled

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H371 - May cause damage to organs

H335 - May cause respiratory irritation

H361 - Suspected of damaging fertility or the unborn child

H372 - Causes damage to organs through prolonged or repeated exposure

H400 - Very toxic to aquatic life

H410 - Very toxic to aquatic life with long lasting effects

H226 - Flammable liquid and vapor

Legend

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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.

Chemical incident response training.

Creation Date 23-Apr-2010

Revision Date 25-Sep-2023

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