

Creation Date 23-Oct-2010

Revision Date 23-Jan-2024

Revision Number 4

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

1.1. Product identifier

Product Description:	4-(Trifluoromethoxy)phenyl isocyanate
Cat No. :	B20033
Synonyms	1-Isocyanato-4-(trifluoromethoxy)benzene
CAS No	35037-73-1
EC No	252-328-0
Molecular Formula	C ₈ H ₄ F ₃ N O ₂
REACH registration number	-

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

Recommended Use	Laboratory chemicals.
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
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E-mail address	begel.sdsdesk@thermofisher.com
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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

Based on available data, the classification criteria are not met

Health hazards

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Acute oral toxicity
Acute dermal toxicity
Acute Inhalation Toxicity - Vapors
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Respiratory Sensitization
Skin Sensitization
Specific target organ toxicity - (single exposure)

Category 4 (H302)
Category 3 (H311)
Category 1 (H330)
Category 1 C (H314)
Category 1 (H318)
Category 1 (H334)
Category 1 (H317)
Category 3 (H335)

Environmental hazards

Chronic aquatic toxicity

Category 3 (H412)

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H302 - Harmful if swallowed
H311 - Toxic in contact with skin
H330 - Fatal if inhaled
H314 - Causes severe skin burns and eye damage
H317 - May cause an allergic skin reaction
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled
H335 - May cause respiratory irritation
H412 - Harmful to aquatic life with long lasting effects
Combustible liquid

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P310 - Immediately call a POISON CENTER or doctor/physician
P301 + P330 + P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

2.3. Other hazards

Lachrymator (substance which increases the flow of tears)
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
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				GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	EEC No. 252-328-0	>95	Acute Tox. 4 (H302) Acute Tox. 3 (H311) Acute Tox. 1 (H330) Skin Corr. 1C (H314) Eye Dam. 1 (H318) Skin Sens. 1 (H317) Resp. Sens. 1 (H334) STOT SE 3 (H335) Aquatic Chronic 3 (H412)

REACH registration number	-
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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	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. Remove to fresh air. 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

Causes burns by all exposure routes. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

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

Notes to Physician	Treat symptomatically.
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SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

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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

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes. Combustible material. Containers may explode when heated.

Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen cyanide (hydrocyanic acid), Gaseous hydrogen fluoride (HF).

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. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

Should not be released into the environment. Do not flush into surface water or sanitary sewer system.

6.3. Methods and material for containment and cleaning up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Wear personal protective equipment/face protection. 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.

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 in a dry place. Keep container tightly closed. Keep away from heat, sparks and flame. Store under an inert atmosphere. Keep refrigerated. Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place.

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

Class 6.1A

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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

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

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

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

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection

Goggles (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
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 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.

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	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.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Clear	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	78 °C / 172.4 °F	@ 22 mmHg
Flammability (liquid)	Combustible liquid	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	69 °C / 156.2 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	1.340	
Bulk Density	Not applicable	Liquid
Vapor Density	7.0	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C8 H4 F3 N O2
Molecular Weight	203.12
Explosive Properties	explosive air/vapour mixtures possible
Refractive index	1.457-1.460

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable. Moisture sensitive.

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10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid

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

10.5. Incompatible materials

Strong oxidizing agents. Alcohols. Amines. Water.

10.6. Hazardous decomposition products

Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid). Gaseous hydrogen fluoride (HF).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;
Oral Category 4
Dermal Category 3
Inhalation Category 1

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	-	LD50 = 670 mg/kg (Rat) LD50 = 268 mg/kg (Rat)	LC50 22.5 - 68.5 mg/m ³ (Rat) 4 h

(b) skin corrosion/irritation; Category 1 C

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;
Respiratory Category 1
Skin Category 1
May cause sensitization by skin contact

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available
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.

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(j) aspiration hazard; No data available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation.

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

12.2. Persistence and degradability No information available

Persistence

Persistence is unlikely, based on information available.

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 Bioaccumulation is unlikely

12.4. Mobility in soil

The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.

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 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.

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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. Do not empty into drains. Large amounts will affect pH and harm aquatic organisms. Do not let this chemical enter the environment.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN3390
14.2. UN proper shipping name TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
Technical Shipping Name 4-(Trifluoromethoxy)phenyl isocyanate
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 8
14.4. Packing group I

ADR

14.1. UN number UN3390
14.2. UN proper shipping name TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
Technical Shipping Name 4-(Trifluoromethoxy)phenyl isocyanate
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 8
14.4. Packing group I

IATA

FORBIDDEN FOR IATA TRANSPORT

14.1. UN number UN3390
14.2. UN proper shipping name TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.* FORBIDDEN FOR IATA TRANSPORT
Technical Shipping Name 4-(Trifluoromethoxy)phenyl isocyanate
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 8
14.4. Packing group I

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	252-328-0	-	-	-	X	-	-	-

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Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	X	ACTIVE	-	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)
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	-	-	-

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
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	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)?

See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin List)
Benzene, 1-isocyanato-4-(trifluoromethoxy)- (CAS #: 35037-73-1)	-	-	Listed	Listed	-

PFAS Legend

Listed = Meets the PFAS definition of the named authority

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
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	WGK2	

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15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

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

H302 - Harmful if swallowed
H311 - Toxic in contact with skin
H330 - Fatal if inhaled
H314 - Causes severe skin burns and eye damage
H317 - May cause an allergic skin reaction
H318 - Causes serious eye damage
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled
H335 - May cause respiratory irritation
H412 - Harmful to aquatic life with long lasting effects

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/NDL - 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

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)

Key literature references and sources for data

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

Suppliers safety data sheet, Chemadviser - 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.

Prepared By

Health, Safety and Environmental Department

Creation Date

23-Oct-2010

Revision Date

23-Jan-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

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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