

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

Creation Date 16-Jul-2014 Revision Date 23-Jan-2024 Revision Number 5

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

1.1. Product identifier

Product Description: Phenyl isothiocyanate

Cat No. : A11596

Synonyms PITC; Phenyl mustard oil

 CAS No
 103-72-0

 EC No
 203-138-1

 Molecular Formula
 C7 H5 N S

REACH registration number -

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

Recommended Use Laboratory chemicals.

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

Product category PC21 - Laboratory chemicals

Process categories PROC15 - Use as a laboratory reagent

Environmental release category ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)

Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company

Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific)

Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom

Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99 **CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

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

Physical hazards

ALFAAA11596

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Phenyl isothiocyanate

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicityCategory 3 (H301)Skin Corrosion/IrritationCategory 1 (H314) BSerious Eye Damage/Eye IrritationCategory 1 (H318)Respiratory SensitizationCategory 1 (H334)Skin SensitizationCategory 1 (H317)

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

H301 - Toxic if swallowed

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

H410 - Very toxic to aquatic life with long lasting effects

Combustible liquid

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection

P284 - Wear respiratory protection

P301 + P330 + P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P310 - Immediately call a POISON CENTER or doctor/physician

2.3. Other hazards

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

Phenyl isothiocyanate

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Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Benzene, isothiocyanato-	103-72-0	EEC No. 203-138-1	<=100	Acute Tox. 3 (H301) Skin Corr. 1B (H314) Eye Dam. 1 (H318) Skin Sens. 1 (H317) Resp. Sens. 1 (H334) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)

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. Get

medical attention.

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.

If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim Inhalation

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 Use personal protective equipment as required.

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: 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: 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

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. CO₂, dry chemical, dry sand, alcohol-resistant foam.

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

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. 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

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.

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.

7.2. Conditions for safe storage, including any incompatibilities

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

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

Class 6.1C

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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

Use only under a chemical fume hood. Use explosion-proof electrical/ventilating/lighting equipment. 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	-	EN 374	(minimum requirement)
Neoprene Natural rubber	recommendations			
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.

To protect the wearer, respiratory protective equipment must be the correct fit and be used

and maintained properly

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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 Yellow Odor pungent

Odor ThresholdNo data availableMelting Point/Range-21 °C / -5.8 °FSoftening PointNo data availableBoiling Point/Range221 °C / 429.8 °F

Boiling Point/Range221 °C / 429.8 °F@ 760 mmHgFlammability (liquid)Combustible liquidOn basis of test dataFlammability (solid,gas)Not applicableLiquid

Explosion Limits No data available

Flash Point 87 °C / 188.6 °F Method - No information available

Autoignition Temperature No data available

Decomposition Temperature > 260°C

pH 7

Viscosity 1.3 mPa s at 20 °C

Water Solubility Insoluble

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure 1.2 mmHg @ 50 °C

Density / Specific Gravity 1.129

Bulk DensityNot applicableLiquidVapor Density4.68 (Air = 1.0)(Air = 1.0)

Particle characteristics Not applicable (liquid)

9.2. Other information

Molecular FormulaC7 H5 N SMolecular Weight135.19

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

Moisture sensitive.

10.3. Possibility of hazardous reactions

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Hazardous Polymerization Hazardous Reactions

Hazardous polymerization does not occur.

None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and

sources of ignition. Exposure to moisture.

10.5. Incompatible materials

Acids. Water. Strong oxidizing agents. Strong bases. Alcohols. Amines.

10.6. Hazardous decomposition products

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

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

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

DermalBased on available data, the classification criteria are not metInhalationBased on available data, the classification criteria are not met

(b) skin corrosion/irritation; Category 1 B

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;

Respiratory Category 1 **Skin** Category 1

No information available

(e) germ cell mutagenicity; Based on available data, the classification criteria are not met

(f) carcinogenicity; Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

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

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

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

Target Organs None known.

(j) aspiration hazard; Based on available data, the classification criteria are not met

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

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Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. delayed

> Possible perforation of stomach or esophagus should be investigated. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation. 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.

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.

12.2. Persistence and degradability Expected to be biodegradable **Persistence**

Degradation in sewage treatment plant

Insoluble in water, May persist, 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

May have some potential to bioaccumulate

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 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. Should not

be released into the environment.

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

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but

application specific.

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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 UN2927

14.2. UN proper shipping name Technical Shipping NameToxic liquid, corrosive, organic, n.o.s. (PHENYL ISOTHIOCYANATE)

14.3. Transport hazard class(es)6.1Subsidiary Hazard Class814.4. Packing groupII

<u>ADR</u>

14.1. UN number UN2927

14.2. UN proper shipping nameToxic liquid, corrosive, organic, n.o.s.Technical Shipping Name(PHENYL ISOTHIOCYANATE)14.3. Transport hazard class(es)6.1

14.3. Transport hazard class(es)6.7Subsidiary Hazard Class814.4. Packing groupII

IATA

<u>14.1. UN number</u> UN2927

14.2. UN proper shipping name TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S.*

Technical Shipping Name (PHENYL ISOTHIOCYANATE)

14.3. Transport hazard class(es)6.1Subsidiary Hazard Class814.4. Packing groupII

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)

- 1										5:000
	Benzene, isothiocyanato-	103-72-0	203-138-1	ı	-	X	X	KE-21760	Χ	X
	Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzene, isothiocyanato-	103-72-0	Х	ACTIVE	Х	-	X	Х	Х

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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) -	REACH (1907/2006) -	REACH Regulation (EC
			Annex XIV - Substances	Annex XVII - Restrictions	1907/2006) article 59 -
			Subject to Authorization	on Certain Dangerous	Candidate List of
				Substances	Substances of Very High
					Concern (SVHC)
ı	Benzene, isothiocyanato-	103-72-0	-	-	=

Seveso III Directive (2012/18/EC)

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
Benzene, isothiocyanato-	103-72-0	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.

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 Water endangering class = 3 (self classification)

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class		
Benzene, isothiocyanato-	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
Benzene, isothiocyanato- 103-72-0 (<=100)	Prohibited and Restricted Substances		

15.2. Chemical safety assessment

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

SECTION 16: OTHER INFORMATION

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H301 - Toxic if swallowed

H314 - Causes severe skin burns and eve 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

H400 - Very toxic to aquatic life

H410 - Very toxic to aquatic life with long lasting effects

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

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, 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.

Prepared By Health, Safety and Environmental Department

Creation Date 16-Jul-2014 Revision Date 16-Jul-2014 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 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