

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

1.1. Product identifier

| | |
|---------------------------|--------------------------------|
| Product Description: | 3-Nitrobenzotrifluoride |
| Cat No. : | L05948 |
| Synonyms | 3-Nitrobenzotrifluoride |
| CAS No | 98-46-4 |
| Molecular Formula | C7 H4 F3 N O2 |
| 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

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

Based on available data, the classification criteria are not met

Health hazards

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| | |
|--|-------------------|
| Acute oral toxicity | Category 4 (H302) |
| Acute dermal toxicity | Category 4 (H312) |
| Acute Inhalation Toxicity - Vapors | Category 3 (H331) |
| Skin Corrosion/Irritation | Category 2 (H315) |
| Serious Eye Damage/Eye Irritation | Category 2 (H319) |
| Specific target organ toxicity - (single exposure) | 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

Warning

Hazard Statements

H331 - Toxic if inhaled
H335 - May cause respiratory irritation
H319 - Causes serious eye irritation
H315 - Causes skin irritation
H412 - Harmful to aquatic life with long lasting effects
H302 + H312 - Harmful if swallowed or in contact with skin
Combustible liquid

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P273 - Avoid release to the environment
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

2.3. Other hazards

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 |
|-------------------------|---------|-------------------|----------|---|
| 3-Nitrobenzotrifluoride | 98-46-4 | EEC No. 202-670-1 | 97 | STOT SE 3 (H335) Skin Irrit. 2 (H315) |

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| | | | | |
|--|--|--|--|--|
| | | | | Eye Irrit. 2 (H319) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 1 (H330) Aquatic Chronic 3 (H412) |
|--|--|--|--|--|

| | |
|----------------------------------|---|
| REACH registration number | - |
|----------------------------------|---|

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

| | |
|---|--|
| Eye Contact | Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. |
| Skin Contact | Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Immediate medical attention is required. |
| Ingestion | Call a physician immediately. Clean mouth with water. |
| Inhalation | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. 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

Difficulty in breathing. 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. Chemical 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

Combustible material. Flammable. Containers may explode when heated.

Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂), 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.

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SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

See Section 12 for additional Ecological Information. Avoid release to the environment. Collect spillage. Do not flush into surface water or sanitary sewer system.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Wear self-contained breathing apparatus and protective suit. Do not let this chemical enter the environment. 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

Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Handle product only in closed system or provide appropriate exhaust ventilation. 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, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 6.1C
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):

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific

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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

Wear appropriate protective gloves and clothing to prevent skin exposure.

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.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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9.1. Information on basic physical and chemical properties

| | | |
|--|---------------------------------------|--|
| Physical State | Liquid | |
| Appearance | Yellow | |
| Odor | aromatic | |
| Odor Threshold | No data available | |
| Melting Point/Range | -5 °C / 23 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | 200 - 205 °C / 392 - 401 °F | @ 760 mmHg |
| Flammability (liquid) | Combustible liquid | On basis of test data |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | Lower 1.2 Upper 18.9 | |
| Flash Point | 87 °C / 188.6 °F | Method - No information available |
| Autoignition Temperature | 475 °C / 887 °F | |
| Decomposition Temperature | > 370°C | |
| pH | No information available | |
| Viscosity | No data available | |
| Water Solubility | 0.4 g/l (20°C) | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Component | log Pow | |
| 3-Nitrobenzotrifluoride | 2.6 | |
| Vapor Pressure | 0.3 hPa @ 20 °C | |
| Density / Specific Gravity | 1.430 | |
| Bulk Density | Not applicable | Liquid |
| Vapor Density | 6.59 | (Air = 1.0) |
| Particle characteristics | Not applicable (liquid) | |

9.2. Other information

| | |
|-----------------------------|--|
| Molecular Formula | C7 H4 F3 N O2 |
| Molecular Weight | 191.11 |
| 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

Stable under normal conditions.

10.3. Possibility of hazardous reactions

| | |
|---------------------------------|---------------------------|
| Hazardous Polymerization | No information available. |
| Hazardous Reactions | No information available. |

10.4. Conditions to avoid

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

10.5. Incompatible materials

Strong oxidizing agents. Strong bases. Strong reducing agents.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Gaseous hydrogen fluoride (HF).

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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 4 |
| Inhalation | Category 3 |

| Component | LD50 Oral | LD50 Dermal | LC50 Inhalation |
|-------------------------|--------------------------|---------------------------|-----------------|
| 3-Nitrobenzotrifluoride | LD50 = 610 mg/kg (Rat) | LD50 = 1900 mg/kg (Rat) | - |

- (b) skin corrosion/irritation; Category 2

- (c) serious eye damage/irritation; Category 2

- (d) respiratory or skin sensitization;
- | | |
|-------------|-------------------|
| Respiratory | No data available |
| Skin | No data available |

- (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.

- (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

Do not empty into drains. Contains a substance which is: Harmful to aquatic organisms.

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

| Component | Freshwater Fish | Water Flea | Freshwater Algae |
|-------------------------|---|------------|------------------|
| 3-Nitrobenzotrifluoride | LC50: = 35 mg/L, 96h static (Brachydanio rerio) | | |

| Component | Microtox | M-Factor |
|-------------------------|------------------------|----------|
| 3-Nitrobenzotrifluoride | EC50 = 129.3 mg/L 16 h | |

12.2. Persistence and degradability

Persistence

Persistence is unlikely.

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

| Component | log Pow | Bioconcentration factor (BCF) |
|-------------------------|---------|-------------------------------|
| 3-Nitrobenzotrifluoride | 2.6 | No data available |

12.4. Mobility in soil

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 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.

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. Do not let this chemical enter the environment.

SECTION 14: TRANSPORT INFORMATION

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IMDG/IMO

14.1. UN number UN2306
14.2. UN proper shipping name NITROBENZOTRIFLUORIDES, LIQUID
14.3. Transport hazard class(es) 6.1
14.4. Packing group II

ADR

14.1. UN number UN2306
14.2. UN proper shipping name NITROBENZOTRI-FLUORIDES, LIQUID
14.3. Transport hazard class(es) 6.1
14.4. Packing group II

IATA

14.1. UN number UN2306
14.2. UN proper shipping name NITROBENZOTRIFLUORIDES, LIQUID
14.3. Transport hazard class(es) 6.1
14.4. Packing group II

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 |
|-------------------------|---------|-----------|--------|-----|-------|------|------|------|------|
| 3-Nitrobenzotrifluoride | 98-46-4 | 202-670-1 | - | - | X | X | - | X | X |

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|-------------------------|---------|------|---|-----|------|------|-------|-------|
| 3-Nitrobenzotrifluoride | 98-46-4 | X | INACTIVE | - | 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) |
|-------------------------|---------|---|---|---|
| 3-Nitrobenzotrifluoride | 98-46-4 | - | - | - |

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 |
|-------------------------|---------|---|--|
| 3-Nitrobenzotrifluoride | 98-46-4 | 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)?

See table for values

| Component | OECD PFAS | US (EPA) PFAS | EU (ECHA) PFAS | UK (HSE) PFAS | Chemsec PFAS (Sin List) |
|---|-----------|---------------|----------------|---------------|-------------------------|
| 3-Nitrobenzotrifluoride (CAS #: 98-46-4) | - | - | 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

See table for values

| Component | Germany - Water Classification (AwSV) | Germany - TA-Luft Class |
|-------------------------|---------------------------------------|-------------------------|
| 3-Nitrobenzotrifluoride | WGK2 | |

| Component | Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81) | Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC) | Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure |
|---|--|---|---|
| 3-Nitrobenzotrifluoride 98-46-4 (97) | 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

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H330 - Fatal 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

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

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IECSC - Chinese Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated 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/MDG - 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.

Prepared By

Health, Safety and Environmental Department

Revision Date

04-Feb-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