

Creation Date 16-Sep-2010

Revision Date 22-Sep-2023

Revision Number 7

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

### 1.1. Product identifier

Product Description:	<b>3-Methylbutyraldehyde</b>
Cat No. :	<b>163970000; 163970025; 163971000; 163975000</b>
Synonyms	Isovaleraldehyde
CAS No	590-86-3
EC No	209-691-5
Molecular Formula	C5 H10 O
REACH registration number	01-2119474890-30

### 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

**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

Flammable liquids

Category 2 (H225)

##### Health hazards

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Serious Eye Damage/Eye Irritation  
Skin Sensitization  
Specific target organ toxicity - (single exposure)

Category 2 (H319)  
Category 1 (H317)  
Category 3 (H335)

## **Environmental hazards**

Chronic aquatic toxicity

Category 2 (H411)

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



Signal Word

Danger

## **Hazard Statements**

H225 - Highly flammable liquid and vapor  
H317 - May cause an allergic skin reaction  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H411 - Toxic to aquatic life with long lasting effects

## **Precautionary Statements**

P333 + P313 - If skin irritation or rash occurs: Get medical advice/attention  
P337 + P313 - If eye irritation persists: Get medical advice/attention  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P312 - Call a POISON CENTER or doctor if you feel unwell  
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**

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
Isopentaldehyde	590-86-3	EEC No. 209-691-5	>95	Flam. Liq. 2 (H225) Skin Sens. 1 (H317)

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				Eye Irrit. 2 (H319) STOT SE 3 (H335) Aq. Acute 2 (H401) Aq. Chron. 2 (H411)
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REACH registration number	01-2119474890-30
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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	If symptoms persist, call a physician.
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. If skin irritation persists, call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Self-Protection of the First Aider	Remove all sources of ignition. Use personal protective equipment as required.

### 4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable. . May cause allergic skin reaction. Inhalation of high vapor concentrations may cause symptoms like 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

### 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

Water spray, carbon dioxide (CO<sub>2</sub>), 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.

#### Hazardous Combustion Products

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Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

## **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.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

### **6.1. Personal precautions, protective equipment and emergency procedures**

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

### **6.2. Environmental precautions**

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. 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. Avoid ingestion and inhalation. Ensure adequate ventilation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

#### **Hygiene Measures**

When using do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

### **7.2. Conditions for safe storage, including any incompatibilities**

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

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

Class 3

### **7.3. Specific end use(s)**

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1. Control parameters**

ACR16397

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## Exposure limits

List source(s):

## Biological limit values

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

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

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

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

### 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	recommendations			
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

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<b>Small scale/Laboratory use</b>	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. <b>Recommended half mask:-</b> Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted
<b>Environmental exposure controls</b>	Do not allow material to contaminate ground water system. Prevent product from entering drains.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

<b>Physical State</b>	Liquid	
<b>Appearance</b>	Colorless, Light yellow	
<b>Odor</b>	Stench	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	-28 °C / -18.4 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	91 - 93 °C / 195.8 - 199.4 °F	@ 760 mmHg
<b>Flammability (liquid)</b>	Highly flammable	On basis of test data
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	<b>Lower</b> 1.4 Vol% <b>Upper</b> 5.6 Vol%	
<b>Flash Point</b>	-5 °C / 23 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	235 °C / 455 °F	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	5.3	
<b>Viscosity</b>	0.6 mPa s at 20 °C	
<b>Water Solubility</b>	Soluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Component</b>	<b>log Pow</b>	
Isopentaldehyde	1.5	
<b>Vapor Pressure</b>	57.9 mbar (20°C)	
<b>Density / Specific Gravity</b>	0.796	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	2.97 (Air = 1.0)	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

### 9.2. Other information

<b>Molecular Formula</b>	C5 H10 O
<b>Molecular Weight</b>	86.13
<b>Explosive Properties</b>	Vapors may form explosive mixtures with air

## SECTION 10: STABILITY AND REACTIVITY

<b>10.1. Reactivity</b>	None known, based on information available
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<b>10.2. Chemical stability</b>	Air sensitive.
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### 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 air.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong bases. Strong reducing agents.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

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

#### Product Information

##### (a) acute toxicity;

Oral

Based on available data, the classification criteria are not met

Dermal

Based on available data, the classification criteria are not met

Inhalation

Based on available data, the classification criteria are not met

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isopentaldehyde	LD50 = 5600 mg/kg ( Rat )	LD50 = 2730 mg/kg ( Rabbit )	LC50 = 42.7 mg/L ( Rat ) 4 h

##### (b) skin corrosion/irritation;

No data available

##### (c) serious eye damage/irritation;

Category 2

##### (d) respiratory or skin sensitization;

Respiratory

No data available

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

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

**Symptoms / effects, both acute and delayed** Inhalation of high vapor concentrations may cause symptoms like 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.

## 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

#### Ecotoxicity effects

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

Component	Freshwater Fish	Water Flea	Freshwater Algae
Isopentaldehyde	LC50 96h 53 mg/L (Leuciscus idus)	EC50: = 177 mg/L, 48h (Daphnia magna)	EC50: = 78 mg/L, 96h (Desmodesmus subspicatus) EC50: = 80 mg/L, 72h (Desmodesmus subspicatus)

### 12.2. Persistence and degradability

#### Persistence

Readily biodegradable

#### Degradation in sewage treatment plant

Soluble in water, Persistence is unlikely, based on information available.

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

### 12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Isopentaldehyde	1.5	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



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## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

<b>Waste from Residues/Unused Products</b>	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.
<b>Contaminated Packaging</b>	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.
<b>European Waste Catalogue (EWC)</b>	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
<b>Other Information</b>	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

<b>14.1. UN number</b>	UN2058
<b>14.2. UN proper shipping name</b>	VALERALDEHYDE
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	II

### ADR

<b>14.1. UN number</b>	UN2058
<b>14.2. UN proper shipping name</b>	VALERALDEHYDE
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	II

### IATA

<b>14.1. UN number</b>	UN2058
<b>14.2. UN proper shipping name</b>	VALERALDEHYDE
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	II

<b>14.5. Environmental hazards</b>	Dangerous for the environment Product is a marine pollutant according to the criteria set by IMDG/IMO
<b>14.6. Special precautions for user</b>	No special precautions required.
<b>14.7. Maritime transport in bulk according to IMO instruments</b>	Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

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## 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
Isopentaldehyde	590-86-3	209-691-5	-	-	X	X	KE-23536	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Isopentaldehyde	590-86-3	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)
Isopentaldehyde	590-86-3	-	-	-

## 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
Isopentaldehyde	590-86-3	Not applicable	Not applicable

## Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

## Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

## WGK Classification

See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Isopentaldehyde	WGK2	

## 15.2. Chemical safety assessment

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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

H317 - May cause an allergic skin reaction  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H411 - Toxic to aquatic life with long lasting effects  
H225 - Highly flammable liquid and vapor

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer  
Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

### Key literature references and sources for data

<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.

**Creation Date** 16-Sep-2010

**Revision Date** 22-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

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materials or in any process, unless specified in the text

**End of Safety Data Sheet**