

according to UN GHS (ST/SG/AC.10/11/Rev.8)

### NATURAL ISOVALERALDEHYDE

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### SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1. Product identifier

NATURAL ISOVALERALDEHYDE

Substance name: NATURAL ISOVALERALDEHYDE

CAS No: 590-86-3

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

#### Use of the substance/mixture

Manufacturing of: - Air care products - Perfumes, fragrances - Pharmaceuticals - Cosmetics, personal care products - Flavouring Substances - Other

### 1.3. Details of the supplier of the safety data sheet

Company name: Axxence Aromatic GmbH

Street: Tackenweide 28

Place: D-46446 Emmerich am Rhein

Telephone: + 49 2822 68561 0 Telefax: + 49 2822 68561 39

e-mail: info@axxence.com

Contact person: Andreas Goertz Telephone: + 49 2822 68561 37

e-mail: andreas.goertz@axxence.com

Internet: www.axxence.de
Responsible Department: QM - Regulatory Affairs

1.4. Emergency telephone +49 2822 68561 99

number:

#### **SECTION 2: Hazards identification**

#### 2.1. Classification of the substance or mixture

### UN GHS (ST/SG/AC.10/11/Rev.8)

Hazard categories:

Flammable liquid: Flam. Liq. 2 Acute toxicity: Acute Tox. 5 Acute toxicity: Acute Tox. 5

Serious eye damage/eye irritation: Eye Irrit. 2 Respiratory or skin sensitisation: Skin Sens. 1

Specific target organ toxicity - single exposure: STOT SE 3 Hazardous to the aquatic environment: Aquatic Acute 2 Hazardous to the aquatic environment: Aquatic Chronic 2

Hazard Statements:

May cause respiratory irritation.

Toxic to aquatic life.

Toxic to aquatic life with long lasting effects.

Highly flammable liquid and vapour. May be harmful in contact with skin.

May be harmful if inhaled.

May cause an allergic skin reaction. Causes serious eye irritation.

## 2.2. Label elements

#### UN GHS (ST/SG/AC.10/11/Rev.8)

Signal word: Danger



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#### Pictograms:







#### **Hazard statements**

H225 Highly flammable liquid and vapour.

H313+H333 May be harmful in contact with skin or if inhaled.

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**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No

smoking.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P264 Wash thoroughly after handling.

P271 Use only outdoors or in a well-ventilated area.

P273 Avoid release to the environment.

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

protection.

P302+P352 IF ON SKIN: Wash with plenty of Water and soap.

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

water or shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if

present and easy to do. Continue rinsing.

P333+P317 If skin irritation or rash occurs: Get medical help.

P337+P317 If eye irritation persists: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P391 Collect spillage.

P403+P235 Store in a well-ventilated place. Keep cool.

P501 Dispose of contents/container to .

## 2.3. Other hazards

No information available.

## **SECTION 3: Composition/information on ingredients**

### 3.1. Substances

Sum formula: C5 H10 O Molecular weight: 86,13

### **Hazardous components**

CAS No	Chemical name	Quantity
	Classification (UN GHS (ST/SG/AC.10/11/Rev.8))	
590-86-3	NATURAL ISOVALERALDEHYDE	100 %
	Flam. Liq. 2, Acute Tox. 5, Acute Tox. 5, Eye Irrit. 2, Skin Sens. 1, STOT SE 3, Aquatic Acute 2, Aquatic Chronic 2; H225 H333 H313 H319 H317 H335 H401 H411	

### **SECTION 4: First aid measures**

#### 4.1. Description of first aid measures



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#### After inhalation

Provide fresh air. When in doubt or if symptoms are observed, get medical advice.

#### After contact with skin

After contact with skin, wash immediately with plenty of water and soap. Take off immediately all contaminated clothing and wash it before reuse. Medical treatment necessary.

#### After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

#### After ingestion

Observe risk of aspiration if vomiting occurs. Rinse mouth immediately and drink 1 glass of of water.

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

No information available.

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

Treat symptomatically.

### **SECTION 5: Firefighting measures**

#### 5.1. Extinguishing media

#### Suitable extinguishing media

Water spray jet, Carbon dioxide (CO2), Foam, Extinguishing powder.

## 5.2. Special hazards arising from the substance or mixture

Highly flammable. Vapours can form explosive mixtures with air.

## 5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

#### Additional information

Use water spray jet to protect personnel and to cool endangered containers. Suppress gases/vapours/mists with water spray jet. Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water

### **SECTION 6: Accidental release measures**

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

#### General advice

Remove all sources of ignition. Provide adequate ventilation. Do not breathe gas/fumes/vapour/spray. Avoid contact with skin, eyes and clothes. Use personal protection equipment.

#### 6.2. Environmental precautions

Do not allow uncontrolled discharge of product into the environment. Explosion risk.

# 6.3. Methods and material for containment and cleaning up

## For cleaning up

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents). Treat the recovered material as prescribed in the section on waste disposal.

#### Other information

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents). Treat the recovered material as prescribed in the section on waste disposal.

#### 6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

## **SECTION 7: Handling and storage**



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#### 7.1. Precautions for safe handling

#### Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fumes/vapour/spray.

#### Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges. Vapours can form explosive mixtures with air.

#### Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff. Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff.

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

#### Requirements for storage rooms and vessels

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaustion at critical locations. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

#### Hints on joint storage

Do not store together with: Oxidizing agent. Pyrophoric or self-heating substances.

## **SECTION 8: Exposure controls/personal protection**

### 8.1. Control parameters

### 8.2. Exposure controls









# Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fumes/vapour/spray.

## Individual protection measures, such as personal protective equipment

#### Eye/face protection

Suitable eye protection: goggles.

#### Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

#### Skin protection

Flame-retardant protective clothing. Wear anti-static footwear and clothing . .

## **Respiratory protection**

In case of inadequate ventilation wear respiratory protection.

#### Thermal hazards

Flame-retardant protective clothing. Wear anti-static footwear and clothing



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#### **SECTION 9: Physical and chemical properties**

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

Physical state: Liquid

Colour:

Melting point/freezing point:

-51 °C

Boiling point or initial boiling point and

92 °C

boiling range: Flammability

Solid/liquid: not applicable not applicable Gas: Lower explosion limits: 1,4 vol. % Upper explosion limits: 5,8 vol. % Flash point: -1 °C Auto-ignition temperature: 210 °C not determined Decomposition temperature: pH-Value (at 20 °C): 3,1 Water solubility: 15 g/L

(at 20 °C)

Solubility in other solvents

not determined

Partition coefficient n-octanol/water: 1,5
Vapour pressure: 61 hPa

(at 20 °C)

Density (at 20 °C): 0,80 g/cm³
Relative vapour density: 2,97

(at 20 °C)

## 9.2. Other information

## Information with regard to physical hazard classes

Explosive properties

The product is not: Explosive.

Oxidizing properties

The product is not: oxidising.

#### Other safety characteristics

Evaporation rate: not determined Solvent content: 0% Solid content: 0% Viscosity / dynamic: 0,69 mPa·s

(at 20 °C)

## **SECTION 10: Stability and reactivity**

### 10.1. Reactivity

Highly flammable.

## 10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

#### 10.3. Possibility of hazardous reactions

No known hazardous reactions.

# 10.4. Conditions to avoid

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames. Vapours can form explosive mixtures with air.



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## 10.5. Incompatible materials

No information available.

## 10.6. Hazardous decomposition products

No known hazardous decomposition products.

## **SECTION 11: Toxicological information**

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

#### **Acute toxicity**

May be harmful in contact with skin.

May be harmful if inhaled.

CAS No	Chemical name	Chemical name					
	Exposure route	Dose		Species	Source	Method	
590-86-3	NATURAL ISOVALERAL	DEHYDE					
	oral	LD50 mg/kg	5740	Rat	REACH Dossier	OECD 401	
	dermal	LD50 mg/kg	2534	Rabbit	REACH Dossier	OECD 402	
	inhalation (4 h) vapour	LC50	42,7 mg/l	Rat	REACH Dossier	OECD 403	
	inhalation dust/mist	ATE	6,25 mg/l				

## Irritation and corrosivity

Causes serious eye irritation.

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

### Sensitising effects

May cause an allergic skin reaction. (NATURAL ISOVALERALDEHYDE)

## Carcinogenic/mutagenic/toxic effects for reproduction

Based on available data, the classification criteria are not met.

## STOT-single exposure

May cause respiratory irritation. (NATURAL ISOVALERALDEHYDE)

# STOT-repeated exposure

Based on available data, the classification criteria are not met.

#### **Aspiration hazard**

Based on available data, the classification criteria are not met.

## 11.2. Information on other hazards

## **Endocrine disrupting properties**

No information available.

### **Further information**

This substance is classified as hazardous according to Regulation (EC) No 1272 (2008).

# **SECTION 12: Ecological information**

## 12.1. Toxicity

Toxic to aquatic life with long lasting effects.



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CAS No	Chemical name						
	Aquatic toxicity	Dose		[h]   [d]	Species	Source	Method
590-86-3	NATURAL ISOVALERALDEHYDE						
	Acute fish toxicity	LC50 mg/l	3,25		Pimephales promelas (fathead minnow)	REACH Dossier	OECD 203
	Acute algae toxicity	ErC50	113 mg/l		Desmodesmus subspicatus	REACH Dossier	German Industrial Standard DIN 38412,
	Acute crustacea toxicity	EC50	177 mg/l		Daphnia magna (Big water flea)	REACH Dossier	Directive 79/831 EEC, C2

#### 12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name							
	Method	Value	d	Source				
	Evaluation		-					
590-86-3	NATURAL ISOVALERALDEHYDE							
	OECD 301D	49,5%	28	REACH Dossier				
	Not readily biodegradable (according to OECD							
	OECD 301D	43,6%	20	REACH Dossier				
	Not readily biodegradable (according to OECD criteria)							
	OECD 301D	36,9%	5	REACH Dossier				
	Not readily biodegradable (according to OECD criteria)							

### 12.3. Bioaccumulative potential

The product has not been tested.

### Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
590-86-3	NATURAL ISOVALERALDEHYDE	1,5

# 12.4. Mobility in soil

The product has not been tested.

### 12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

No information available.

# 12.7. Other adverse effects

No information available.

## **Further information**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

# **SECTION 13: Disposal considerations**

# 13.1. Waste treatment methods

## **Disposal recommendations**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation.

## Contaminated packaging

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself.

## **SECTION 14: Transport information**



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Marine transport (IMDG)

14.1. UN number or ID number: UN 2058

**14.2. UN proper shipping name:** VALERALDEHYDE

14.3. Transport hazard class(es):314.4. Packing group:IIHazard label:3



Special Provisions:

Limited quantity:

Excepted quantity:

E2

EmS:

F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 2058

**14.2. UN proper shipping name:** VALERALDEHYDE

14.3. Transport hazard class(es):314.4. Packing group:IIHazard label:3



Limited quantity Passenger: 1 L
Passenger LQ: Y341
Excepted quantity: E2

IATA-packing instructions - Passenger:353IATA-max. quantity - Passenger:5 LIATA-packing instructions - Cargo:364IATA-max. quantity - Cargo:60 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



Danger releasing substance: ISOVALERALDEHYD

14.6. Special precautions for user

Warning: Combustible liquid.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

# **SECTION 15: Regulatory information**

**National regulatory information** 

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile

work protection guideline' (94/33/EC).

Skin resorption/Sensitization: Causes allergic hypersensitivity reactions.

### **SECTION 16: Other information**

## Abbreviations and acronyms

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)



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IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service LC50: Lethal concentration, 50%

LD50: Lethal dose, 50%

CLP: Classification, labelling and Packaging

REACH: Registration, Evaluation and Authorization of Chemicals

GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals

**UN: United Nations** 

DNEL: Derived No Effect Level
DMEL: Derived Minimal Effect Level
PNEC: Predicted No Effect Concentration

ATE: Acute toxicity estimate LL50: Lethal loading, 50% EL50: Effect loading, 50%

EC50: Effective Concentration 50%

ErC50: Effective Concentration 50%, growth rate NOEC: No Observed Effect Concentration

BCF: Bio-concentration factor

PBT: persistent, bioaccumulative, toxic vPvB: very persistent, very bioaccumulative

RID: Regulations concerning the international carriage of dangerous goods by rail

ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures)

EmS: Emergency Schedules MFAG: Medical First Aid Guide

ICAO: International Civil Aviation Organization

MARPOL: International Convention for the Prevention of Marine Pollution from Ships

IBC: Intermediate Bulk Container VOC: Volatile Organic Compounds SVHC: Substance of Very High Concern

For abbreviations and acronyms, see table at http://abbrev.esdscom.eu

#### Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.