Material Safety Data Sheet

1. PRODUCT AND COMPANY IDENTIFICATION

Identification of the substance/preparation **Isovaleraldehyde**

CAS-No	590-86-3
EINECS-No	209-691-5
Registration number (REACh)	01-2119474890-30-0000
Use of the Substance /Preparation	Intermediate.
Identified uses	Transported isolated intermediate (1907/2006)

Company/Undertaking Identification

OXEA GmbH
Otto-Roelen-Str. 3
D-46147 Oberhausen
Germany

Product Information

Product Stewardship
FAX: +49 (0)208 693 2053
email: psq@oxea-chemicals.com

Emergency telephone number +44 (0) 1235 239 670 (UK)

2. HAZARDS IDENTIFICATION

GHS / CLP

Basis for Classification This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation, GHS)

Classification

Flammable liquid	Category 2
Serious eye damage/eye irritation	Category 2
Skin sensitization	Category 1
Target Organ Systemic Toxicant - Single exposure	Category 3
Environmental hazard	Chronic aquatic toxicity 2

Hazard symbols

Signal word **Danger**

Hazard statements	H225: Highly flammable liquid and vapour H319: Causes serious eye irritation H317: May cause an allergic skin reaction H335: May cause respiratory irritation H411: Toxic to aquatic life with long lasting effects
Precautionary statements	P210: Keep away from sources of ignition - No smoking P233: Keep container tightly closed P235: Keep cool P261: Avoid breathing dust/fume/gas/mist/vapours/spray P273: Avoid release to the environment P280: Wear protective gloves and eye/face protection P303+P361+P353: IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower P304+P340: IF INHALED: Remove victim to fresh air and keep at rest in a position 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 P312: Call a POISON CENTRE or doctor if you feel unwell P501: Dispose of contents/container in accordance with local regulation
Other Hazards	Vapours may form explosive mixture with air Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

Classification and labelling according to Directive 67/548/EEC or 1999/45/EC

Basis for Classification	The product is classified in accordance with Annex VI to Directive 67/548/EEC.
contains	3-Methylbutanal (CAS 590-86-3)
Symbol(s)	F - Highly flammable Xi - Irritant
R-phrase(s)	R11 - Highly flammable R36/37 - Irritating to eyes and respiratory system R43 - May cause sensitization by skin contact
S-phrase(s)	S 9 - Keep container in a well-ventilated place S16 - Keep away from sources of ignition - No smoking S24 - Avoid contact with skin S26 - In case of contact with eyes, rinse immediately with plenty of water and seek medical advice S37 - Wear suitable gloves
Other hazards	Vapours may form explosive mixture with air Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS-No	REACh-No	67/548/EEC	1272/2008/EC	Concentration (%)
Isovaleraldehyde	590-86-3	01-2119474890-30-0000	F;R11 Xi;R36/37 Xi;R43	Flam. Liq. 2; H225 Eye Irrit. 2; H319 Skin Sens. 1; H317 STOT SE 3; H335 Aquatic Chronic 2; H411	> 99,0

Remarks
3-Methylbutanal.

4. FIRST AID MEASURES

General advice
Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Inhalation
Keep at rest. Aerate with fresh air. When symptoms persist or in all cases of doubt seek medical advice.

Eyes
Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Obtain medical attention.

Skin
Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

Ingestion
Do not induce vomiting without medical advice. Call a physician immediately.

Main symptoms
shortness of breath, vomiting, headache, nausea.

Special hazard
Lung oedema, Lung irritation.

Notes to physician
Treat symptomatically. In case of lung irritation, first treatment with cortisone spray.

5. FIRE-FIGHTING MEASURES

Suitable extinguishing media
alcohol-resistant foam, dry chemical, carbon dioxide (CO2), water spray

Extinguishing media which must not be used for safety reasons
Do not use a solid water stream as it may scatter and spread fire.

Special exposure hazards arising from the substance or preparation itself, its combustion products, or released gases
Under conditions giving incomplete combustion, hazardous gases produced may consist of:
carbon monoxide (CO)
carbon dioxide (CO2)
Combustion gases of organic materials must in principle be graded as inhalation poisons
Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback
Vapours may form explosive mixtures with air

Special protective equipment for fire-fighters
Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

Precautions for fire-fighting
Cool containers / tanks with water spray. Water run-off and vapor cloud may be corrosive. Water run-off can cause environmental damage. Dike and collect water used to fight fire. Keep people away from and upwind of fire.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition. For emergency responders: Personal protection see section 8.

Environmental precautions
Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant). Water runoff can cause environmental damage.

Methods for containment
Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

Methods for cleaning up
Soak up with inert absorbent material. DO NOT use combustible materials such as sawdust. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

7. HANDLING AND STORAGE

Handling

Advice on safe handling
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms. Refill and handle product only in closed system. Do not use compressed air for filling, discharging or handling.

Advice on protection against fire and explosion
Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material. Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback. Vapours may form explosive mixture with air.

Advice on the protection of the environment
See Section 8: Environmental exposure controls.

Storage

Technical measures/Storage conditions
Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Handle under nitrogen, protect from moisture. Store at temperatures not exceeding 38 °C/ 100 °F.

Suitable material
stainless steel

Unsuitable material
mild steel

Advice on common storage
Incompatible products:
acids and bases
amines
oxidizing agents

Temperature class
T3

Identified uses

Transported isolated intermediate (1907/2006)

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

DNEL & PNEC

This substance is registered as intermediate under strictly controlled conditions.

Exposure limits European Union

No exposure limits established.

Exposure limits UK

No exposure limits established.

Occupational exposure controls

Engineering measures

General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

Personal protective equipment

General industrial hygiene practice
Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene measures
When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Respiratory protection
Respirator with A filter. Full mask with above mentioned filter according to producers using requirements or self-contained breathing apparatus. Equipment should conform to EN 136 or EN 140 and EN 143.

Hand protection
Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

Suitable material	butyl-rubber
Evaluation	according to EN 374: level 3
Glove thickness	approx 0.3 mm
Break through time	approx 60 min

Suitable material	polyvinylchloride
Evaluation	Information derived from practical experience
Glove thickness	approx 0.8 mm

Eye protection
Tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face.
Equipment should conform to EN 166

Skin and body protection
Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. Observe the exposure limits, clean exhaust air if needed. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.

Additional advice
Further details on substance data can be found in the registration dossier under the following link: http://apps.echa.europa.eu/registered/registered-sub.aspx.

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state	liquid
Colour	colourless

Odour	strong
Odour threshold	0,1 - 2 ppb
Molecular weight	86,13
Molecular formula	C5 H10 O

Flash point	0,5 °C
Method	EU A.9
Autoignition temperature	210 °C
Method	DIN 51794
Melting point/range	< -90 °C (Pour point)
Boiling point/range	92 °C @ 1013 hPa

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F
75	7,5***	0,074***	20	68
255	25,5***	0,252***	50	122

Density

Values [g/cm³]	@ °C	@ °F	Method
0,797	20	68	DIN 51757

Refractive index	1,387 @ 20 °C
Viscosity	0,56 mPa*s @ 20 °C
Method	DIN 51562, dynamic
pH	3,1 (15 g/l in water @ 20 °C (68 °F))
Water solubility	15 g/l @ 20 °C, OECD 105
log Pow	1,5 (measured), OECD 117
Vapour density	2,96 (Air = 1) @ 20 °C (68 °F)
Surface tension	46,1 mN/m (1 g/l @ 20°C)

10. STABILITY AND REACTIVITY

Stability
Stable under recommended storage conditions.

Hazardous reactions
Hazardous polymerisation may occur. Polymerization is a highly exothermic reaction and may generate sufficient heat to cause thermal decomposition and/or rupture containers. May form explosive peroxides. When finely distributed, self-ignition is possible. Vapours may form explosive mixture with air.

Conditions to avoid
Avoid contact with heat, sparks, open flame and static discharge. Avoid any source of ignition.

Materials to avoid
bases, amines, acids, oxidizing agents.

11. TOXICOLOGICAL INFORMATION

Principle Routes of Exposure Inhalation, Eye contact, Skin contact, Ingestion

Acute toxicity				
Isovaleraldehyde (590-86-3)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	~ 5740 mg/kg	rat, male/female	OECD 401
Oral	LD50	7100 mg/kg	rat, male	OECD 401
Dermal	LD50	2534 mg/kg	rabbit	OECD 402
Inhalative	LC50	42,7 mg/l (4h)	rat	OECD 403

Irritation and corrosion				
Isovaleraldehyde (590-86-3)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	Mild skin irritation	OECD 404	4h
Eyes	rabbit	irritating		

Sensitization				
Isovaleraldehyde (590-86-3)				
Target Organ Effects	Species	Evaluation	Method	
Skin	mouse	mildly sensitizing	OECD 429	read across

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Isovaleraldehyde (590-86-3)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		human lymphocytes	positive (without metabolic activation)	SCE	In vitro study
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	read across
Mutagenicity		mouse	negative	OECD 474	Bone marrow
Carcinogenicity	LOAEC: 500 ppm	rat, male/female		OECD 451, Inhalative	read across
Carcinogenicity	LOAEC: 500 ppm	mouse		OECD 451, Inhalative	read across

Isovaleraldehyde, CAS: 590-86-3

Main symptoms

shortness of breath, vomiting, nausea, headache.

Other adverse effects

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin.

Note

Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:
http://apps.echa.europa.eu/registered/registered-sub.aspx.

12. ECOLOGICAL INFORMATION

Acute aquatic toxicity			
Isovaleraldehyde (590-86-3)			
Species	Exposure time	Dose	Method
Daphnia magna (Water flea)	24h	EC50: 210 mg/l	84/449/EEC C.2

Daphnia magna (Water flea)	48h	EC50: 177 mg/l	84/449/EEC C.2
Pimephales promelas (fathead minnow)	96h	LC50: 3,25 mg/l	OECD 203
Desmodesmus subspicatus	72h	EC50: 80 mg/l (Biomass)	DIN 38412, part 9
Desmodesmus subspicatus	72h	EC50: 112,78 mg/l (Growth rate)	DIN 38412, part 9
Pseudomonas putida	17 h	EC10: 310 mg/l	DIN 38412, part 8

Isovaleraldehyde, CAS: 590-86-3
Biodegradation
50 % (28 d), Sewage, aerobic, OECD 301 D.
Note
Avoid release to the environment.

13. DISPOSAL CONSIDERATIONS

Product Information
Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.
Hazardous waste according to European Waste Catalogue (EWC)

Uncleaned empty packaging
Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

14. TRANSPORT INFORMATION

ADR/RID
UN/ID No UN 2058
Proper shipping name Valeraldehyde
Class 3
Packing group II
ADR Tunnel restriction code (D/E)
Classification Code F1
Hazard Number 33

ADN ADN Container
UN/ID No UN 2058
Proper shipping name Valeraldehyde
Class 3
Packing group II
Classification Code F1
Hazard Number 33

ADN ADN Tanker
forbidden

ICAO/IATA
UN/ID No UN 2058
Proper shipping name Valeraldehyde***
Class 3

Packing group II

IMDG

UN/ID No	UN 2058
Proper shipping name	Valeraldehyde***
Class	3
Packing group	II
EmS	F-E, S-D

IBC-Code

Product name	Valeraldehyde
Ship type	3
Pollution category	Y

15. REGULATORY INFORMATION

GHS / CLP

Basis for Classification This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation, GHS). (See chapter 2)

Water contaminating class (Germany)

Water contaminating class (Germany)	1
KBwS Number	1356
KBwS Classification	Annex 1 or 2

DI 96/82/EC (Seveso II)

Category	Annex I, part 2: 7b

Chemical Safety Assessment (CSA)

The Chemical Safety Report (CSR) is not required.***

International Inventories

Isovaleraldehyde, CAS: 590-86-3

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2096915 (EU)
ENCS (2)-494 (JP)
ISHL (2)-494 (JP)
KECI KE-23536 (KR)

PICCS (PH)
TSCA (US)
NZIoC (NZ)

National regulatory information Great Britain

This classification following EG guidelines is also in accordance with the Chemicals (Hazard Information and Packaging for Supply) Regulation CHIP (as amended).

Releases to air (Pollution Inventory Substances)
not subject***

Releases to water (Pollution Inventory Substances)
not subject***

Releases to sewer (Pollution Inventory Substances)
not subject***
For details and further information please refer to the original regulation***

16. OTHER INFORMATION

Full text of H-Statements referred to under section 3
H225: Highly flammable liquid and vapour
H319: Causes serious eye irritation
H317: May cause an allergic skin reaction
H335: May cause respiratory irritation
H411: Toxic to aquatic life with long lasting effects

Full text of R-phrases referred to under sections 2 and 3
R11 - Highly flammable
R36/37 - Irritating to eyes and respiratory system
R43 - May cause sensitization by skin contact

Revision Date 15-Nov-2010
Issuing date 14-Dec-2012

Training advice
For effective first-aid, special training / education is needed.

Sources of key data used to compile the datasheet
Information contained in this safety data sheet is based on Oxea owned data and public sources deemed valid or acceptable. The absence of data elements required by ANSI or 2001/58/EC indicates, that no data meeting these requirements is available.

Further information for the safety data sheet
Changes against the previous version are marked by ***. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the Oxea homepage (www.oxea-chemicals.com).
The annex is not required because the substance is registered as an intermediate under REACh.

Disclaimer

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