

SAFETY DATA SHEET



Isovaleraldehyde

10150

Version / Revision

5

Revision Date

25-Jun-2021

Supersedes Version

4.01***

Issuing date

25-Jun-2021

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

1.1. Product identifier

Identification of the substance/preparation

Isovaleraldehyde

Chemical Name

3-Methylbutanal

CAS-No

590-86-3

EC No.

209-691-5

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

Identified uses

Transported isolated intermediate (1907/2006)

Other uses

Uses advised against

None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking Identification

OQ Chemicals GmbH
Rheinpromenade 4A
D-40789 Monheim
Germany

Product Information

Product Stewardship
FAX: +49 (0)208 693 2053
email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number +44 (0) 1235 239 670 (UK)
available 24/7

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation)

Flammable liquid Category 2, H225

Serious eye damage/eye irritation Category 2, H319

Skin sensitization Category 1, H317

Target Organ Systemic Toxicant - Single exposure Category 3, H335

Environmental hazard Aquatic Chronic 2; H411

Additional information

For full text of Hazard- and EU Hazard-statements see SECTION 16.

2.2. Label elements

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

Labelling according to Regulation 1272/2008/EC and its amendments (CLP Regulation).

Hazard pictograms



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 heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233: Keep container tightly closed.
P261: Avoid breathing gas/mist/vapours.
P273: Avoid release to the environment.
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.
P363: Wash contaminated clothing before reuse.
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.
P312: Call a POISON CENTRE/doctor if you feel unwell.
P391: Collect spillage.
P403 + P235: Store in a well ventilated place. Keep cool.

2.3. 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

PBT and vPvB assessment Not required

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	1272/2008/EC	Concentration (%)
Isovaleraldehyde	590-86-3	Flam. Liq. 2; H225 Eye Irrit. 2; H319 Skin Sens. 1; H317 STOT SE 3; H335	> 99,0

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

		Aquatic Chronic 2; H411	
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Remarks

3-Methylbutanal.

For full text of Hazard- and EU Hazard-statements see SECTION 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

Inhalation

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

Skin

Wash off immediately with soap and plenty of water. 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.

Ingestion

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

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

Main symptoms

shortness of breath, vomiting, headache, nausea.

Special hazard

Lung oedema, Lung irritation.

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

General advice

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

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

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

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

Unsuitable Extinguishing Media

Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

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

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback
Vapours may form explosive mixture with air

5.3. Advice for firefighters

Special protective equipment for firefighters

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

Precautions for firefighting

Keep people away from and upwind of fire. Cool containers / tanks with water spray. Dike and collect water used to fight fire. Water run-off can cause environmental damage.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: For personal protective equipment see section 8. 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.

6.2. 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.

6.3. Methods and material for containment and cleaning up

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).

6.4. Reference to other sections

For personal protective equipment see section 8.

SECTION 7: Handling and storage

7.1. Precautions for safe 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.

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.

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

Advice on the protection of the environment

See Section 8: Environmental exposure controls.

Incompatible products

acids and bases
amines
oxidizing agents

7.2. Conditions for safe storage, including any incompatibilities

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.

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

Temperature class

T3

7.3. Specific end use(s)

Transported isolated intermediate (1907/2006)
Other uses

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits European Union

No exposure limits established

Exposure limits UK

No exposure limits established.

DNEL & PNEC

This substance is registered as intermediate under strictly controlled conditions.

8.2. Exposure controls

Special adaptations (REACH)

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

The substance has been registered as an transported isolated intermediate and must be handled throughout its life cycle under strictly controlled conditions in accordance with Article 18.4, REACH.

Appropriate Engineering controls

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.

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

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

Skin and body protection

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

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.

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. 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://echa.europa.eu/information-on-chemicals/registered-substances>.

SECTION 9: Physical and chemical properties

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

9.1. Information on basic physical and chemical properties

Appearance	liquid
Colour	colourless
Odour	strong
Odour threshold	0,1 - 2 ppb
pH	3,1 (15 g/l in water @ 20 °C (68 °F))
Melting point/range	< -90 °C (Pour point)
Method	DIN ISO 3016
Boiling point/range	92 °C @ 1013 hPa
Method	OECD 103
Flash point	0,5 °C @ 1013 hPa
Method	EU A.9
Evaporation rate	No data available
Flammability (solid, gas)	Does not apply, the substance is a liquid
Lower explosion limit	No data available
Upper explosion limit	No data available

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
75	7,5	0,074	20	68	DIN EN 13016-2
255	25,5	0,252	50	122	DIN EN 13016-2

Vapour density 2,96 (Air = 1) @ 20 °C (68 °F)

Relative density

Values	@ °C	@ °F	Method
0,797	20	68	DIN 51757

Solubility 15 g/l @ 20 °C, in water, OECD 105

log Pow 1,5 @ 25 °C (77 °F), OECD 117

Autoignition temperature 210 °C @ 1020 hPa

Method DIN 51794

Decomposition temperature No data available

Viscosity 0,69 mm²/s @ 20°C

Method OECD 114, kinematic

Explosive properties Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties

Oxidizing properties Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties

9.2. Other information

Molecular weight 86,13

Molecular formula C₅ H₁₀ O

Refractive index 1,387 @ 20 °C

Surface tension 46,1 mN/m (1 g/l @ 20°C (68°F)), OECD 115

SECTION 10: Stability and Reactivity

10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

any text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous polymerisation does not occur.

10.4. Conditions to avoid

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

10.5. Incompatible materials

bases, amines, acids, oxidizing agents.

10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely 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
Dermal	LD50	2534 mg/kg	rabbit male	OECD 402
Inhalative	LC50	42,7 mg/l (4h)	rat	OECD 403

Isovaleraldehyde, CAS: 590-86-3

Assessment

Based on available data, the classification criteria are not met for:

Acute oral toxicity

Acute dermal toxicity

Acute inhalation toxicity

Irritation and corrosion				
Isovaleraldehyde (590-86-3)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	Mild skin irritation	OECD 404	4h in vivo
Eyes	rabbit	irritating		in vivo
Respiratory tract	mouse	RD50: 757-1008 ppm		10 min in vivo

Isovaleraldehyde, CAS: 590-86-3

Assessment

The available data lead to the classification given in section 2

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

Sensitization				
Isovaleraldehyde (590-86-3)				
Target Organ Effects	Species	Evaluation	Method	
Skin	mouse guinea pig	sensitizing	Weight of evidence	read across

Isovaleraldehyde, CAS: 590-86-3

Assessment

The available data lead to a classification as skin sensitizer (see section 2)

For respiratory sensitization, no data are available

Subacute, subchronic and prolonged toxicity				
Isovaleraldehyde (590-86-3)				
Type	Dose	Species	Method	
no data available				

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Isovaleraldehyde (590-86-3)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		human lymphocytes	positive (without metabolic activation)	Similar to: OECD 479 (SCE)	In vitro study
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study read across
Mutagenicity		mouse	negative	OECD 474 Chromosomal Aberration	in vivo
Carcinogenicity	LOAEC: 500 ppm	rat, male/female	negative	OECD 451, Inhalative	read across
Carcinogenicity	LOAEC: 500 ppm	mouse male/female	negative	OECD 451, Inhalative	read across
Reproductive toxicity	No data available				

Isovaleraldehyde, CAS: 590-86-3

CMR Classification

The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B

Evaluation

Did not show carcinogenic or mutagenic effects in animal experiments

Isovaleraldehyde, CAS: 590-86-3

Main symptoms

shortness of breath, vomiting, nausea, headache.

Target Organ Systemic Toxicant - Single exposure

The available data lead to the classification given in section 2

Target Organ Systemic Toxicant - Repeated exposure

Based on available data, the classification criteria are not met for:

STOT RE

Aspiration toxicity

According to experience not expected

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

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

found in the registration dossier under the following link:
<http://echa.europa.eu/information-on-chemicals/registered-substances>.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
Isovaleraldehyde (590-86-3)			
Species	Exposure time	Dose	Method
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

Long term toxicity				
Isovaleraldehyde (590-86-3)				
Type	Species	Dose	Method	
Aquatic toxicity	Desmodesmus subspicatus	EC10: 32.62 mg/l (72 h) Biomass	DIN 38412 / part 9	
Aquatic toxicity	Desmodesmus subspicatus	EC10: 71,89 mg/l (72 h) Growth inhibition	DIN 38412 / part 9	

12.2. Persistence and degradability

Isovaleraldehyde, CAS: 590-86-3

Biodegradation

50 % (28 d), Sewage, aerobic, OECD 301 D.

Abiotic Degradation		
Isovaleraldehyde (590-86-3)		
Type	Result	Method
Hydrolysis	No data available	
Photolysis	No data available	

12.3. Bioaccumulative potential

Isovaleraldehyde (590-86-3)		
Type	Result	Method
log Pow	1,5 @ 25 °C (77 °F)	OECD 117
BCF	No data available	

12.4. Mobility in soil

Isovaleraldehyde (590-86-3)		
Type	Result	Method
Surface tension	46,1 mN/m (1 g/l @ 20°C (68°F))	OECD 115

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

Adsorption/Desorption	no data available	
Distribution to environmental compartments	no data available	

12.5. Results of PBT and vPvB assessment

Isovaleraldehyde, CAS: 590-86-3

PBT and vPvB assessment

Not required

12.6. Other adverse effects

Isovaleraldehyde, CAS: 590-86-3

No data available

Note

Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

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.

SECTION 14: Transport information

ADR/RID

14.1. UN number	UN 2058
14.2. UN proper shipping name	Valeraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
ADR Tunnel restriction code	(D/E)
Classification Code	F1
Hazard Number	33

ADN

ADN Container

14.1. UN number	UN 2058
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SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

14.2. UN proper shipping name	Valeraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
Classification Code	F1
Hazard Number	33

ADN ADN Tanker
forbidden

ICAO-TI / IATA-DGR

14.1. UN number	UN 2058
14.2. UN proper shipping name	Valeraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	no data available

IMDG

14.1. UN number	UN 2058
14.2. UN proper shipping name	Valeraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
EmS	F-E, S-D
14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code	
Product name	Valeraldehyde
Ship type	3
Pollution category	Y

SECTION 15: Regulatory information

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

Regulation 1272/2008, Annex VI

not listed

DI 2012/18/EU (Seveso III)

Category

Annex I, part 1:
P5a - c; depending on conditions
E2

DI 1999/13/EC (VOC Guideline)

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

Component	Status
Isovaleraldehyde CAS: 590-86-3	regulated

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)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC (NZ)
TCSI (TW)

National regulatory information Great Britain

Releases to air (Pollution Inventory Substances)

not subject

Releases to water (Pollution Inventory Substances)

not subject

Releases to sewer (Pollution Inventory Substances)

not subject

The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019 No. 758 ***

Component	Status
Isovaleraldehyde CAS: 590-86-3	The substance is/will be pre-registered.***

For details and further information please refer to the original regulation

15.2. Chemical safety assessment

The Chemical Safety Report (CSR) is not required.

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 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.

SAFETY DATA SHEET



Isovaleraldehyde
10150

Version / Revision 5

Abbreviations

A table of terms and abbreviations can be found under the following link:
http://echa.europa.eu/documents/10162/13632/information_requirements_r20_en.pdf

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 OQ owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/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 OQ homepage (www.chemicals.oq.com).

The annex is not required because the substance is registered as an intermediate under REACH

Disclaimer

For industrial use only. The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. OQ makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards.

End of Safety Data Sheet