SAFETY DATA SHEET

Isovaleraldehyde
10150

Version / Revision	6	**Revision Date**	28-Feb-2023
Supersedes Version	5.01***	**Issuing date**	28-Feb-2023

SECTION 1: Identification

1.1. Product identifier

Identification of the substance/preparation **Isovaleraldehyde**

Chemical Name 3-Methylbutanal
CAS-No 590-86-3

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

Use of the Substance / Preparation Intermediate
Uses advised against None

1.3. Details of the supplier of the safety data sheet

Supplier

OQ Chemicals Corporation
15375 Memorial Drive
West Memorial Place I
Suite 300
Houston, TX 77079
USA

Product Information

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

1.4. Emergency telephone number

Emergency telephone number NCEC +1 202 464 2554
available 24/7

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).

Serious eye damage/eye irritation Category 2A, H319
Skin sensitization Category 1, H317
Target Organ Systemic Toxicant - Single exposure Category 3, H335
Flammable liquid Category 2, H225
Environmental hazard Aquatic Chronic 2; H411; Aquatic Acute 2; H401

OSHA Specified Hazards Not applicable.

2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).

Hazard symbol(s)

Signal word **Danger**

Hazard statements

H225: Highly flammable liquid and vapor.
H319: Causes serious eye irritation.
H317: May cause an allergic skin reaction.
H335: May cause respiratory irritation.
H401: Toxic to aquatic life
H411: Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233: Keep container tightly closed.
P240: Ground and bond container and receiving equipment.
P241: Use explosion-proof electrical/ ventilating/ lighting equipment.
P242: Use non-sparking tools.
P243: Take precautionary measures against static discharge.
P280: Wear protective gloves/eye protection/face protection.
P264: Wash hands thoroughly after handling.
P261: Avoid breathing gas/mist/vapours.
P271: Use only outdoors or in a well ventilated area.
P272: Contaminated work clothing must not be allowed out of the workplace.
P273: Avoid release to the environment.

Response

P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P333 + P313: If skin irritation or rash occurs: Get medical advice/attention.
P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
P363: Wash contaminated clothing before reuse.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
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 CENTRE/doctor if you feel unwell. P391: Collect spillage.
Storage	P403 + P235: Store in a well ventilated place. Keep cool. P405: Store locked up.
Disposal	P501: Dispose of contents/container in accordance with local regulation.

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

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	Concentration (%)
Isovaleraldehyde	590-86-3	> 99,0

Remarks
3-Methylbutanal.

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
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.

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

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits United States of America

No exposure limits established regarding ACGIH, OSHA Z-1 and OSHA Z-2.

8.2. Exposure controls

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.

Individual protection measures, such as 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.

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 filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (vapor or mist). Equipment should conform to NIOSH.

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.

SECTION 9: Physical and chemical properties

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/freezing point	< -130 °F (< -90 °C) (Pour point)
Method	DIN ISO 3016
Boiling point or initial boiling point and boiling range	197,6 °F (92 °C) @ 1 atm (101,3 kPa)
Method	OECD 103
Flash point	32,9 °F (0,5 °C) @ 1 atm (101,3 kPa)
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

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

Density and/or relative density

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

Solubility 15 g/l @ 20 °C (68 °F), in water, OECD 105
Partition coefficient n-octanol/water (log value) 1,5 @ 25 °C (77 °F) OECD 117

Autoignition temperature	410 °F (210 °C)
Method	DIN 51794
Decomposition temperature	No data available
Viscosity	0,69 mm²/s @ 68 °F (20 °C)
Method	OECD 114, kinematic

9.2. Other information

Molecular weight	86,13
Molecular formula	C5 H10 O
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties
Refractive Index	1,387 @ 68 °F (20 °C)
Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties
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 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

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

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

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
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 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
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.

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

D.O.T. (49CFR)

14.1. UN number or ID 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	***
Marking	Fish and tree***
Marine pollutant	yes***
14.6. Special precautions for user	
Emergency Response Guide	129

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)	3
14.4. Packing group	II
14.5. Environmental hazards	*** Fish and tree***
14.6. Special precautions for user	no data available

IMDG

14.1. UN number or ID 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	***
Marking	Fish and tree***
Marine pollutant	yes***
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

Federal and State Regulations

Components of the product are listed in the quoted regulations. For details please refer to the regulations directly. This list is not exhaustive, please check for other applicable regulations.

Federal Regulations

This product is listed on the TSCA inventory

Isovaleraldehyde, CAS: 590-86-3

CERCLA Hazardous Substance

CERCLA RQ	100 LBS

State Regulations

Isovaleraldehyde, CAS: 590-86-3

MA RTK List
NY RTK List
PA RTK List

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)

SECTION 16: Other information

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Hazard Rating Systems

NFPA (National Fire Protection Association)

Health Hazard	1
Fire Hazard	3
Reactivity	0

HMIS (Hazardous Material Information System)

Health Hazard	1
Flammability	3
Physical Hazard	0

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 use of a comma in section 3 and section 7 to 12 is the same as a period.

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End of Safety Data Sheet