SAFETY DATA SHEET

Isopentanoic acid
11560

Version / Revision	5	**Revision Date**	15-Nov-2021
Supersedes Version	4.00***	**Issuing date**	15-Nov-2021

SECTION 1: Identification

1.1. Product identifier

Identification of the substance/preparation **Isopentanoic acid**

CAS-No -

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
Phone +1 346 378 7300

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

Skin corrosion/irritation Category 1B, H314
Serious eye damage/eye irritation Category 1, H318
Flammable liquid Category 4, H227
Environmental hazard Aquatic Acute 3; H402***

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
H227: Combustible liquid
H314: Causes severe skin burns and eye damage.
H402: Harmful to aquatic life***

Precautionary statements

Prevention
P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P260: Do not breathe gas/mist/vapours.
P264: Wash hands thoroughly after handling.
P273: Avoid release to the environment.

Response
P301 + P330 + P331: IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
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.
P310: Immediately call a POISON CENTER/doctor.
P363: Wash contaminated clothing before reuse.

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.

contains n-Valeric acid (CAS 109-52-4), 2-Methylbutyric acid (CAS 116-53-0)

2.3. Other hazards

Components of the product may be absorbed into the body by inhalation and ingestion
Vapour/air-mixtures are explosive at intense warming

SECTION 3: Composition / information on ingredients

3.2. Mixtures

Component	CAS-No	Concentration (%)
Valeric acid	109-52-4	< 70
2-Methylbutyric acid***	116-53-0	34 - 37

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. Immediate medical attention is required.

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

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

Main symptoms
central nervous system depression, unconsciousness, shortness of breath, vomiting, cough, dizziness, nausea, gastrointestinal discomfort.

Special hazard
Lung irritation, Lung oedema, Dermatitis.

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. If ingested, flush stomach and compensate acidosis.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media
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
Vapours are heavier than air and may spread along floors
Vapour/air-mixtures are explosive at intense warming

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
Cool containers / tanks with water spray. Keep people away from and upwind of fire. Dike and collect water used to fight fire. Water run-off and vapor cloud may be corrosive. 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. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Dispose of in accordance with local regulations. 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.

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
bases
amines
strong 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/air-mixtures are explosive at intense warming.

Technical measures/Storage conditions
Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care.

Suitable material
stainless steel

Unsuitable material
copper, nickel

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	nitrile rubber
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,55 mm
Break through time	> 480 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	unpleasant
Odour threshold	No data available
pH	3,1 - 3,3 (10 g/l in water @ 25 °C (77 °F))***
Melting point/range	-130 - -31 °F (-90 - -35 °C) (Pour point)
Method	DIN ISO 3016***
Boiling point/range	350,6 - 366,8 °F (177 - 186 °C) @ 1 atm (101,3 kPa)
Method	OECD 103***
Flash point	170,6 - 192,2 °F (77 - 89 °C)
Method	EN 22719, ISO 2719***
Evaporation rate	No data available
Flammability (solid, gas)	Does not apply, the substance is a liquid
Lower explosion limit	1,6 Vol %
Upper explosion limit	7,6 Vol %

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
0,2 - 1,68***	0,02 - 1,168***	< 0,001 - 0,002***	20	68	DIN EN 13016-2***

Vapour density	~ 3,5 (Air = 1) @ 20 °C (68 °F)

Relative density

Values	@ °C	@ °F	Method
0,9360 - 0,94***	20	68	DIN 51757

Solubility	37 - 45 g/l @ 20 °C (68 °F), in water, OECD 105
log Pow	1,8 @ 25 °C (77 °F) measured OECD 117***
Autoignition temperature	770 - 815 °F (410 - 435 °C) @ 1003 - 1007 hPa***
Method	DIN 51794
Decomposition temperature	No data available
Viscosity	2,1 - 2,173 mPa*s @ 68 °F (20 °C)
Method	DIN 51562, dynamic

9.2. Other information

Molecular weight	102,13
Molecular formula	C5 H10 O2
Dissociation constant	pKa 4,8 @ 20 - 22,5 °C (68 - 72,5 °F), OECD 112***
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties
Refractive Index	1,405 - 1,408 @ 68 °F (20 °C)
Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties
Surface tension	51,6 - 64,2 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, strong 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 Ingestion, Inhalation, Eye contact, Skin contact

Valeric acid, CAS: 109-52-4
Main symptoms
central nervous system depression, unconsciousness, shortness of breath, vomiting.
Target Organ Systemic Toxicant - Single exposure
Based on available data, the classification criteria are not met for:
STOT SE
Target Organ Systemic Toxicant - Repeated exposure
Due to lack of data, a classification is not possible for:
STOT RE
2-Methylbutyric acid*, CAS: 116-53-0**
Main symptoms
cough, dizziness, nausea, shortness of breath, unconsciousness, gastrointestinal discomfort.
Target Organ Systemic Toxicant - Single exposure
Based on available data, the classification criteria are not met for:
STOT SE

Target Organ Systemic Toxicant - Repeated exposure
Based on available data, the classification criteria are not met for:
STOT RE

Acute toxicity				
Valeric acid (109-52-4)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	4600 mg/kg	rat, male/female	OECD 401
Dermal	LD50	> 2000 mg/kg (24 h)	rat, male/female	OECD 402
Inhalative***	LC0***	11,63 mg/l (7 h)***	rat, male/female***	

2-Methylbutyric acid (116-53-0)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	1750 mg/kg	rat, male/female	OECD 401
Dermal	LD50	2228 mg/kg	rabbit male	OECD 402
Dermal	LD50	1367 mg/kg	rabbit female	OECD 402
Inhalative	LC0	8375 mg/m³ (6 h)	rat, male/female	OECD 403

Valeric acid, CAS: 109-52-4
Assessment
Based on available data, the classification criteria are not met for:
Acute oral toxicity
Acute dermal toxicity
STOT SE
An LC50/inhalation/4h/rat could not be determined because no mortality of rats was observed at the maximum achievable concentration
2-Methylbutyric acid*, CAS: 116-53-0**
Assessment
The available data lead to the classification given in section 2
An LC50/inhalation/4h/rat could not be determined because no mortality of rats was observed at the maximum achievable concentration

Irritation and corrosion				
Valeric acid (109-52-4)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive		3 min
Eyes	rabbit	corrosive		

2-Methylbutyric acid (116-53-0)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	corrosive	OECD 404	3 min

Valeric acid, CAS: 109-52-4
Assessment
The available data lead to the classification given in section 2
For respiratory irritation, no data are available
2-Methylbutyric acid*, CAS: 116-53-0**
Assessment

The available data lead to the classification given in section 2
Available skin corrosion data suffice for classification of eye corrosion without further testing
For respiratory irritation, no data are available

Valeric acid, CAS: 109-52-4
Assessment
Skin sensitization was not tested due to the corrosive properties of the substance
For skin sensitization, no data are available
For respiratory sensitization, no data are available

2-Methylbutyric acid*, CAS: 116-53-0**
Assessment
Skin sensitization was not tested due to the corrosive properties of the substance
For respiratory sensitization, no data are available

Subacute, subchronic and prolonged toxicity				
Valeric acid (109-52-4)				
Type	Dose	Species	Method	
no data available				

Valeric acid, CAS: 109-52-4
Assessment
Due to lack of data, a classification is not possible for:
STOT RE

2-Methylbutyric acid*, CAS: 116-53-0**
Assessment
Based on available data, the classification criteria are not met for:
STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Valeric acid (109-52-4)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study
Mutagenicity		CHO (Chinese Hamster Ovary) cells	positive (with metabolic activation)***	OECD 473 (Chromosomal Aberration)	In vitro study
Mutagenicity		CHO (Chinese Hamster Ovary) cells	positive	OECD 479 (SCE)	In vitro study
Mutagenicity		CHO (Chinese Hamster Ovary) cells	negative	OECD 476 (Mammalian Gene Mutation)	In vitro study
Mutagenicity		mouse	negative	OECD 474	in vivo
Developmental Toxicity***	NOEL 50 mg/kg/d***	rat***		Oral***	Developmental toxicity***
Developmental Toxicity***	NOAEL 750 mg/kg/d***	rat***		OECD 414, Oral***	Maternal toxicity, Embryotoxicity***

2-Methylbutyric acid (116-53-0)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium Escherichia coli***	negative	OECD 471 (Ames)***	

Valeric acid, CAS: 109-52-4
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
No developmental effects in the absence of maternal toxicity
Did not show mutagenic effects in animal experiments***
2-Methylbutyric acid*, CAS: 116-53-0**
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
In vitro tests did not show mutagenic effects

Valeric acid, CAS: 109-52-4
Aspiration toxicity
no data available
Other adverse effects
Components of the product may be absorbed into the body by inhalation and ingestion.
2-Methylbutyric acid*, CAS: 116-53-0**
Aspiration toxicity
no data available
Note
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
Valeric acid (109-52-4)			
Species	Exposure time	Dose	Method
Daphnia magna (Water flea)	48h	EC50: 88,1 mg/l***	OECD 202 read across
Pseudokirchneriella subcapitata	72h	EC50: 29,3 mg/l (Growth rate)***	OECD 201
Pimephales promelas (fathead minnow)	96h	LC50: 39 mg/l	OECD 203

2-Methylbutyric acid (116-53-0)			
Species	Exposure time	Dose	Method
Danio rerio (Zebra fish)	96h	LC50: > 1000 mg/l	OECD 203

Bacteria / Sewage	24h	TTC: 1250 mg/l	ETAD Fermentation tube method
Daphnia magna (Water flea)***	48h***	LC50: 88,1 mg/l***	OECD 202 read across***
Pseudokirchneriella subcapitata***	72h***	EC50: 73,2 mg/l (Growth rate)***	OECD 201 read across***

Long term toxicity				
Valeric acid (109-52-4)				
Type	Species	Dose	Method	
Aquatic toxicity	Pseudokirchneriella subcapitata	NOAEC: 12,6 mg/l (3d)	OECD 201	

2-Methylbutyric acid (116-53-0)				
Type	Species	Dose	Method	
Aquatic toxicity***	Pseudokirchneriella subcapitata***	NOEC: 54,4 mg/l (3d) Growth inhibition***	OECD 201 read across***	

12.2. Persistence and degradability

Valeric acid, CAS: 109-52-4
Biodegradation
72 % (10 d), activated sludge, non-adapted, aerobic.
2-Methylbutyric acid*, CAS: 116-53-0**
Biodegradation
67,9 % (10 d), Sewage, domestic, non-adapted, Readily biodegradable, OECD 301 D.

Abiotic Degradation		
Valeric acid (109-52-4)		
Type	Result	Method
Hydrolysis	not expected	
Photolysis	No data available	

2-Methylbutyric acid (116-53-0)		
Type	Result	Method
Hydrolysis***	No data available***	
Photolysis***	No data available***	

12.3. Bioaccumulative potential

Valeric acid (109-52-4)		
Type	Result	Method
log Pow	1,8 @ 25 °C (77 °F)***	measured, OECD 117
BCF***	No data available***	

2-Methylbutyric acid (116-53-0)		
Type	Result	Method

log Pow	1,8 @ 25 °C (77 °F)***	measured, OECD 117
BCF***	No data available***	

12.4. Mobility in soil

Valeric acid (109-52-4)		
Type	Result	Method
Surface tension	51,6 mN/m (1 g/l @ 20°C (68°F))	OECD 115
Adsorption/Desorption	no data available	
Distribution to environmental compartments	no data available	

2-Methylbutyric acid (116-53-0)		
Type	Result	Method
Surface tension	64,2 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

Valeric acid, CAS: 109-52-4
PBT and vPvB assessment
This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)
2-Methylbutyric acid*, CAS: 116-53-0**
PBT and vPvB assessment
This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

12.6. Other adverse effects

Valeric acid, CAS: 109-52-4
No data available
2-Methylbutyric acid*, CAS: 116-53-0**
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	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (2-Methylbutyric acid / n-Valeric acid)
14.3. Transport hazard class(es)	8
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
Emergency Response Guide	153

ICAO-TI / IATA-DGR

14.1. UN number	UN 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (2-Methylbutyric acid / n-Valeric acid)
14.3. Transport hazard class(es)	8
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 3265
14.2. UN proper shipping name	Corrosive liquid, acidic, organic, n.o.s. (2-Methylbutyric acid / n-Valeric acid)
14.3. Transport hazard class(es)	8
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
EmS	F-A, S-B

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code not applicable

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

State Regulations

Valeric acid, CAS: 109-52-4

MA RTK List
NY RTK List
PA RTK List

International Inventories

Valeric acid, CAS: 109-52-4

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2036772 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-35263 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC (NZ)***
TCSI (TW)

2-Methylbutyric acid*, CAS: 116-53-0**

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2041452 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-23544 (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	3
Fire Hazard	2
Reactivity	0

HMIS (Hazardous Material Information System)

Health Hazard	3
Flammability	2
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