

SAFETY DATA SHEET

Creation Date 16-Sep-2010

Revision Date 18-Jan-2018

Revision Number 4

1. Identification

Product Name 3-Methylbutyraldehyde

Cat No. : AC163970000; AC163970025; AC163971000; AC163975000

CAS-No 590-86-3
Synonyms Isovaleraldehyde

Recommended Use Laboratory chemicals.
Uses advised against Not for food, drug, pesticide or biocidal product use

Details of the supplier of the safety data sheet

Company

Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Skin Sensitization	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Danger

Hazard Statements

Highly flammable liquid and vapor
May cause an allergic skin reaction
Causes serious eye irritation
May cause respiratory irritation

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
 Avoid breathing dust/fume/gas/mist/vapors/spray
 Contaminated work clothing should not be allowed out of the workplace
 Use only outdoors or in a well-ventilated area
 Keep away from heat/sparks/open flames/hot surfaces. - No smoking
 Keep container tightly closed
 Ground/bond container and receiving equipment
 Use explosion-proof electrical/ventilating/lighting/equipment
 Use only non-sparking tools
 Take precautionary measures against static discharge
 Wear protective gloves/protective clothing/eye protection/face protection
 Keep cool

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
 Call a POISON CENTER or doctor/physician if you feel unwell

Skin

If skin irritation or rash occurs: Get medical advice/attention
 Wash contaminated clothing before reuse
 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
 If eye irritation persists: Get medical advice/attention

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

Store in a well-ventilated place. Keep container tightly closed
 Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Toxic to aquatic life
 Toxic to aquatic life with long lasting effects

Other hazards

Stench.

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Isopentaldehyde	590-86-3	>95

4. First-aid measures

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Move to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	None reasonably foreseeable. . May cause allergic skin reaction. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray.
Unsuitable Extinguishing Media	No information available
Flash Point	-5 °C / 23 °F
Method -	No information available
Autoignition Temperature	235 °C / 455 °F
Explosion Limits	
Upper	5.6 vol %
Lower	1.4 vol %
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Carbon monoxide (CO) Carbon dioxide (CO₂)

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
2	3	1	N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Do not flush into surface water or sanitary sewer system.
Methods for Containment and Clean Up	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling	Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Ensure adequate ventilation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by
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static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Storage

Flammables area. Keep away from heat and sources of ignition. Store under an inert atmosphere. Keep refrigerated. Keep container tightly closed in a dry and well-ventilated place.

8. Exposure controls / personal protection

Exposure Guidelines

This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment.

Personal Protective Equipment**Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection

Long sleeved clothing.

Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Hygiene Measures

When using, do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless, Light yellow
Odor	Stench
Odor Threshold	No information available
pH	5.3
Melting Point/Range	-28 °C / -18.4 °F
Boiling Point/Range	91 - 93 °C / 195.8 - 199.4 °F @ 760 mmHg
Flash Point	-5 °C / 23 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	5.6 vol %
Lower	1.4 vol %
Vapor Pressure	57.9 mbar (20°C)
Vapor Density	2.97 (Air = 1.0)
Specific Gravity	0.796
Solubility	soluble
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	235 °C / 455 °F
Decomposition Temperature	No information available
Viscosity	0.6 mPa s at 20 °C
Molecular Formula	C5 H10 O
Molecular Weight	86.13

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Air sensitive.
Conditions to Avoid	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition. Exposure to air.
Incompatible Materials	Strong oxidizing agents, Strong bases, Strong reducing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isopentaldehyde	LD50 = 5600 mg/kg (Rat)	LD50 = 2730 mg/kg (Rabbit)	LC50 = 42700 mg/m ³ (Rat) 4 h

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation Irritating to eyes, respiratory system and skin

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Isopentaldehyde	590-86-3	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

The product contains following substances which are hazardous for the environment. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Isopentaldehyde	EC50: = 78 mg/L, 96h (Desmodesmus subspicatus) EC50: = 80 mg/L, 72h (Desmodesmus subspicatus)	LC50 96h 53 mg/L (Leuciscus idus)	Not listed	EC50: = 177 mg/L, 48h (Daphnia magna)

Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility . Will likely be mobile in the environment due to its water solubility.

Component	log Pow
Isopentaldehyde	1.31

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No UN2058
 Proper Shipping Name VALERALDEHYDE
 Hazard Class 3
 Packing Group II

TDG

UN-No UN2058
 Proper Shipping Name VALERALDEHYDE
 Hazard Class 3
 Packing Group II

IATA

UN-No UN2058
 Proper Shipping Name VALERALDEHYDE
 Hazard Class 3
 Packing Group II

IMDG/IMO

UN-No UN2058
 Proper Shipping Name VALERALDEHYDE
 Hazard Class 3
 Packing Group II

15. Regulatory information

All of the components in the product are on the following Inventory lists: X = listed

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
Isopentaldehyde	X	X	-	209-691-5	-		X	X	X	X	X

Legend:

X - Listed

E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.

F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.

N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.

P - Indicates a commenced PMN substance

R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.

S - Indicates a substance that is identified in a proposed or final Significant New Use Rule

T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.

XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B)).

Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.

Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations

TSCA 12(b)	Not applicable
SARA 313	Not applicable
SARA 311/312 Hazard Categories	See section 2 for more information
CWA (Clean Water Act)	Not applicable
Clean Air Act	Not applicable
OSHA Occupational Safety and Health Administration	Not applicable
CERCLA	Not applicable
California Proposition 65	This product does not contain any Proposition 65 chemicals

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Isopentaldehyde	X	X	X	-	-

U.S. Department of Transportation

Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

U.S. Department of Homeland Security

This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade	Serious risk, Grade 3
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16. Other information

Prepared By	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
Creation Date	16-Sep-2010
Revision Date	18-Jan-2018
Print Date	18-Jan-2018
Revision Summary	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the

date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS