Chemical Safety Data Sheet MSDS / SDS

2-ethylhexanal SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: 2-ethylhexanal

CAS: 123-05-7

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 3
Skin sensitization, Sub-category 1B

Reproductive toxicity, Category 2

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Warning

Hazard statement(s)

H226 Flammable liquid and vapour
H317 May cause an allergic skin reaction
H361 Suspected of damaging fertility or the unborn child

Precautionary statement(s)

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 action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P203 Obtain, read and follow all safety instructions before use.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P333+P317 If skin irritation or rash occurs: Get medical help.
P321 Specific treatment (see ... on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.
P318 IF exposed or concerned, get medical advice.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	2-ethylhexanal
Common names and synonyms:	2-ethylhexanal
CAS number:	123-05-7
EC number:	204-596-5
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Rest. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Inhalation may be irritating to mucous membrane; overexposure may cause dizziness and collapse. Ingestion causes irritation of mouth and stomach. Contact with eyes or skin causes irritation. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aldehydes and Related Compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Use dry chemical, carbon dioxide or foam extinguishers.

Specific hazards arising from the chemical

Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (ERG, 2016)

Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then

store and dispose of according to local regulations. Do NOT let this chemical enter the environment. Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance.

Environmental precautions

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment. Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance.

Methods and materials for containment and cleaning up

Absorb liquids in vermiculite, dry sand, earth, peat, carbon, or a similar material and deposit in sealed containers. Keep ethyl hexaldehyde out of a confined space, such as a sewer, because of the possibility of an explosion ...

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. NO contact with hot surfaces. Above 46°C use a closed system, ventilation and explosion-proof electrical equipment. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from acids, bases and oxidants. Cool. Well closed.Store in tightly closed containers in a cool, well ventilated area away from oxidizers, strong bases and combustible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Colorless.
Odour:	Mild odor
Melting point/freezing point:	< -100 °C.
Boiling point or initial boiling point and boiling range:	159.6 °C. Atm. press.:760 mm Hg.
Flammability:	Flammable.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 0.85% by volume @ 93 deg C (200 deg F); Upper flammable limit: 7.2% by volume @135 deg C (275 deg F)

Flash point:	44 °C. Atm. press.:1 013.25 hPa.
Auto-ignition temperature:	190 °C. Atm. press.:1 013.25 hPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 1. Temperature:20°C.
Solubility:	less than 1 mg/mL at 70° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = 3.07. Temperature:25 °C.
Vapour pressure:	2 hPa. Temperature:18.5 °C.;2.8 hPa. Temperature:23.4 °C.
Density and/or relative density:	0.85 g/cm3. Temperature:20 °C.
Relative vapour density:	4.42 (NTP, 1992) (Relative to Air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance can form explosive peroxides on prolonged contact with oxygen or air. The substance polymerizes on contact with sodium hydroxide, ammonia, butyl- and dibutylamine and inorganic acids. Reacts with oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

Dangerous fire hazard; spontaneously flammable in air.The vapour is heavier than air.2-ETHYLHEXALDEHYDE is an aldehyde. Aldehydes are frequently involved in self-condensation or polymerization reactions. These reactions are exothermic; they are

often catalyzed by acid. Aldehydes are readily oxidized to give carboxylic acids. Flammable and/or toxic gases are generated by the combination of aldehydes with azo, diazo compounds, dithiocarbamates, nitrides, and strong reducing agents. Aldehydes can react with air to give first peroxo acids, and ultimately carboxylic acids. These autoxidation reactions are activated by light, catalyzed by salts of transition metals, and are autocatalytic (catalyzed by the products of the reaction). The addition of stabilizers (antioxidants) to shipments of aldehydes retards autoxidation.

Conditions to avoid

no data available

Incompatible materials

Forms explosive mixture with air. Violent reaction with oxidizers. Incompatible with strong acids, caustics, ammonia, amines.

Hazardous decomposition products

When heated to decomposition it emits acrid and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - ca. 3.2 mL/kg bw.

Inhalation: LC50 - rat (male/female) - > 6.83 mg/L air.

Dermal: LD50 - rat (male/female) - > 16 440 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes and skin. The vapour is irritating to the respiratory tract.

STOT-repeated exposure

Repeated or prolonged contact with skin may cause dermatitis.

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Oncorhynchus mykiss (previous name: Salmo gairdneri) - 5.5 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 4.7 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 6.9 mg/L - 72 h.

Toxicity to microorganisms: EC0 - activated sludge, domestic - 48.8 mg/L - 30 min. Remarks:Respiration rate.

Persistence and degradability

AEROBIC: Using OECD Method 301F (Ready Biodegradability, Manometric Respirometry Test) with a domestic activated sludge inoculum and a 28-day incubation period, 2-ethylhexaldehyde had a theoretical BODT of 71.8%(1) which classifies it as readily

biodegradable(SRC). By analogy, isobutyraldehyde (a structurally similar branched saturated aldehyde to 2-ethylhexaldhyde), present at 30 mg/L, reached 81% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 100 mg/L in the Japanese MITI test(2).

Bioaccumulative potential

An estimated BCF of 49 was calculated in fish for 2-ethylhexaldehyde(SRC), using a log Kow of 3.07(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 2-ethylhexaldehyde can be estimated to be 18(SRC). According to a classification scheme(2), this estimated Koc value suggests that 2-ethylhexaldehyde is expected to have very high mobility in soil(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1191 (For reference only, please check.)

IMDG: UN1191 (For reference only, please check.)
IATA: UN1191 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: OCTYL ALDEHYDES (For reference only, please check.)
IMDG: OCTYL ALDEHYDES (For reference only, please check.)
IATA: OCTYL ALDEHYDES (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)
IMDG: 3 (For reference only, please check.)
IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)
IMDG: III (For reference only, please check.)
IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No
IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Other Information

Check for peroxides prior to distillation; eliminate if found.