

Chemical Safety Data Sheet MSDS / SDS

2-Ethylhexanoic acid

Revision Date:2024-08-17 Revision Number:1

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

Product identifier

Product name : 2-Ethylhexanoic acid
CBnumber : CB5425330
CAS : 149-57-5
EINECS Number : 205-743-6
Synonyms : 2-ethylhexanoic acid, Hexanoic acid, 2-ethyl-

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
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

Classification of the substance or mixture

Reproductive toxicity, Category 2

Label elements

Pictogram(s)

Signal word : Warning

Hazard statement(s)

H290 May be corrosive to metals
H302 Harmful if swallowed
H312 Harmful in contact with skin
H314 Causes severe skin burns and eye damage
H360 May damage fertility or the unborn child
H361 Suspected of damaging fertility or the unborn child
H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

P201 Obtain special instructions before use.

P202 Do not handle until all safety precautions have been read and understood.

P234 Keep only in original container.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P264 Wash hands thoroughly after handling.

P264 Wash skin thoroughly after handling.

P273 Avoid release to the environment.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P390 Absorb spillage to prevent material damage.

P308+P313 IF exposed or concerned: Get medical advice/attention.

P405 Store locked up.

P406 Store in corrosive resistant/... container with a resistant inner liner.

P501 Dispose of contents/container to....

Prevention

P203 Obtain, read and follow all safety instructions before use.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

Response

P318 IF exposed or concerned, get medical advice.

Storage

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2-Ethylhexanoic acid
Synonyms	: 2-ethylhexanoic acid, Hexanoic acid, 2-ethyl-
CAS	: 149-57-5
EC number	: 205-743-6
MF	: C ₈ H ₁₆ O ₂
MW	: 144.21

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

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. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Harmful if swallowed, inhaled or absorbed through skin. Material is extremely destructive to tissues of mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx, bronchii, chemical pneumonitis and pulmonary edema. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. (USCG, 1999)

Indication of any immediate medical attention and special treatment needed

Call for medical aid. Vapor irritating to eyes, nose, and throat. If inhaled, will cause coughing or difficult breathing. If breathing stopped, give artificial respiration. If breathing is difficult, give oxygen. Liquid will burn skin and eyes. If swallowed will cause nausea and vomiting. Remove contaminated clothing and shoes. Flush affected areas with plenty of water. If in eyes, hold eyelids open, and flush with plenty of water.

SECTION 5: Firefighting measures

Extinguishing media

Combustible. Water may be ineffective on fire. Wear self-contained breathing apparatus and protective clothing. Extinguish with dry chemical, alcohol foam, or carbon dioxide.

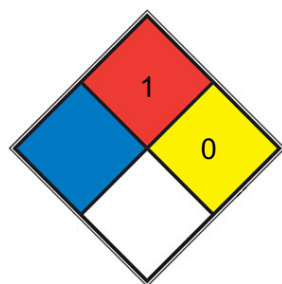
Specific Hazards Arising from the Chemical

This chemical is combustible. (NTP, 1992)

Advice for firefighters

Use water spray, powder, foam, carbon dioxide.

NFPA 704



■ HEALTH

Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion

■ FIRE 1 can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

☐ SPEC.
☐ HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Do NOT absorb in saw-dust or other combustible absorbents. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Do NOT absorb in saw-dust or other combustible absorbents. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent and remove to safe place. Do NOT absorb in saw-dust or other combustible absorbents. Do NOT let this chemical enter the environment.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. 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

Separated from strong oxidants. Store in an area without drain or sewer access. Separated from strong oxidants. Store in an area without drain or sewer access.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 5 mg/m³, as TWA

Biological limit values

no data available

Exposure 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

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Liquid
Colour	Clear
Odour	Mild odor
Melting point/freezing point	-57 °C.
Boiling point or initial boiling point and boiling range	226 - 229 °C. Atm. press.:1 013 hPa.
Flammability	Combustible.
Lower and upper explosion limit/flammability limit	1.04%, 135°F
Flash point	118 °C. Atm. press.:1 013.25 hPa.
Auto-ignition temperature	310 °C. Atm. press.:1 013.25 hPa.
Decomposition temperature	no data available
pH	3 (1.4g/l, H ₂ O, 20°C)
Kinematic viscosity	dynamic viscosity (in mPa s) = 8.4. Temperature:20.3°C.;dynamic viscosity (in mPa s) = 4.2. Temperature:40°C.
Solubility	1.4g/l
Partition coefficient n-octanol/water	log Pow = 2.7. Temperature:25 °C.
Vapour pressure	<0.01 mm Hg (20 °C)
Density and/or relative density	906.7 kg/m ³ . Temperature:20 °C.
Relative vapour density	4.98 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance is a strong reducing agent. It reacts violently with oxidants. Decomposes on heating. This produces irritating fumes.

Chemical stability

no data available

Possibility of hazardous reactions

ETHYLHEXOIC ACID is a carboxylic acid. Carboxylic acids donate hydrogen ions if a base is present to accept them. They react in this way with all bases, both organic (for example, the amines) and inorganic. Their reactions with bases, called "neutralizations", are accompanied by the evolution of substantial amounts of heat. Neutralization between an acid and a base produces water plus a salt. Carboxylic acids with six or fewer carbon atoms are freely or moderately soluble in water; those with more than six carbons are slightly soluble in water. Soluble carboxylic acid dissociate to an extent in water to yield hydrogen ions. The pH of solutions of carboxylic acids is therefore less than 7.0. Many insoluble carboxylic acids react rapidly with aqueous solutions containing a chemical base and dissolve as the neutralization generates a soluble salt. Carboxylic acids in aqueous solution and liquid or molten carboxylic acids can react with active metals to form gaseous hydrogen and a metal salt. Such reactions occur in principle for solid carboxylic acids as well, but are slow if the solid acid remains dry. Even "insoluble" carboxylic acids may absorb enough water from the air and dissolve sufficiently in it to corrode or dissolve iron, steel, and aluminum parts and containers. Carboxylic acids, like other acids, react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slower for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H₂S and SO₃), dithionites (SO₂), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions.

Conditions to avoid

no data available

Incompatible materials

The substance is a strong reducing agent and reacts with oxidants.

Hazardous decomposition products

When heated to decomposition, it emits acrid and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD₅₀ - rat (female) - 2 043 mg/kg bw.
- Inhalation: LC₀ - rat (male/female) - 0.11 mg/L air (nominal).
- Dermal: LD₅₀ - rat (male/female) - > 2 000 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, skin and respiratory tract.

STOT-repeated exposure

Animal tests show that this substance possibly causes toxicity to human reproduction or development.

Aspiration hazard

A harmful contamination of the air will be reached on evaporation of this substance at 20°C; on spraying or dispersing, however, much faster.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oryzias latipes* - > 100 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 910 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 49.3 mg/L - 72 h.

Toxicity to microorganisms: EC10 - *Pseudomonas putida* - 71.7 mg/L - 17 h.

Persistence and degradability

AEROBIC: Using an enrichment sediment consortium from the Pearl River, Guangzhou City, China and incubated using a shake-flask technique, 2-ethylhexanoic acid exhibited a biodegradation rate constant of 6.3×10^{-3} mmol/hr(1), corresponding to a half-life of approximately 5 days(SRC). Products included butanoic acid and ethanoic acid(1). A 4% decrease in the initial 2-ethylhexanoic acid concn of 5.1 mg/L was observed after 21 days incubation in an aerobic mixed bacterial culture obtained from trench leachate at a low-level radioactive waste disposal site in Maxey Flats, KY(2). A 50% decrease in the initial 2-ethylhexanoic acid concn of 59.5 mg/L was observed after 21 days incubation in an aerobic mixed bacterial culture obtained from trench leachate at a low-level radioactive waste disposal site in West Valley, NY(2). Decreases of 16 and 24% in the initial 2-ethylhexanoic acid concn of 67.8 mg/L were observed after 21 days incubation in an aerobic mixed bacterial culture and a nitrogen amended bacterial culture, respectively obtained from trench leachate at a low-level radioactive waste disposal site in West Valley, NY(2).

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for 2-ethylhexanoic acid(SRC), using a log Kow of 2.64(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of 2-ethylhexanoic acid is estimated as 650(SRC), using a log Kow of 2.64(1)((1,SRC) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 2-ethylhexanoic acid is expected to have low mobility in soil. The estimated pKa of 2-ethylhexanoic acid is 4.70(4), indicating that this compound will partially exist in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

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: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (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

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Listed.

Korea Existing Chemicals List (KECL)

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?pagelD=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/>

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