Safety Data Sheet



According to the UN GHS revision 8

Creation Date: August 12, 2024 Revision Date: August 12, 2024

1. IDENTIFICATION

1.1 GHS Product identifier

Product name: Estrone

Catalog Number: T1009

CAS Number: 53-16-7

1.2 Other means of identification

Other names:

1.3 Recommended use of the chemical and restrictions on use

Identified uses: no data available

1.4 Supplier's details

Company: Targetmol Chemicals Inc.

Uses advised against: 36 Washington Street, Wellesley Hills, Massachusetts 02481 USA

Tel/Fax: (781) 999-4286

1.5 Emergency phone number

Emergency phone number: 781-999-4286

Service hours: Monday to Friday, 9am-5pm (Standard timezone: UTC/GMT -5hours).

2. HAZARD IDENTIFICATION

2.1 Classification of the substance or mixture

Carcinogenicity, Category 2 Reproductive toxicity, Category 1A

Reproductive toxicity, Additional category for effects on or via lactation

2.2 GHS label elements, including precautionary statements

Pictogram(s):



Signal word: Dange

H351 Suspected of causing cancer

Hazard statement(s): H360 May damage fertility or the unborn child

H362 May cause harm to breast-fed children

Precautionary statement(s):

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

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

protection/...

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

P263 Avoid contact during pregnancy and while nursing.

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

Response: P318 IF exposed or concerned, get medical advice.

Storage: P405 Store locked up.

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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.

2.3 Other hazards which do not resultin classification

no data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number
Estrone	-	53-16-7	200-164-5

4. FIRST-AID MEASURES

4.1 Description of necessary first-aid measures

General advice

no data available

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

4.2 Most important symptoms/effects, acute and delayed

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 if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the 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. Poisons A and B

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

no data available

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Water spray, dry chemical, carbon dioxide, or foam as appropriate for surrounding fire and materials. ... As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing.

5.2 Specific hazards arising from the chemical

no data available

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

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6.2 Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Wear approved respiratory protection, chemically compatible gloves, and protective clothing. Wipe up spillage or collect spillage using a high-efficiency vacuum cleaner. Avoid breathing dust. Place spillage in appropriately labeled container for disposal. Wash spill site.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

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.

7.2 Conditions for safe storage, including any incompatibilities

Store in the original package. Do not store above 25 deg C.

EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

8.

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 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.

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

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state Solid

Color Small, white crystals, or white to creamy white, crystalline powder

Odour Odorless

Melting point/ freezing point 217°C(lit.)

Boilingpoint or initial boiling point

and boiling range

183°C

Flammability no data available

Lower and upper explosion

limit/flammability limit

no data available

Flash point 9°C

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Auto-ignition temperature no data available

Decomposition temperature no data available

pH no data available

Kinematic viscosity no data available

Solubility DMSO: 6.88 mg/mL (25.43 mM), Sonication is recommended.

Ethanol: < 1 mg/mL (insoluble or slightly soluble),

N-octanol-water partition

coefficient

no data available

Vapour pressure 2.49X10-10 mm Hg at 25 deg C (est)

Density and/ or relative density 1.164 g/cm3

Relative vapour density no data available

Particle characteristics no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

Stable in air.

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral: no data available Inhalation: no data available Dermal: no data available

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

Estrogens, Steroidal: known to be human carcinogens. Estrogens, Steroidal

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish: EC50; Species: Danio rerio (Zebra danio, age 20 days posthatch); Conditions: freshwater, renewal, 26 deg C;

Concentration: 0.078 ug/L for 18 days; Effect: whole body vitellogenin induction /100% purity

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC: Estrone exhibited approximately 38% mineralization in 33 days using 4 Mile Creek sediment, 56% mineralization in 33 days using Boulder Creek sediment, and up 90% mineralization using South Platte River sediments, Colorado. Sediments were collected downstream of local waste water treatment plants. Upstream sediments exhibited approximately 1, 1, and 1% mineralization, respectively(1). Estrone is biodegraded by sewage bacteria via ring cleavage, ultimately to carbon dioxide through a tricarboxylic acid cycle(2). C14-labeled estrone, present at 0.1 mg/kg, reached 2.0-17.4% mineralization in 21 days using natural German and Austrian soils in microcosm incubations maintained at 20 deg C(3,4). Soil-specific percent 14CO2 evolution values of 5.4, 4.6, 11.1, 2.0, and 17.4 were reported using Metelan (grassland, 3.3% SOC), Koeln (crop field, 0.7% SOC), Halle (crop field, 1.3% SOC), Gumpenstein (crop field, 2.2% SOC), and Hamapil (orchard, 1.5% SOC) soil microcosms, respectively(4).

12.3 Bioaccumulative potential

An estimated BCF of 54 was calculated in fish for estrone(SRC), using a log Kow of 3.13(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).

12.4 Mobility in soil

The Koc of estrone was reported as 2,000-18,000, using a Chelsea, MI topsoil (total organic carbon 5.45%)(1). Natural estrogens such as estrone are mainly removed from the aqueous phase by adsorption onto solids such as sludge in wastewater or soil in cases of land application(2). Sorption of estrone from CaCl2 solution and artificial urine in pastoral soils from North Island, New Zealand was studied. The log Koc values using Horotiu silt loam (pH 5.4; % OC 8.2; % Sand 34; % Silt 48; % Clay 17), Hamilton clay loam (pH 5.1; % OC 4; % Sand 19; % Silt 51; % Clay 30), and TeKowhai silt loam (pH 5.1; % OC 5; % Sand 9; % Silt 54; % Clay 37) were 2.66 and 2.75, 2.93 and 3.04, and 3.15 and 2.9, respectively(3), corresponding to Koc values of 457 and 562, 851 and 1096, and 1412 and 794, respectively(SRC). According to a classification scheme(4), these Koc values suggest that estrone mobility in soil is moderate to immobile. In soils with a long history of treatment with manure, biosolids, or wastewater, sorption of estrone becomes dependent on soil organic carbon content (SOC). Kd values of 122, 46, 134, 72, and 67 mL/g were reported using Metelan (grassland, SOC 3.3%), Koeln (crop field, 0.7% SOC), Halle (crop field, 1.3% SOC), Gumpenstein (crop field, 2.2% SOC), and Hamapil (orchard, 1.5% SOC) soils in Germany, respectively(5). A Kd of 402 L/kg was reported using activated sludge(6).

12.5 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 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.

14. TRANSPORT INFORMATION

14.1 UN Number

no data available

14.2 UN Proper Shipping Name

no data available

14.3 Transport hazard class(es)

no data available

14.4 Packing group, if applicable

no data available

14.5 Environmental hazards

no data available

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

15. REGULATORY INFORMATION

15.1 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.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Not Listed.
Vietnam National Chemical Inventory	Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Not Listed.
Korea Existing Chemicals List (KECL)	Not Listed.

16. OTHER INFORMATION

Information on revision

Creation Date August 12, 2024

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Abbreviations and acronyms

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- · 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

no data available

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product. All products are for Research Use Only · Not For Human or Veterinary or Therapeutic Use

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