

Chemical Safety Data Sheet MSDS / SDS

Estrone

Revision Date:2024-12-21 Revision Number:1

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

Product name : Estrone
CBnumber : CB5741416
CAS : 53-16-7
EINECS Number : 200-164-5
Synonyms : Estrone,Oestrone

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**

Carcinogenicity, Category 2
Reproductive toxicity, Category 1A
Reproductive toxicity, Additional category for effects on or via lactation

Label elements**Pictogram(s)**

☐☐☐

Signal word : Danger

Hazard statement(s)

H225 Highly Flammable liquid and vapour
H351 Suspected of causing cancer
H360 May damage fertility or the unborn child
H362 May cause harm to breast-fed children
H370 Causes damage to organs

Precautionary statement(s)

P201 Obtain special instructions before use.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

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

P263 Avoid contact during pregnancy/while nursing.

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

P281 Use personal protective equipment as required.

P311 Call a POISON CENTER or doctor/physician.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

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

P370+P378 In case of fire: Use ... for extinction.

Prevention

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

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

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.

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	: Estrone
Synonyms	: Estrone, Oestrone
CAS	: 53-16-7
EC number	: 200-164-5
MF	: C ₁₈ H ₂₂ O ₂
MW	: 270.37

SECTION 4: First aid measures

Description of first aid measures

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.

Most important symptoms and effects, both acute and delayed

no data available

Indication of any immediate medical attention and special treatment needed

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

SECTION 5: Firefighting measures

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.

Specific Hazards Arising from the Chemical

no data available

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

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.

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.

Odour	Odorless
Melting point/freezing point	217°C(lit.)
Boiling point 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
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Chloroform (Slightly), Dioxane (Slightly), Ethanol (Slightly), Methanol (Slightl
Partition coefficient n-octanol/water	no data available
Vapour pressure	2.49X10 ⁻¹⁰ mm Hg at 25 deg C (est)
Density and/or relative density	1.164 g/cm ³
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

Stable in air.

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 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

SECTION 12: Ecological information

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

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).

Bioaccumulative potential

An estimated BCF of 54 was calculated in fish for estrone(SRC), using a log K_{ow} 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).

Mobility in soil

The K_{oc} 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 K_{oc} 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 K_{oc} values of 457 and 562, 851 and 1096, and 1412 and 794, respectively(SRC). According to a classification scheme(4), these K_{oc} 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). K_d 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 K_d of 402 L/kg was reported using activated sludge(6).

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

Not Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Not 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?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/>

Disclaimer:

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