

## 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

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## SECTION 3: Composition/information on ingredients

### **Substance**

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

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## 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

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## 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.

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## 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 <sup>-10</sup> mm Hg at 25 deg C (est)
Density and/or relative density	1.164 g/cm <sup>3</sup>
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

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## 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 <sup>14</sup>CO<sub>2</sub> 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<sub>ow</sub> 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<sub>oc</sub> 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 CaCl<sub>2</sub> solution and artificial urine in pastoral soils from North Island, New Zealand was studied. The log K<sub>oc</sub> 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<sub>oc</sub> values of 457 and 562, 851 and 1096, and 1412 and 794, respectively(SRC). According to a classification scheme(4), these K<sub>oc</sub> 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<sub>d</sub> 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<sub>d</sub> of 402 L/kg was reported using activated sludge(6).

### **Other adverse effects**

no data available

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## 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.

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## 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

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## 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.

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# 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](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/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.