

According to the UN GHS revision 8

Creation Date: April 20, 2026

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1. IDENTIFICATION

1.1 GHS Product identifier

Product name: (-)-Alkannin

Catalog Number: T4958

CAS Number: 517-88-4

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.

Address: 34 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 -5 hours).

2. HAZARD IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, oral (Category 4),H302

Skin corrosion/irritation (Category 2),H315

Serious eye damage/eye irritation (Category 2A),H319

Specific target organ toxicity, single exposure; Respiratory tract irritation (Category 3),H335

2.2 GHS label elements, including precautionary statements

Pictogram(s):



Signal word:

Warning

Hazard statement(s):

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

Precautionary statement(s):

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P264 Wash hands thoroughly after handling

Prevention:

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

P271 Use only outdoors or in a well-ventilated area.

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

Response:

P302+P352 IF ON SKIN: Wash with plenty of soap and water.

P304+P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for

breathing.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P330 Rinse mouth.

P362+P364 Take off contaminated clothing and wash it before reuse.

Storage:

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

Disposal:

P501 Dispose of contents/container to in accordance with local regulation.

2.3 Other hazards which do not result in classification

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number
(-)-Alkannin	-	517-88-4	208-245-7

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

Extinguishing Media: Carbon dioxide, dry chemical powder, polymer foam, water spray.

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.

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

For spill clean up, wear suitable protective clothing, chemical resistant rubber gloves, rubber boots, and chemical safety goggles. Self contained breathing apparatus or NIOSH/MSHA approved respirator is required.

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

Keep container tightly closed in a dry and well-ventilated place. Recommended storage temperature: 2-8 deg C. Store with desiccant.

Keep away from direct sunlight

Powder: -20°C for 3 years | In solvent: -80°C for 1 year

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

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	no data available
Odour	no data available
Melting point/freezing point	147 deg C

Boiling point or initial boiling point and boiling range	567.4°C at 760mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	311°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	DMSO: 50 mg/mL (173.43 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
N-octanol-water partition coefficient	log Kow = 3.56 (est)
Vapour pressure	5.1X10-11 mm Hg at 25 deg C (est)
Density and/or relative density	1.373g/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

no data available

10.3 Possibility of hazardous reactions

Not flammable or combustible.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. Carbon oxides.

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

no data available

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: no data available

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

no data available

12.3 Bioaccumulative potential

An estimated BCF of 15 was calculated in fish for shikonin(SRC), using an estimated log Kow of 3.56(1) and a regression-derived equation (1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of shikonin can be estimated to be 1800(SRC).

According to a classification scheme(2), this estimated Koc value suggests that shikonin is expected to have low mobility in soil.

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	Not Listed.
China Catalog of Hazardous chemicals 2015	Not Listed.
New Zealand Inventory of Chemicals (NZIoC)	Not Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Not Listed.
Vietnam National Chemical Inventory	Not 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**

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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.com>

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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

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