

According to the UN GHS revision 8

Creation Date: April 29, 2026

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1. IDENTIFICATION

1.1 GHS Product identifier

Product name: (3E)-4-(1H-indol-3-yl)but-3-en-2-one

Catalog Number: TN7139

CAS Number: 57598-80-8

1.2 Other means of identification

Other names: -

1.3 Recommended use of the chemical and restrictions on use

Identified uses: Industrial and scientific research uses

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

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s): unknown

Signal word: no data available

Hazard statement(s): no data available

Precautionary statement(s):

Prevention: no data available

Response: no data available

Storage: no data available

Disposal: no data available

2.3 Other hazards which do not result in classification

no data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number
(3E)-4-(1H-indol-3-yl)but-3-en-2-one	-	57598-80-8	-

4. FIRST-AID MEASURES

4.1 Description of necessary first-aid measures

General advice

Medical attention is required. Consult a doctor. Show this safety data sheet (SDS) to the doctor in attendance.

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 water. Consult a doctor immediately.

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

no data available

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

Wear personal protective equipment.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam

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

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.

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use sparkproof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

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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 the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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)

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state	Solid
Color	Yellow
Odour	no data available
Melting point/freezing point	no data available
Boiling point or initial boiling point and boiling range	no data available
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	no data available
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	DMSO: 55 mg/mL (296.94 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
N-octanol-water partition coefficient	no data available
Vapour pressure	no data available
Density and/or relative density	1.183 g/cm ³ (Predicted)
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

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

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

no data available

12.2 Persistence and degradability

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no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

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

16. OTHER INFORMATION

Information on revision

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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

no data available

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