

## Safety Data Sheet

according to UK REACH Regulation

### Estragol-N-Acetylcystein-13C3,15N

Revision date: 19.03.2026

Product code: OP133

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#### SECTION 1: Identification of the substance/mixture and of the company/undertaking

##### 1.1. Product identifier

Estragol-N-Acetylcystein-13C3,15N

##### Further trade names

(E)-N-Acetyl-S-[3-(4-methoxyphenyl)allyl]-L-cysteine-13C3,15N

Substance name: Estragol-N-Acetylcystein-13C3,15N

CAS No: na

##### 1.2. Relevant identified uses of the substance or mixture and uses advised against

##### Use of the substance/mixture

Reference standard for analysis.

##### 1.3. Details of the supplier of the safety data sheet

Company name: WITEGA Laboratorien Berlin-Adlershof GmbH

Street: James-Franck-Strasse 4

Place: D-12489 Berlin

Telephone: +493063922001

Telefax: +493063922007

E-mail: witega@witega.de

Internet: www.witega.de

**1.4. Emergency telephone number:** +493063922001

#### SECTION 2: Hazards identification

##### 2.1. Classification of the substance or mixture

##### GB CLP Regulation

Skin Irrit. 2; H315

Eye Irrit. 2; H319

STOT SE 3; H335

Full text of hazard statements: see SECTION 16.

##### 2.2. Label elements

##### GB CLP Regulation

Signal word: Warning

Pictograms:



##### Hazard statements

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

##### Precautionary statements

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

P262 Do not get in eyes, on skin, or on clothing.

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

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

##### 2.3. Other hazards

No data available

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## SECTION 3: Composition/information on ingredients

### 3.1. Substances

Sum formula: C1213C3H1915NO4S  
Molecular weight: 313.35 g/mol g/mol

#### Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
na	Estragol-N-Acetylcystein-13C3,15N			100 %
	Skin Irrit. 2, Eye Irrit. 2, STOT SE 3; H315 H319 H335			

Full text of H and EUH statements: see section 16.

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

#### General information

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

#### After inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

#### After contact with skin

Remove contaminated, saturated clothing immediately. Subsequently wash off with: Water and soap

#### After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

#### After ingestion

Rinse mouth immediately and drink plenty of water. Get immediate medical advice/attention.

Do NOT induce vomiting. Never give anything by mouth to an unconscious person or a person with cramps.

### 4.2. Most important symptoms and effects, both acute and delayed

No data available

### 4.3. Indication of any immediate medical attention and special treatment needed

No data available

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

#### Suitable extinguishing media

Water spray jet. Foam. Dry extinguishing powder. Carbon dioxide (CO2).

### 5.2. Special hazards arising from the substance or mixture

In case of fire may be liberated: Pyrolysis products, toxic. In case of fire and/or explosion do not breathe fumes.

### 5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

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#### General advice

Use personal protection equipment. Do not breathe gas/fumes/vapour/spray.

#### 6.2. Environmental precautions

Do not allow to enter into surface water or drains.

#### 6.3. Methods and material for containment and cleaning up

##### Other information

Take up dust-free and set down dust-free.

#### 6.4. Reference to other sections

Disposal: see section 13

### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

##### Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation should be used if possible.

##### Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

##### Advice on general occupational hygiene

Use personal protection equipment.

#### 7.2. Conditions for safe storage, including any incompatibilities

##### Requirements for storage rooms and vessels

Keep container tightly closed in a cool, well-ventilated place. Avoid: UV-radiation/sunlight

##### Further information on storage conditions

storage temperature: 2-8°C  
under inert gas

#### 7.3. Specific end use(s)

none

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

#### 8.2. Exposure controls

##### Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation should be used if possible. If local exhaust ventilation is not possible or not sufficient, the entire working area should be ventilated by technical means.

##### Individual protection measures, such as personal protective equipment

##### Eye/face protection

Eye glasses with side protection

##### Hand protection

Wear suitable gloves. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances.

##### Skin protection

lab coat

##### Respiratory protection

In case of inadequate ventilation wear respiratory protection.

### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

Physical state: solid

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Colour:	white	
Odour:	odourless	
Melting point/freezing point:		123-125 °C
Boiling point or initial boiling point and boiling range:		No data available
Flammability:		No data available
Lower explosion limits:		No data available
Upper explosion limits:		No data available
Flash point:		No data available
Auto-ignition temperature:		No data available
Decomposition temperature:		No data available
pH-Value:		No data available
Water solubility:		No data available
Solubility in other solvents:		No data available
Partition coefficient n-octanol/water:		No data available
Vapour pressure:		No data available
Density:		No data available
Relative vapour density:		No data available

#### **9.2. Other information**

##### **Information with regard to physical hazard classes**

Explosive properties

No data available

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

##### **Other safety characteristics**

Evaporation rate:

No data available

##### **Further Information**

none

### **SECTION 10: Stability and reactivity**

#### **10.1. Reactivity**

Reacts with : Oxidising agent, Alkali (lye), Etchant and acids

#### **10.2. Chemical stability**

The product is chemically stable under recommended conditions of storage, use and temperature.

#### **10.3. Possibility of hazardous reactions**

No known hazardous reactions.

#### **10.4. Conditions to avoid**

Do not expose to temperatures exceeding 50 °C/122 °F.

#### **10.5. Incompatible materials**

Oxidising agent, Alkali (lye), Etchant and acids

#### **10.6. Hazardous decomposition products**

In case of fire may be liberated: Pyrolysis products, toxic.

### **SECTION 11: Toxicological information**

#### **11.1. Information on hazard classes as defined in GB CLP Regulation**

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#### Acute toxicity

Based on available data, the classification criteria are not met.

#### Irritation and corrosivity

Skin corrosion/irritation: Causes skin irritation.

Serious eye damage/eye irritation: Causes serious eye irritation.

#### Sensitising effects

Based on available data, the classification criteria are not met.

#### Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

Reproductive toxicity: Based on available data, the classification criteria are not met.

#### STOT-single exposure

May cause respiratory irritation. (Estragol-N-Acetylcystein-13C3,15N)

#### STOT-repeated exposure

Based on available data, the classification criteria are not met.

#### Aspiration hazard

Based on available data, the classification criteria are not met.

#### Specific effects in experiment on an animal

No data available

## SECTION 12: Ecological information

### 12.1. Toxicity

Based on available data, the classification criteria are not met.

No data available

### 12.2. Persistence and degradability

No data available

### 12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

### 12.4. Mobility in soil

No data available

### 12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of UK REACH.

This substance does not meet the PBT/vPvB criteria of REACH, Annex XIII.

### 12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

### 12.7. Other adverse effects

No data available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Disposal recommendations

Dispose of waste according to applicable legislation.

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

#### Contaminated packaging

This material and its container must be disposed of as hazardous waste.

## SECTION 14: Transport information

### Land transport (ADR/RID)

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- 14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.
- Inland waterways transport (ADN)**
- 14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.
- Marine transport (IMDG)**
- 14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.
- Air transport (ICAO-TI/IATA-DGR)**
- 14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.
- 14.5. Environmental hazards**
- ENVIRONMENTALLY HAZARDOUS: No
- 14.6. Special precautions for user**
- No data available
- 14.7. Maritime transport in bulk according to IMO instruments**
- No dangerous good in sense of this transport regulation.

### SECTION 15: Regulatory information

#### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

##### National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

#### 15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

### SECTION 16: Other information

#### Abbreviations and acronyms

Skin Irrit: Skin irritation

Eye Irrit: Eye irritation

STOT SE: Specific target organ toxicity - single exposure

#### Relevant H and EUH statements (number and full text)

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

#### Further Information

This information is based on our present state of knowledge. However, it should not constitute a guarantee for any specific product properties and shall not establish a legally valid relationship. The substances are only for R&D. Do not use as a drug, in household or other applications.