

SAFETY DATA SHEET
Z-Ligustilide - in acetonitrile**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1. Product identifier**

Product name	Z-Ligustilide - in acetonitrile
Product number	FL65531
Synonyms; trade names	3-Butyliden-4,5-dihydro-3H-isobenzofuran-1-one
CAS number	81944-09-4
EC number	694-690-6

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

Identified uses	Laboratory reagent. Manufacture of substances. Research and development.
-----------------	--

1.3. Details of the supplier of the safety data sheet

Supplier	Carbosynth Ltd 8&9 Old Station Business Park Compton Berkshire RG20 6NE UK +44 1635 578444 +44 1635 579444 info@carbosynth.com
----------	--

1.4. Emergency telephone number

Emergency telephone	+44 7887 998634
---------------------	-----------------

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Classification (EC 1272/2008)**

Physical hazards	Not Classified
Health hazards	Acute Tox. 3 - H301
Environmental hazards	Not Classified

2.2. Label elements

EC number	694-690-6
-----------	-----------

Pictogram

Signal word	Danger
Hazard statements	H301 Toxic if swallowed.

Z-Ligustilide - in acetonitrile

Precautionary statements	P264 Wash contaminated skin thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. P321 Specific treatment (see medical advice on this label). P330 Rinse mouth. P501 Dispose of contents/ container in accordance with national regulations.
---------------------------------	---

2.3. Other hazards

No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	Z-Ligustilide - in acetonitrile
CAS number	81944-09-4
EC number	694-690-6
Chemical formula	C ₁₂ H ₁₄ O ₂

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical advice/attention if you feel unwell.
Inhalation	Remove person to fresh air and keep comfortable for breathing. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. If breathing stops, provide artificial respiration. Get medical attention if symptoms are severe or persist.
Ingestion	Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.
Skin contact	Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.
Eye contact	Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

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

General information	See Section 11 for additional information on health hazards.
----------------------------	--

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

Notes for the doctor	Treat symptomatically.
-----------------------------	------------------------

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
-------------------------------------	--

5.2. Special hazards arising from the substance or mixture

Specific hazards	None known.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Oxides of carbon.

5.3. Advice for firefighters

Z-Ligustilide - in acetonitrile

Special protective equipment for firefighters Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of vapours. Provide adequate ventilation. Keep unnecessary and unprotected personnel away from the spillage.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up Wear protective clothing as described in Section 8 of this safety data sheet. Absorb spillage with sand or other inert absorbent. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Provide adequate ventilation. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid contact with skin and eyes. Avoid inhalation of vapours.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions Keep container tightly closed. Store in a cool and well-ventilated place. Store contents under inert gas. Store at temperatures not exceeding -20°C.

7.3. Specific end use(s)

Specific end use(s) The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure Controls/personal protection

8.1. Control parameters

Occupational exposure limits

No exposure limits known for ingredient(s).

8.2. Exposure controls

Appropriate engineering controls Provide adequate ventilation.

Eye/face protection Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.

Z-Ligustilide - in acetonitrile

Hand protection	Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.
Other skin and body protection	Wear appropriate clothing to prevent repeated or prolonged skin contact.
Respiratory protection	Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is 'CE'-marked. Gas and combination filter cartridges should comply with European Standard EN14387. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.
Environmental exposure controls	Keep container tightly sealed when not in use.

SECTION 9: Physical and Chemical Properties

9.1. Information on basic physical and chemical properties

Appearance	Liquid.
Odour	No data available.
Odour threshold	No data available.
pH	No data available.
Melting point	No data available.
Initial boiling point and range	No data available.
Flash point	No data available.
Evaporation rate	No data available.
Flammability (solid, gas)	No data available.
Upper/lower flammability or explosive limits	No data available.
Vapour pressure	No data available.
Vapour density	No data available.
Relative density	No data available.
Solubility(ies)	Almost insoluble in the following materials: Chloroform. Ethyl Acetate
Partition coefficient	log Pow: 2.574
Auto-ignition temperature	No data available.
Decomposition Temperature	No data available.
Viscosity	No data available.
Explosive properties	No data available.
Oxidising properties	No data available.

9.2. Other information

Molecular weight	190.24
-------------------------	--------

SECTION 10: Stability and reactivity

Z-Ligustilide - in acetonitrile

10.1. Reactivity

Reactivity No data available.

10.2. Chemical stability

Stability Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions No data available.

10.4. Conditions to avoid

Conditions to avoid No data available.

10.5. Incompatible materials

Materials to avoid Strong oxidising agents.

10.6. Hazardous decomposition products

Hazardous decomposition products Oxides of carbon.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Notes (oral LD₅₀) Acute Tox. 3 - H301 Toxic if swallowed.

ATE oral (mg/kg) 100.0

Acute toxicity - dermal

Notes (dermal LD₅₀) Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC₅₀) Based on available data the classification criteria are not met.

Skin corrosion/irritation

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

Serious eye damage/irritation

Serious eye damage/irritation Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation Based on available data the classification criteria are not met.

Germ cell mutagenicity

Genotoxicity - in vitro Based on available data the classification criteria are not met.

Carcinogenicity

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

IARC carcinogenicity

None of the ingredients are listed or exempt.

Reproductive toxicity

Reproductive toxicity - fertility Based on available data the classification criteria are not met.

Z-Ligustilide - in acetonitrile

Reproductive toxicity - development Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard

Aspiration hazard Based on available data the classification criteria are not met.

General information The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation No specific symptoms known.

Ingestion May cause stomach pain or vomiting. May cause severe internal injury.

Skin contact No specific symptoms known.

Eye contact No specific symptoms known.

Route of exposure Ingestion Inhalation Skin and/or eye contact

Target organs No specific target organs known.

RTECS # NP6810000

Z-Ligustilide - in acetonitrile

SECTION 12: Ecological Information

Ecotoxicity Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity

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

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient log Pow: 2.574

12.4. Mobility in soil

Mobility No data available.

12.5. Results of PBT and vPvB assessment

Results of PBT and vPvB assessment No data available.

12.6. Other adverse effects

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

SECTION 14: Transport information

14.1. UN number

UN No. (ADR/RID) 1648

UN No. (IMDG) 1648

UN No. (ICAO) 1648

UN No. (ADN) 1648

14.2. UN proper shipping name

Proper shipping name (ADR/RID) ACETONITRILE

Proper shipping name (IMDG) ACETONITRILE

Proper shipping name (ICAO) ACETONITRILE

Proper shipping name (ADN) ACETONITRILE

14.3. Transport hazard class(es)

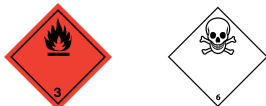
ADR/RID class 3

ADR/RID classification code F1

Z-Ligustilide - in acetonitrile

ADR/RID label	3
IMDG class	3
ICAO class/division	3
ADN class	3

Transport labels



14.4. Packing group

ADR/RID packing group	II
IMDG packing group	II
ADN packing group	II
ICAO packing group	II

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

14.6. Special precautions for user

EmS	F-E, S-D
ADR transport category	2
Emergency Action Code	•2YE
Hazard Identification Number (ADR/RID)	33
Tunnel restriction code	(D/E)

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

SECTION 15: Regulatory information

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

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
EU legislation	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (as amended). Commission Regulation (EU) No 2015/830 of 28 May 2015. Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures (as amended).

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Z-Ligustilide - in acetonitrile

Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road. ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways. RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail. IATA: International Air Transport Association. ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air. IMDG: International Maritime Dangerous Goods. CAS: Chemical Abstracts Service. ATE: Acute Toxicity Estimate. LC ₅₀ : Lethal Concentration to 50 % of a test population. LD ₅₀ : Lethal Dose to 50% of a test population (Median Lethal Dose). EC ₅₀ : 50% of maximal Effective Concentration. PBT: Persistent, Bioaccumulative and Toxic substance. vPvB: Very Persistent and Very Bioaccumulative.
Training advice	Only trained personnel should use this material.
Revision date	17/07/2019
Revision	1
SDS number	144929
Hazard statements in full	H301 Toxic if swallowed.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.