

1 Identification

Product identifier

Product name: 3,5-Dimethoxyphenyl isothiocyanate

Stock number: A15728, L12129

CAS Number:
104968-58-3

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

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS06 Skull and crossbones

Acute Tox. 3 H331 Toxic if inhaled.



GHS05 Corrosion

Skin Corr. 1B H314 Causes severe skin burns and eye damage.

Eye Dam. 1 H318 Causes serious eye damage.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS05 GHS06

Signal word

Danger

Hazard statements

H302+H312 Harmful if swallowed or in contact with skin.

H331 Toxic if inhaled.

H314 Causes severe skin burns and eye damage.

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

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

P301+P330+P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

D1B - Toxic material causing immediate and serious toxic effects

D2B - Toxic material causing other toxic effects

E - Corrosive material



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 2 Health (acute effects) = 2

FIRE 1 Flammability = 1

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

104968-58-3 3,5-Dimethoxyphenyl isothiocyanate

Product name: 3,5-Dimethoxyphenyl isothiocyanate

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4 First-aid measures

Description of first aid measures

General information Immediately remove any clothing soiled by the product.

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Seek medical treatment.

Information for doctor

Most important symptoms and effects, both acute and delayed

Causes severe skin burns.

Causes serious eye damage.

Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media

Suitable extinguishing agents CO2, sand, extinguishing powder. Do not use water.

Special hazards arising from the substance or mixture

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Nitrogen oxides (NOx)

Sulfur oxides (SOx)

Hydrogen cyanide (HCN)

Advice for firefighters

Protective equipment:

Wear self-contained respirator.

Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.

Methods and material for containment and cleaning up:

Use neutralizing agent.

Dispose of contaminated material as waste according to section 13.

Ensure adequate ventilation.

Prevention of secondary hazards: No special measures required.

Reference to other sections

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

7 Handling and storage

Handling

Precautions for safe handling

Handle under dry protective gas.

Keep container tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation at the workplace.

Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities

Storage

Requirements to be met by storerooms and receptacles: No special requirements.

Information about storage in one common storage facility:

Store away from oxidizing agents.

Store away from water/moisture.

Further information about storage conditions:

Store under dry inert gas.

This product is moisture sensitive.

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

Protect from humidity and water.

Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace: Not required.

Additional information: No data

Exposure controls

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

Breathing equipment: Use suitable respirator when high concentrations are present.

Protection of hands:

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

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USA

Product name: **3,5-Dimethoxyphenyl isothiocyanate**

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Eye protection:
Tightly sealed goggles
Full face protection
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form: Powder
Color: White
Odor: Irritating
Odor threshold: Not determined.

pH-value: Not applicable.

Change in condition

Melting point/Melting range: 49-52 °C (120-126 °F)
Boiling point/Boiling range: 130-132 °C (266-270 °F) (3mm Hg)
Sublimation temperature / start: Not determined

Flash point: Not applicable
Flammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined.

Danger of explosion: Product does not present an explosion hazard.

Explosion limits:

Lower: Not determined
Upper: Not determined

Vapor pressure: Not applicable.

Density: Not determined

Relative density Not determined.

Vapor density Not applicable.

Evaporation rate Not applicable.

Solubility in / Miscibility with

Water: Hydrolyzes

Partition coefficient (n-octanol/water): Not determined.

Viscosity:

dynamic: Not applicable.

kinematic: Not applicable.

Other information No further relevant information available.

10 Stability and reactivity

Reactivity No information known.

Chemical stability Stable under recommended storage conditions.

Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.

Possibility of hazardous reactions No dangerous reactions known

Conditions to avoid No further relevant information available.

Incompatible materials:

Alcohols

Amines

Oxidizing agents

Water/moisture

Hazardous decomposition products:

Carbon monoxide and carbon dioxide

Nitrogen oxides

Sulfur oxides (SOx)

Hydrogen cyanide

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful in contact with skin.

Harmful if swallowed.

Toxic if inhaled.

Danger through skin absorption.

Swallowing will lead to a strong corrosive effect on mouth and throat and to the danger of perforation of esophagus and stomach.

LD/LC50 values that are relevant for classification: No data

Skin irritation or corrosion: Causes severe skin burns.

Eye irritation or corrosion: Causes serious eye damage.

Sensitization: No sensitizing effects known.

Germ cell mutagenicity: No effects known.

Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

Reproductive toxicity: No effects known.

Specific target organ system toxicity - repeated exposure: No effects known.

Specific target organ system toxicity - single exposure: No effects known.

Aspiration hazard: No effects known.

Subacute to chronic toxicity: No effects known.

Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity

Aquatic toxicity: No further relevant information available.

Persistence and degradability No further relevant information available.

Bioaccumulative potential No further relevant information available.

Mobility in soil No further relevant information available.

Additional ecological information:

General notes:

Do not allow material to be released to the environment without proper governmental permits.

Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.

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USA

Product name: 3,5-Dimethoxyphenyl isothiocyanate	
Avoid transfer into the environment. Results of PBT and vPvB assessment PBT: Not applicable. vPvB: Not applicable. Other adverse effects No further relevant information available.	
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13 Disposal considerations	
Waste treatment methods Recommendation Consult state, local or national regulations to ensure proper disposal. Uncleaned packagings: Recommendation: Disposal must be made according to official regulations.	
14 Transport information	
UN-Number DOT, IMDG, IATA	UN2923
UN proper shipping name DOT IMDG, IATA	Corrosive solids, toxic, n.o.s. (3,5-Dimethoxyphenyl isothiocyanate) CORROSIVE SOLID, TOXIC, N.O.S. (3,5-Dimethoxyphenyl isothiocyanate)
Transport hazard class(es) DOT	
 	
Class Label Class Label IMDG, IATA	8 Corrosive substances. 8+6.1 8 (CT2) Corrosive substances 8+6.1
 	
Class Label	8 Corrosive substances. 8+6.1
Packing group DOT, IMDG, IATA	III
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Corrosive substances
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	UN2923, Corrosive solids, toxic, n.o.s. (3,5-Dimethoxyphenyl isothiocyanate), 8 (6.1), III
15 Regulatory information	
Safety, health and environmental regulations/legislation specific for the substance or mixture	
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)	
Hazard pictograms	
 	
GHS05 GHS06	
Signal word Danger	
Hazard statements	
H302+H312 Harmful if swallowed or in contact with skin.	
H331 Toxic if inhaled.	
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Precautionary statements	
P260 Do not breathe dust/fume/gas/mist/vapours/spray.	
P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.	
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P301+P330+P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.	
P405 Store locked up.	
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.	
National regulations	
This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.	
SARA Section 313 (specific toxic chemical listings) Substance is not listed.	
California Proposition 65	
Prop 65 - Chemicals known to cause cancer Substance is not listed.	
Prop 65 - Developmental toxicity Substance is not listed.	
Prop 65 - Developmental toxicity, female Substance is not listed.	
Prop 65 - Developmental toxicity, male Substance is not listed.	
Information about limitation of use: For use only by technically qualified individuals.	
Other regulations, limitations and prohibitive regulations	
Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.	
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.	
Substance is not listed.	
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.	
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Product name: 3,5-Dimethoxyphenyl isothiocyanate

Chemical safety assessment: A Chemical Safety Assessment has not been carried out. (Contd. of page 4)

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department

Date of preparation / last revision 11/24/2015 / -

Abbreviations and acronyms:

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IATA-DSR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

CAS: Chemical Abstracts Service (division of the American Chemical Society)

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

vPvB: very Persistent and very Bioaccumulative

ACGIH: American Conference of Governmental Industrial Hygienists (USA)

OSHA: Occupational Safety and Health Administration (USA)

NTP: National Toxicology Program (USA)

IARC: International Agency for Research on Cancer

EPA: Environmental Protection Agency (USA)

USA