

SAFETY DATA SHEET

Revision Date 01-Sep-2023

Revision Number 3

1. Identification

Product Name 3,5-Dimethylphenyl isothiocyanate

Cat No. : TL00501DA; TL00501EA; TL00501EB; TL00501ZZ

Synonyms No information available

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Thermo Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Warning

Hazard Statements

Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation
Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water
Call a POISON CENTER or doctor/physician if you feel unwell
If skin irritation occurs: Get medical advice/attention
Take off contaminated clothing and wash before reuse

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Storage

Store in a well-ventilated place. Keep container tightly closed
Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS No	Weight %
3,5-Dimethylphenyl isothiocyanate	40046-30-8	97

4. First-aid measures

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Carbon dioxide (CO ₂). Dry chemical. Chemical foam.
Unsuitable Extinguishing Media	No information available
Flash Point	No information available
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required.
Environmental Precautions	Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

7. Handling and storage

Handling	Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.
Storage.	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Store under an inert atmosphere. Incompatible Materials. Bases. Amines. Reducing Agent.

8. Exposure controls / personal protection

Exposure Guidelines	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
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Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended Filter type: Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Light yellow
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	140 °C / 284 °F @ 15 mmHg
Flash Point	No information available
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	No information available
Specific Gravity	No information available
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C9 H9 N S
Molecular Weight	163.24

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Moisture sensitive.
Conditions to Avoid	Incompatible products. Exposure to moist air or water.
Incompatible Materials	Bases, Amines, Reducing Agent
Hazardous Decomposition Products	Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO ₂), Sulfur oxides
Hazardous Polymerization	No information available.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
3,5-Dimethylphenyl isothiocyanate	40046-30-8	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed No information available

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No UN2810
Proper Shipping Name TOXIC LIQUIDS, ORGANIC, N.O.S.
Hazard Class 6.1
Packing Group III

TDG

UN-No UN2810
Proper Shipping Name Toxic liquid, organic, n.o.s.
Hazard Class 6.1
Packing Group III

IATA

UN-No UN2810
Proper Shipping Name Toxic liquid, organic, n.o.s.
Hazard Class 6.1
Packing Group III

IMDG/IMO

UN-No UN2810
Proper Shipping Name Toxic liquid, organic, n.o.s.
Hazard Class 6.1
Packing Group III

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
3,5-Dimethylphenyl isothiocyanate	40046-30-8	-	-	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
3,5-Dimethylphenyl isothiocyanate	40046-30-8	-	-	-	-	-	-	-	-	-

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3,5-Dimethylphenyl isothiocyanate	40046-30-8	-	-	-

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
3,5-Dimethylphenyl isothiocyanate	40046-30-8	Not applicable	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
3,5-Dimethylphenyl isothiocyanate	40046-30-8	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

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Revision Summary

This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The 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, unless specified in the text

End of SDS