

SAFETY DATA SHEET

Creation Date 16-Nov-2010

Revision Date 19-Dec-2025

Revision Number 6

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name 4-Methoxybenzyl isothiocyanate

Cat No. : AC413810000; AC413810050

CAS No 3694-57-3
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

Acros Organics
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 according to [US] OSHA (29 CFR 1910.1200, 2024)

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 person to fresh air and keep comfortable for breathing
Call a POISON CENTER or doctor if you feel unwell

Skin

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

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)

Lachrymator (substance which increases the flow of tears)

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
4-Methoxybenzyl isothiocyanate	3694-57-3	>95

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	Water spray. 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
1

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.

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 place. Keep container tightly closed. Store under an inert atmosphere. Air sensitive. To maintain product quality: Keep refrigerated. Incompatible Materials. Strong oxidizing agents.

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.
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

Appearance		
Physical State	Liquid	
Color	Yellow	
Odor	No information available	
Odor Threshold	No information available	
Property	Values	Remarks • Method
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	170 - 175 °C / 338 - 347 °F	@ 16 mmHg
Flash Point	No information available	Method - No information available
Flammability (liquid)	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Autoignition Temperature	No data available	
Decomposition Temperature	> 300°C	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	1.087	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	
Other Information		
Molecular Formula	C9 H9 N O S	
Molecular Weight	179.24	

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions. Hygroscopic.
Conditions to Avoid	Incompatible products. Exposure to moist air or water.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Nitrogen oxides (NO _x), Carbon monoxide (CO), Carbon dioxide (CO ₂), Sulfur oxides
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	Not an expected route of exposure.
Ingestion	May be harmful if swallowed.
Eyes	Avoid contact with eyes. Irritating to eyes. Lachrymator (substance which increases the flow of tears).
Skin	Avoid contact with skin. May cause irritation. Harmful in contact with skin.

Toxicology data for the components

Toxicologically Synergistic Products	No information available
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(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory	No data available
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity;

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

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
4-Methoxybenzyl isothiocyanate	3694-57-3	Not listed	Not listed	Not listed	Not listed	Not listed

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs	Respiratory system.
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	No data available
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects, both acute and delayed	No information available.
Other Adverse Effects	The toxicological properties have not been fully investigated.
Endocrine Disrupting Properties	This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability	No information available
Bioaccumulation/ Accumulation	No information available.
Mobility	No information available.

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.
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14. Transport information

DOT

UN-No	UN2810
Proper Shipping Name	TOXIC LIQUIDS, ORGANIC, N.O.S.
Technical Shipping Name	4-Methoxybenzyl isothiocyanate
Hazard Class	6.1
Packing Group	III

TDG

UN-No	UN2810
Proper Shipping Name	Toxic liquid, organic, n.o.s.
Technical Shipping Name	4-Methoxybenzyl isothiocyanate
Hazard Class	6.1
Packing Group	III

IATA

UN-No	UN2810
Proper Shipping Name	Toxic liquid, organic, n.o.s.
Technical Shipping Name	4-Methoxybenzyl isothiocyanate
Hazard Class	6.1
Packing Group	III

IMDG/IMO

UN-No	UN2810
Proper Shipping Name	Toxic liquid, organic, n.o.s.
Technical Shipping Name	4-Methoxybenzyl isothiocyanate
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
4-Methoxybenzyl isothiocyanate	3694-57-3	-	-	-

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

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
4-Methoxybenzyl isothiocyanate	3694-57-3	-	-	-	-	-	-	-	-	-

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

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act)

Not applicable

Clean Air Act

Not applicable

OSHA - Occupational Safety and Health Administration

Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

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)
4-Methoxybenzyl isothiocyanate	3694-57-3	-	-	-

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)
4-Methoxybenzyl isothiocyanate	3694-57-3	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)
4-Methoxybenzyl isothiocyanate	3694-57-3	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By Product stewardship (Regulatory Affairs)
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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