



5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate

Apollo Scientific

Part Number: OR22982

Version No: 2.2

Safety Data Sheet

Chemwatch Hazard Alert Code: 2

Issue Date: 07/07/2023

Print Date: 07/07/2023

S.GHS.GB-NIR.EN

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

Product Identifier

Product name	5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate
Chemical Name	5-METHYL-3-PHENYL-4-ISOXAZOLYL ISOTHIOCYANATE
Synonyms	Not Available
Other means of identification	Not Available
CAS number	306934-97-4*

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

Relevant identified uses	Not Available
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Details of the manufacturer or supplier of the safety data sheet

Registered company name	Apollo Scientific	Apollo Scientific Ltd
Address	Whitefield Road, Bredbury SK62QR United Kingdom	Whitefield Road, Bredbury Cheshire SK6 2QR United Kingdom (NI)
Telephone	01614060505	+44(0) 161 406 0505
Fax	0161 406 0506	Not Available
Website	http://www.apolloscientific.co.uk/	apolloscientific.co.uk
Email	sales@apolloscientific.co.uk	sales@apolloscientific.co.uk

Emergency telephone number

Association / Organisation	Not Available
Emergency telephone numbers	Not Available
Other emergency telephone numbers	Not Available

SECTION 2 Hazards identification

Classification of the substance or mixture

Classification according to regulation (EC) No 1272/2008 [CLP] and amendments [1]	H312 - Acute Toxicity (Dermal) Category 4, H332 - Acute Toxicity (Inhalation) Category 4, H335 - Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3, H302 - Acute Toxicity (Oral) Category 4, H319 - Serious Eye Damage/Eye Irritation Category 2
Legend:	1. Classified by Chemwatch; 2. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate

Label elements

Hazard pictogram(s)	
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Signal word	Warning
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Hazard statement(s)

H312	Harmful in contact with skin.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H302	Harmful if swallowed.
H319	Causes serious eye irritation.

Precautionary statement(s) Prevention

P271	Use only outdoors or in a well-ventilated area.
P261	Avoid breathing dust/fumes.
P264	Wash all exposed external body areas thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P280	Wear protective gloves, protective clothing, eye protection and face protection.

Precautionary statement(s) Response

P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313	If eye irritation persists: Get medical advice/attention.
P301+P312	IF SWALLOWED: Call a POISON CENTER/doctor/physician/first aider if you feel unwell.
P302+P352	IF ON SKIN: Wash with plenty of water.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P330	Rinse mouth.
P362+P364	Take off contaminated clothing and wash it before reuse.

Precautionary statement(s) Storage

P405	Store locked up.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.

Precautionary statement(s) Disposal

P501	Dispose of contents/container to authorised hazardous or special waste collection point in accordance with any local regulation.
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SECTION 3 Composition / information on ingredients

Substances

CAS No	%[weight]	Name	Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	SCL / M-Factor
306934-97-4*	100	<u>5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate</u>	Acute Toxicity (Dermal) Category 4, Acute Toxicity (Inhalation) Category 4, Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3 , Acute Toxicity (Oral) Category 4, Serious Eye Damage/Eye Irritation Category 2; H312, H332, H335, H302, H319 ^[1]	Not Available

Legend: 1. Classified by Chemwatch; 2. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI; 3. Classification drawn from C&L; * EU IOELVs available; [e] Substance identified as having endocrine disrupting properties

Mixtures

See section above for composition of Substances

SECTION 4 First aid measures

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate**Description of first aid measures**

Eye Contact	<p>If this product comes in contact with the eyes:</p> <ul style="list-style-type: none">▸ Wash out immediately with fresh running water.▸ Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.▸ Seek medical attention without delay; if pain persists or recurs seek medical attention.▸ Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.
Skin Contact	<p>If skin or hair contact occurs:</p> <ul style="list-style-type: none">▸ Flush skin and hair with running water (and soap if available).▸ Seek medical attention in event of irritation.
Inhalation	<ul style="list-style-type: none">▸ If fumes or combustion products are inhaled remove from contaminated area.▸ Lay patient down. Keep warm and rested.▸ Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.▸ Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary.▸ Transport to hospital, or doctor, without delay.
Ingestion	<ul style="list-style-type: none">▸ Immediately give a glass of water.▸ First aid is not generally required. If in doubt, contact a Poisons Information Centre or a doctor.

Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5 Firefighting measures**Extinguishing media**

- There is no restriction on the type of extinguisher which may be used.
- Use extinguishing media suitable for surrounding area.

Special hazards arising from the substrate or mixture

Fire Incompatibility	None known.
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Advice for firefighters

Fire Fighting	<ul style="list-style-type: none">▸ Alert Fire Brigade and tell them location and nature of hazard.▸ Wear breathing apparatus plus protective gloves in the event of a fire.▸ Prevent, by any means available, spillage from entering drains or water courses.▸ Use fire fighting procedures suitable for surrounding area.▸ DO NOT approach containers suspected to be hot.▸ Cool fire exposed containers with water spray from a protected location.▸ If safe to do so, remove containers from path of fire.▸ Equipment should be thoroughly decontaminated after use.
Fire/Explosion Hazard	<ul style="list-style-type: none">▸ Non combustible.▸ Not considered a significant fire risk, however containers may burn. <p>May emit poisonous fumes.</p> <p>May emit corrosive fumes.</p>

SECTION 6 Accidental release measures**Personal precautions, protective equipment and emergency procedures**

See section 8

Environmental precautions

See section 12

Methods and material for containment and cleaning up

Minor Spills	<ul style="list-style-type: none">▸ Clean up all spills immediately.▸ Avoid breathing dust and contact with skin and eyes.▸ Wear protective clothing, gloves, safety glasses and dust respirator.
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	<ul style="list-style-type: none">▸ Use dry clean up procedures and avoid generating dust.▸ Sweep up, shovel up or▸ Vacuum up (consider explosion-proof machines designed to be grounded during storage and use).▸ Place spilled material in clean, dry, sealable, labelled container.
Major Spills	<p>Moderate hazard.</p> <ul style="list-style-type: none">▸ CAUTION: Advise personnel in area.▸ Alert Emergency Services and tell them location and nature of hazard.▸ Control personal contact by wearing protective clothing.▸ Prevent, by any means available, spillage from entering drains or water courses.▸ Recover product wherever possible.▸ IF DRY: Use dry clean up procedures and avoid generating dust. Collect residues and place in sealed plastic bags or other containers for disposal. IF WET: Vacuum/shovel up and place in labelled containers for disposal.▸ ALWAYS: Wash area down with large amounts of water and prevent runoff into drains.▸ If contamination of drains or waterways occurs, advise Emergency Services.

Personal Protective Equipment advice is contained in Section 8 of the SDS.

SECTION 7 Handling and storage

Precautions for safe handling

Safe handling	<ul style="list-style-type: none">▸ Avoid all personal contact, including inhalation.▸ Wear protective clothing when risk of exposure occurs.▸ Use in a well-ventilated area.▸ Prevent concentration in hollows and sumps.▸ DO NOT enter confined spaces until atmosphere has been checked.▸ DO NOT allow material to contact humans, exposed food or food utensils.▸ Avoid contact with incompatible materials.▸ When handling, DO NOT eat, drink or smoke.▸ Keep containers securely sealed when not in use.▸ Avoid physical damage to containers.▸ Always wash hands with soap and water after handling.▸ Work clothes should be laundered separately. Launder contaminated clothing before re-use.▸ Use good occupational work practice.▸ Observe manufacturer's storage and handling recommendations contained within this SDS.▸ Atmosphere should be regularly checked against established exposure standards to ensure safe working conditions are maintained.
Other information	<ul style="list-style-type: none">▸ Store in original containers.▸ Keep containers securely sealed.▸ Store in a cool, dry area protected from environmental extremes.▸ Store away from incompatible materials and foodstuff containers.▸ Protect containers against physical damage and check regularly for leaks.▸ Observe manufacturer's storage and handling recommendations contained within this SDS. <p>For major quantities:</p> <ul style="list-style-type: none">▸ Consider storage in bunded areas - ensure storage areas are isolated from sources of community water (including stormwater, ground water, lakes and streams).▸ Ensure that accidental discharge to air or water is the subject of a contingency disaster management plan; this may require consultation with local authorities.

Conditions for safe storage, including any incompatibilities

Suitable container	<ul style="list-style-type: none">▸ Polyethylene or polypropylene container.▸ Check all containers are clearly labelled and free from leaks.
Storage incompatibility	<p>None known</p> <ul style="list-style-type: none">▸ Moisture sensitive▸ Store under argon

SECTION 8 Exposure controls / personal protection

Control parameters

Occupational Exposure Limits (OEL)

INGREDIENT DATA

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate

Not Available

Emergency Limits

Ingredient	TEEL-1	TEEL-2	TEEL-3
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	Not Available	Not Available	Not Available

Ingredient	Original IDLH	Revised IDLH
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	Not Available	Not Available

Occupational Exposure Banding

Ingredient	Occupational Exposure Band Rating	Occupational Exposure Band Limit
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	E	≤ 0.01 mg/m³

Notes:	Occupational exposure banding is a process of assigning chemicals into specific categories or bands based on a chemical's potency and the adverse health outcomes associated with exposure. The output of this process is an occupational exposure band (OEB), which corresponds to a range of exposure concentrations that are expected to protect worker health.
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Exposure controls

Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.

The basic types of engineering controls are:

Process controls which involve changing the way a job activity or process is done to reduce the risk.

Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment. Ventilation can remove or dilute an air contaminant if designed properly. The design of a ventilation system must match the particular process and chemical or contaminant in use.

Employers may need to use multiple types of controls to prevent employee overexposure.

- ▶ Local exhaust ventilation is required where solids are handled as powders or crystals; even when particulates are relatively large, a certain proportion will be powdered by mutual friction.
- ▶ If in spite of local exhaust an adverse concentration of the substance in air could occur, respiratory protection should be considered.

Such protection might consist of:

(a): particle dust respirators, if necessary, combined with an absorption cartridge;

(b): filter respirators with absorption cartridge or canister of the right type;

(c): fresh-air hoods or masks.

Air contaminants generated in the workplace possess varying "escape" velocities which, in turn, determine the "capture velocities" of fresh circulating air required to effectively remove the contaminant.

Appropriate engineering controls

Type of Contaminant:	Air Speed:
direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)	1-2.5 m/s (200-500 f/min.)
grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).	2.5-10 m/s (500-2000 f/min.)

Within each range the appropriate value depends on:

Lower end of the range	Upper end of the range
1: Room air currents minimal or favourable to capture	1: Disturbing room air currents
2: Contaminants of low toxicity or of nuisance value only.	2: Contaminants of high toxicity
3: Intermittent, low production.	3: High production, heavy use
4: Large hood or large air mass in motion	4: Small hood-local control only

Simple theory shows that air velocity falls rapidly with distance away from the opening of a simple extraction pipe. Velocity generally decreases with the square of distance from the extraction point (in simple cases). Therefore the air speed at the extraction point should be adjusted, accordingly, after reference to distance from the contaminating source. The air velocity at the extraction fan, for example, should be a minimum of 4-10 m/s (800-2000 f/min) for extraction of crusher dusts generated 2 metres distant from the extraction point. Other mechanical considerations, producing performance deficits within the extraction apparatus, make it essential that theoretical air velocities are multiplied by factors of 10 or more when extraction systems are installed or used.

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Individual protection measures, such as personal protective equipment	
Eye and face protection	<ul style="list-style-type: none"> ▶ Safety glasses with side shields. ▶ Chemical goggles. [AS/NZS 1337.1, EN166 or national equivalent] ▶ Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lenses or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience. Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59].
Skin protection	See Hand protection below
Hands/feet protection	<p>The selection of suitable gloves does not only depend on the material, but also on further marks of quality which vary from manufacturer to manufacturer. Where the chemical is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.</p> <p>The exact break through time for substances has to be obtained from the manufacturer of the protective gloves and has to be observed when making a final choice.</p> <p>Personal hygiene is a key element of effective hand care. Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.</p> <p>Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include:</p> <ul style="list-style-type: none"> • frequency and duration of contact, • chemical resistance of glove material, • glove thickness and • dexterity <p>Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739, AS/NZS 2161.1 or national equivalent).</p> <ul style="list-style-type: none"> • When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374, AS/NZS 2161.10.1 or national equivalent) is recommended. • When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374, AS/NZS 2161.10.1 or national equivalent) is recommended. • Some glove polymer types are less affected by movement and this should be taken into account when considering gloves for long-term use. • Contaminated gloves should be replaced. <p>As defined in ASTM F-739-96 in any application, gloves are rated as:</p> <ul style="list-style-type: none"> • Excellent when breakthrough time > 480 min • Good when breakthrough time > 20 min • Fair when breakthrough time < 20 min • Poor when glove material degrades <p>For general applications, gloves with a thickness typically greater than 0.35 mm, are recommended.</p> <p>It should be emphasised that glove thickness is not necessarily a good predictor of glove resistance to a specific chemical, as the permeation efficiency of the glove will be dependent on the exact composition of the glove material. Therefore, glove selection should also be based on consideration of the task requirements and knowledge of breakthrough times.</p> <p>Glove thickness may also vary depending on the glove manufacturer, the glove type and the glove model. Therefore, the manufacturers technical data should always be taken into account to ensure selection of the most appropriate glove for the task.</p> <p>Note: Depending on the activity being conducted, gloves of varying thickness may be required for specific tasks. For example:</p> <ul style="list-style-type: none"> • Thinner gloves (down to 0.1 mm or less) may be required where a high degree of manual dexterity is needed. However, these gloves are only likely to give short duration protection and would normally be just for single use applications, then disposed of. • Thicker gloves (up to 3 mm or more) may be required where there is a mechanical (as well as a chemical) risk i.e. where there is abrasion or puncture potential <p>Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.</p> <p>Experience indicates that the following polymers are suitable as glove materials for protection against undissolved, dry solids, where abrasive particles are not present.</p> <ul style="list-style-type: none"> ▶ polychloroprene. ▶ nitrile rubber. ▶ butyl rubber. ▶ fluorocautchouc. ▶ polyvinyl chloride. <p>Gloves should be examined for wear and/ or degradation constantly.</p>
Body protection	See Other protection below
Other protection	<ul style="list-style-type: none"> ▶ Overalls. ▶ P.V.C apron. ▶ Barrier cream. ▶ Skin cleansing cream. ▶ Eye wash unit.

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Respiratory protection

Type -P Filter of sufficient capacity. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

Required Minimum Protection Factor	Half-Face Respirator	Full-Face Respirator	Powered Air Respirator
up to 10 x ES	P1 Air-line*	- -	PAPR-P1 -
up to 50 x ES	Air-line**	P2	PAPR-P2
up to 100 x ES	-	P3	-
		Air-line*	-
100+ x ES	-	Air-line**	PAPR-P3

* - Negative pressure demand ** - Continuous flow

A(All classes) = Organic vapours, B AUS or B1 = Acid gasses, B2 = Acid gas or hydrogen cyanide(HCN), B3 = Acid gas or hydrogen cyanide(HCN), E = Sulfur dioxide(SO₂), G = Agricultural chemicals, K = Ammonia(NH₃), Hg = Mercury, NO = Oxides of nitrogen, MB = Methyl bromide, AX = Low boiling point organic compounds(below 65 degC)

- Respirators may be necessary when engineering and administrative controls do not adequately prevent exposures.
- The decision to use respiratory protection should be based on professional judgment that takes into account toxicity information, exposure measurement data, and frequency and likelihood of the worker's exposure - ensure users are not subject to high thermal loads which may result in heat stress or distress due to personal protective equipment (powered, positive flow, full face apparatus may be an option).
- Published occupational exposure limits, where they exist, will assist in determining the adequacy of the selected respiratory protection. These may be government mandated or vendor recommended.
- Certified respirators will be useful for protecting workers from inhalation of particulates when properly selected and fit tested as part of a complete respiratory protection program.
- Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU)
- Use approved positive flow mask if significant quantities of dust becomes airborne.
- Try to avoid creating dust conditions.

SECTION 9 Physical and chemical properties

Information on basic physical and chemical properties

Appearance	Not Available		
Physical state	Solid	Relative density (Water = 1)	Not Available
Odour	Not Available	Partition coefficient n-octanol / water	Not Available
Odour threshold	Not Available	Auto-ignition temperature (°C)	Not Available
pH (as supplied)	Not Available	Decomposition temperature (°C)	Not Available
Melting point / freezing point (°C)	73-77	Viscosity (cSt)	Not Available
Initial boiling point and boiling range (°C)	Not Available	Molecular weight (g/mol)	Not Available
Flash point (°C)	Not Available	Taste	Not Available
Evaporation rate	Not Available	Explosive properties	Not Available
Flammability	Not Available	Oxidising properties	Not Available
Upper Explosive Limit (%)	Not Available	Surface Tension (dyn/cm or mN/m)	Not Applicable
Lower Explosive Limit (%)	Not Available	Volatile Component (%vol)	Not Available
Vapour pressure (kPa)	Not Available	Gas group	Not Available
Solubility in water	Not Available	pH as a solution (1%)	Not Available
Vapour density (Air = 1)	Not Available	VOC g/L	Not Available

SECTION 10 Stability and reactivity

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate

Reactivity	See section 7
Chemical stability	<ul style="list-style-type: none"> ▸ Unstable in the presence of incompatible materials. ▸ Product is considered stable. ▸ Hazardous polymerisation will not occur.
Possibility of hazardous reactions	See section 7
Conditions to avoid	See section 7
Incompatible materials	See section 7
Hazardous decomposition products	See section 5

SECTION 11 Toxicological information

Information on toxicological effects

Inhaled	<p>The material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.</p> <p>Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.</p> <p>If prior damage to the circulatory or nervous systems has occurred or if kidney damage has been sustained, proper screenings should be conducted on individuals who may be exposed to further risk if handling and use of the material result in excessive exposures.</p>
Ingestion	The material has NOT been classified by EC Directives or other classification systems as "harmful by ingestion". This is because of the lack of corroborating animal or human evidence.
Skin Contact	<p>The material is not thought to produce adverse health effects or skin irritation following contact (as classified by EC Directives using animal models). Nevertheless, good hygiene practice requires that exposure be kept to a minimum and that suitable gloves be used in an occupational setting.</p> <p>Open cuts, abraded or irritated skin should not be exposed to this material</p> <p>Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.</p>
Eye	This material can cause eye irritation and damage in some persons.
Chronic	<p>Long-term exposure to respiratory irritants may result in airways disease, involving difficulty breathing and related whole-body problems.</p> <p>Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.</p>
Legend:	<p>1. Value obtained from Europe ECHA Registered Substances - Acute toxicity 2. Value obtained from manufacturer's SDS.</p> <p>Unless otherwise specified data extracted from RTECS - Register of Toxic Effect of chemical Substances</p>

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	<p>Asthma-like symptoms may continue for months or even years after exposure to the material ends. This may be due to a non-allergic condition known as reactive airways dysfunction syndrome (RADS) which can occur after exposure to high levels of highly irritating compound. Main criteria for diagnosing RADS include the absence of previous airways disease in a non-atopic individual, with sudden onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. Other criteria for diagnosis of RADS include a reversible airflow pattern on lung function tests, moderate to severe bronchial hyperreactivity on methacholine challenge testing, and the lack of minimal lymphocytic inflammation, without eosinophilia. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. On the other hand, industrial bronchitis is a disorder that occurs as a result of exposure due to high concentrations of irritating substance (often particles) and is completely reversible after exposure ceases. The disorder is characterized by difficulty breathing, cough and mucus production.</p>
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Acute Toxicity	✓	Carcinogenicity	✗
Skin Irritation/Corrosion	✗	Reproductivity	✗
Serious Eye Damage/Irritation	✓	STOT - Single Exposure	✓
Respiratory or Skin sensitisation	✗	STOT - Repeated Exposure	✗
Mutagenicity	✗	Aspiration Hazard	✗

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate

Legend: ✗ – Data either not available or does not fill the criteria for classification
✔ – Data available to make classification

SECTION 12 Ecological information

Toxicity

Legend: Extracted from 1. IUCLID Toxicity Data 2. Europe ECHA Registered Substances - Ecotoxicological Information - Aquatic Toxicity
 4. US EPA, Ecotox database - Aquatic Toxicity Data 5. ECETOC Aquatic Hazard Assessment Data 6. NITE (Japan) -
 Bioconcentration Data 7. METI (Japan) - Bioconcentration Data 8. Vendor Data

DO NOT discharge into sewer or waterways.

Persistence and degradability

Ingredient	Persistence: Water/Soil	Persistence: Air
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	HIGH	HIGH

Bioaccumulative potential

Ingredient	Bioaccumulation
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	HIGH (LogKOW = 4.7169)

Mobility in soil

Ingredient	Mobility
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	LOW (KOC = 2621)

SECTION 13 Disposal considerations

Waste treatment methods

Product / Packaging disposal	
	<ul style="list-style-type: none"> Recycle wherever possible or consult manufacturer for recycling options. Consult State Land Waste Management Authority for disposal. Bury residue in an authorised landfill. Recycle containers if possible, or dispose of in an authorised landfill.

SECTION 14 Transport information

Labels Required

Marine Pollutant	NO
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Land transport (ADR): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Air transport (ICAO-IATA / DGR): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Sea transport (IMDG-Code / GGVSee): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Inland waterways transport (ADN): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Transport in bulk according to Annex II of MARPOL and the IBC code

Not Applicable

Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

Product name	Group
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	Not Available

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate

Transport in bulk in accordance with the IGC Code

Product name	Ship Type
5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate	Not Available

SECTION 15 Regulatory information

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

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate is found on the following regulatory lists

Not Applicable

National Inventory Status

National Inventory	Status
Australia - AIIC / Australia Non-Industrial Use	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Canada - DSL	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Canada - NDSL	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
China - IECSC	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Europe - EINEC / ELINCS / NLP	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Japan - ENCS	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Korea - KECI	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
New Zealand - NZIoC	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Philippines - PICCS	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
USA - TSCA	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Taiwan - TCSI	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Mexico - INSQ	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Vietnam - NCI	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Russia - FBEPH	No (5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate)
Legend:	Yes = All CAS declared ingredients are on the inventory No = One or more of the CAS listed ingredients are not on the inventory. These ingredients may be exempt or will require registration.

SECTION 16 Other information

Revision Date	07/07/2023
Initial Date	08/07/2023

SDS Version Summary

Version	Date of Update	Sections Updated
1.2	07/07/2023	Toxicological information - Acute Health (inhaled), Toxicological information - Acute Health (skin), Physical and chemical properties - Appearance, CAS Number, Toxicological information - Chronic Health, Hazards identification - Classification, Ecological Information - Environmental, Exposure controls / personal protection - Exposure Standard, Firefighting measures - Fire Fighter (fire/explosion hazard), First Aid measures - First Aid (inhaled), Composition / information on ingredients - Ingredients, Stability and reactivity - Instability Condition, Korean MSDS Number, Handling and storage - Storage (suitable container), Identification of the substance / mixture and of the company / undertaking - Supplier Information, Identification of the substance / mixture and of the company / undertaking - Synonyms

Other information

Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

The SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

5-Methyl-3-phenyl-4-isoxazolyl isothiocyanate

For detailed advice on Personal Protective Equipment, refer to the following EU CEN Standards:

EN 166 Personal eye-protection

EN 340 Protective clothing

EN 374 Protective gloves against chemicals and micro-organisms

EN 13832 Footwear protecting against chemicals

EN 133 Respiratory protective devices

Definitions and abbreviations

PC - TWA: Permissible Concentration-Time Weighted Average

PC - STEL: Permissible Concentration-Short Term Exposure Limit

IARC: International Agency for Research on Cancer

ACGIH: American Conference of Governmental Industrial Hygienists

STEL: Short Term Exposure Limit

TEEL: Temporary Emergency Exposure Limit

IDLH: Immediately Dangerous to Life or Health Concentrations

ES: Exposure Standard

OSF: Odour Safety Factor

NOAEL :No Observed Adverse Effect Level

LOAEL: Lowest Observed Adverse Effect Level

TLV: Threshold Limit Value

LOD: Limit Of Detection

OTV: Odour Threshold Value

BCF: BioConcentration Factors

BEI: Biological Exposure Index

AIIC: Australian Inventory of Industrial Chemicals

DSL: Domestic Substances List

NDSL: Non-Domestic Substances List

IECSC: Inventory of Existing Chemical Substance in China

EINECS: European INventory of Existing Commercial chemical Substances

ELINCS: European List of Notified Chemical Substances

NLP: No-Longer Polymers

ENCS: Existing and New Chemical Substances Inventory

KECI: Korea Existing Chemicals Inventory

NZIoC: New Zealand Inventory of Chemicals

PICCS: Philippine Inventory of Chemicals and Chemical Substances

TSCA: Toxic Substances Control Act

TCSI: Taiwan Chemical Substance Inventory

INSQ: Inventario Nacional de Sustancias Químicas

NCI: National Chemical Inventory

FBEPH: Russian Register of Potentially Hazardous Chemical and Biological Substances

Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]

Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	Classification Procedure
Acute Toxicity (Dermal) Category 4, H312	Expert judgement
Acute Toxicity (Inhalation) Category 4, H332	Expert judgement
Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3 , H335	Calculation method
Acute Toxicity (Oral) Category 4, H302	Expert judgement
Serious Eye Damage/Eye Irritation Category 2, H319	Calculation method