

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

### 1.1 Product identifier

Trade name **(R)-(-)-3-Methyl-2-butyl isothiocyanate**

Stock number: L20071

CAS Number:

737001-02-4

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

Identified use: SU24 Scientific research and development

### 1.3 Details of the supplier of the safety data sheet

#### Manufacturer/Supplier:

Alfa Aesar  
Avocado Research Chemicals, Ltd.  
Shore Road  
Port of Heysham Industrial Park  
Heysham Lancashire LA3 2XY  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608  
Email: uktech@alfa.com  
www.alfa.com

Informing department: Product safety department.

1.4 Emergency telephone number: Call Carechem 24 at +44 (0) 1865 407333 (English only); +44 (0) 1235 239670 (Multi-language)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008



GHS02 flame

Flam. Liq. 3 H226 Flammable liquid and vapour.



GHS06 skull and crossbones

Acute Tox. 3 H331 Toxic if inhaled.



GHS05 corrosion

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



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Other hazards that do not result in classification No information known.

### 2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 The substance is classified and labelled according to the CLP regulation.

#### Hazard pictograms



GHS02 GHS05 GHS06

Signal word Danger

#### Hazard statements

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H312 Harmful in contact with skin.

H331 Toxic if inhaled.

H314 Causes severe skin burns and eye damage.

#### Precautionary statements

P280 Wear protective gloves/protective clothing/eye protection/face protection.

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

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER/doctor/...

### 2.3 Other hazards

#### Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

CAS# Designation:

737001-02-4 (R)-(-)-3-Methyl-2-butyl isothiocyanate

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

General information Instantly remove any clothing soiled by the product.

#### After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

Seek immediate medical advice.

#### After skin contact

Instantly 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 doctor.

After swallowing Seek medical treatment.

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

Causes severe skin burns.

Causes serious eye damage.

Trade name **(R)-(-)-3-Methyl-2-butyl isothiocyanate**

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

(Contd. of page 1)

### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

**Suitable extinguishing agents** CO<sub>2</sub>, sand, extinguishing powder. Do not use water.

#### 5.2 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 (NO<sub>x</sub>)

Possibly Hydrogen cyanide (HCN)

Sulphur oxides (SO<sub>x</sub>)

#### 5.3 Advice for firefighters

##### Protective equipment:

Wear self-contained breathing apparatus.

Wear full protective suit.

### SECTION 6: Accidental release measures

#### 6.1 Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Keep away from ignition sources

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

#### 6.3 Methods and material for containment and cleaning up:

Keep away from ignition sources.

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Use neutralizing agent.

Dispose of contaminated material as waste according to section 13.

Ensure adequate ventilation.

**Prevention of secondary hazards:** Keep away from ignition sources.

#### 6.4 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 information on disposal.

### SECTION 7: Handling and storage

#### 7.1 Precautions for safe handling

Handle under dry protective gas.

Keep containers tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation/exhaustion at the workplace.

#### Information about protection against explosions and fires:

Protect against electrostatic charges.

Fumes can combine with air to form an explosive mixture.

Keep ignition sources away - Do not smoke.

#### 7.2 Conditions for safe storage, including any incompatibilities

##### Storage

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

#### Information about storage in one common storage facility:

Store away from oxidising agents.

Store away from water.

#### 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 keep away from water.

Store in a locked cabinet or with access restricted to technical experts or their assistants.

#### 7.3 Specific end use(s)

 No further relevant information available.

### SECTION 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.

#### 8.1 Control parameters

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

**Additional information:** No data

#### 8.2 Exposure controls

##### Personal protective equipment

##### General protective and hygienic measures

The usual precautionary measures should be adhered to in handling the chemicals.

Keep away from foodstuffs, beverages and food.

Instantly remove any soiled and impregnated garments.

Wash hands during breaks and at the end of the work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

**Breathing equipment:** Use breathing protection with high concentrations.

##### Protection of hands:

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

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

**Material of gloves** Impervious gloves

**Penetration time of glove material (in minutes)** Not determined

##### Eye protection:

Tightly sealed safety glasses.

Full face protection

**Body protection:** Protective work clothing.

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

##### General Information

##### Appearance:

**Form:** Liquid

**Colour:** Colourless

**Smell:** Not determined

**Odour threshold:** Not determined.

(Contd. on page 3)  
GB

**Trade name (R)-(-)-3-Methyl-2-butyl isothiocyanate**

(Contd. of page 2)

<b>pH-value:</b>	Not determined.
<b>Change in condition</b>	
<b>Melting point/Melting range:</b>	Not determined
<b>Boiling point/Boiling range:</b>	Not determined
<b>Sublimation temperature / start:</b>	Not determined
<b>Flash point:</b>	< 55 °C
<b>Inflammability (solid, gaseous)</b>	Not applicable.
<b>Ignition temperature:</b>	Not determined
<b>Decomposition temperature:</b>	Not determined
<b>Self-inflammability:</b>	Not determined.
<b>Danger of explosion:</b>	Product is not explosive. However, formation of explosive air/steam mixtures is possible.
<b>Critical values for explosion:</b>	
<b>Lower:</b>	Not determined
<b>Upper:</b>	Not determined
<b>Steam pressure:</b>	Not determined
<b>Density at 20 °C</b>	0.924 g/cm <sup>3</sup>
<b>Relative density</b>	Not determined.
<b>Vapour density</b>	Not determined.
<b>Evaporation rate</b>	Not determined.
<b>Solubility in / Miscibility with</b>	
<b>Water:</b>	Hydrolyzes
<b>Partition coefficient (n-octanol/water):</b>	Not determined.
<b>Viscosity:</b>	
<b>dynamic:</b>	Not determined.
<b>kinematic:</b>	Not determined.
<b>9.2 Other information</b>	No further relevant information available.

**SECTION 10: Stability and reactivity**

**10.1 Reactivity** No information known.  
**10.2 Chemical stability** Stable under recommended storage conditions.  
**Thermal decomposition / conditions to be avoided:** No decomposition if used and stored according to specifications.  
**10.3 Possibility of hazardous reactions** No dangerous reactions known  
**10.4 Conditions to avoid** No further relevant information available.  
**10.5 Incompatible materials:**  
Alcohols  
Amines  
Oxidising agents  
Water/moisture  
**10.6 Hazardous decomposition products:**  
Carbon monoxide and carbon dioxide  
Nitrogen oxides (NOx)  
Sulphur oxides (SOx)  
Possibly Hydrogen cyanide (HCN)

**SECTION 11: Toxicological information**

**11.1 Information on toxicological effects**  
**Acute toxicity:**  
Harmful if swallowed.  
Toxic if inhaled.  
Danger by skin resorption.  
Swallowing will lead to a strong caustic 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 effect 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.

**SECTION 12: Ecological information**





**12.1 Toxicity**  
**Aquatic toxicity:** No further relevant information available.  
**12.2 Persistence and degradability** No further relevant information available.  
**12.3 Bioaccumulative potential** No further relevant information available.  
**12.4 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.  
Water hazard class 1 (Self-assessment): slightly hazardous for water.  
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.  
Avoid transfer into the environment.  
**12.5 Results of PBT and vPvB assessment**  
**PBT:** Not applicable.  
**vPvB:** Not applicable.  
**12.6 Other adverse effects** No further relevant information available.

**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**  
**Recommendation**  
Hand over to disposers of hazardous waste.  
Must be specially treated under adherence to official regulations.  
Consult state, local or national regulations for proper disposal.  
**Uncleaned packagings:**  
**Recommendation:** Disposal must be made according to official regulations.

Trade name (R)-(-)-3-Methyl-2-butyl isothiocyanate

(Contd. of page 3)

SECTION 14: Transport information	
UN-Number ADR, IMDG, IATA	UN2924
14.2 UN proper shipping name ADR	2924 FLAMMABLE LIQUID, CORROSIVE, N.O.S. ((R)-(-)-3-Methyl-2-butyl isothiocyanate)
IMDG, IATA	FLAMMABLE LIQUID, CORROSIVE, N.O.S. ((R)-(-)-3-Methyl-2-butyl isothiocyanate)
14.3 Transport hazard class(es) ADR	
 	
Class Label IMDG, IATA	3 (FC) Flammable liquids. 3+8
 	
Class Label	3 Flammable liquids. 3+8
Packing group ADR, IMDG, IATA	III
14.5 Environmental hazards:	Not applicable.
14.6 Special precautions for user Kemler Number: EMS Number:	Warning: Flammable liquids. 38 F-E,S-C
14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
ADR Excepted quantities (EQ): Limited quantities (LQ) Transport category Tunnel restriction code	E1 5L 3 D/E
UN "Model Regulation":	UN2924, FLAMMABLE LIQUID, CORROSIVE, N.O.S. ((R)-(-)-3-Methyl-2-butyl isothiocyanate), 3 (8), III

SECTION 15: Regulatory information	
15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture	
Australian Inventory of Chemical Substances Substance is not listed.	
Standard for the Uniform Scheduling of Drugs and Poisons Substance is not listed.	
National regulations	
Information about limitation of use: For use only by technically qualified individuals. Employment restrictions concerning young persons must be observed.	
Water hazard class: Water hazard class 1 (Self-assessment): slightly hazardous for water.	
Other regulations, limitations and prohibitive regulations	
ELINCS (European List of Notified Chemical Substances) Substance is not listed.	
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.	
15.2 Chemical safety assessment: A Chemical Safety Assessment has not been carried out.	

SECTION 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	
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-DGR: 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 IATA: International Air Transport Association GHS: Globally Harmonized System of Classification and Labelling of Chemicals CAS: Chemical Abstracts Service (division of the American Chemical Society) 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)	