

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

Product Description: **3-(Methoxycarbonyl)phenyl isocyanate**  
 Cat No. : **L18709**  
 Synonyms 3-(Methoxycarbonyl)phenyl isocyanate; 3-Carbomethoxyphenyl isocyanate  
 CAS No 41221-47-0  
 Molecular Formula C9 H7 N O3  
 REACH registration number -

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

Recommended Use Laboratory chemicals.  
 Uses advised against No Information available

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

Company Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
 Shore Road, Heysham  
 Lancashire, LA3 2XY,  
 United Kingdom  
 Office Tel: +44 (0) 1524 850506  
 Office Fax: +44 (0) 1524 850608

E-mail address [begel.sdsdesk@thermofisher.com](mailto:begel.sdsdesk@thermofisher.com)

### 1.4. 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

##### Physical hazards

Based on available data, the classification criteria are not met

##### Health hazards

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

Acute oral toxicity	Category 4 (H302)
Acute dermal toxicity	Category 4 (H312)
Acute Inhalation Toxicity - Dusts and Mists	Category 4 (H332)
Skin Corrosion/Irritation	Category 2 (H315)
Serious Eye Damage/Eye Irritation	Category 2 (H319)
Respiratory Sensitization	Category 1 (H334)
Skin Sensitization	Category 1 (H317)
Specific target organ toxicity - (single exposure)	Category 3 (H335)

## Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements



Signal Word

Danger

## Hazard Statements

- H315 - Causes skin irritation
- H317 - May cause an allergic skin reaction
- H319 - Causes serious eye irritation
- H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled
- H335 - May cause respiratory irritation
- H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

## Precautionary Statements

- P280 - Wear protective gloves/protective clothing/eye protection/face protection
- P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting
- P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
- P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
- P312 - Call a POISON CENTER or doctor if you feel unwell
- P333 + P313 - If skin irritation or rash occurs: Get medical advice/attention

## 2.3. Other hazards

- Water reactive
- Lachrymator (substance which increases the flow of tears)
- This product does not contain any known or suspected endocrine disruptors

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
3-Carbomethoxyphenyl isocyanate	41221-47-0		>95	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Skin Irrit. 2 (H315)

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

				Skin Sens. 1 (H317) Eye Irrit. 2 (H319) Acute Tox. 4 (H332) Resp. Sens. 1 (H334) STOT SE 3 (H335)
--	--	--	--	---

<b>REACH registration number</b>	-
----------------------------------	---

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>General Advice</b>	If symptoms persist, call a physician.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
<b>Self-Protection of the First Aider</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

### 4.3. Indication of any immediate medical attention and special treatment needed

**Notes to Physician** Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

### 5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors.

#### **Hazardous Combustion Products**

Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

## 5.3. Advice for firefighters

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

## SECTION 6: ACCIDENTAL RELEASE MEASURES

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

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

### 6.2. Environmental precautions

Should not be released into the environment.

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

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Ensure adequate ventilation. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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

Keep in a dry place. Keep container tightly closed.  
To maintain product quality. Protect from moisture. Keep refrigerated.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 11  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

## Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

### Personal protective equipment

#### Eye Protection

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

#### Skin and body protection

Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

#### Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

#### Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

**Recommended Filter type:** Particulates filter conforming to EN 143

#### Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

**Recommended half mask:-** Particle filtering: EN149:2001

When RPE is used a face piece Fit Test should be conducted

#### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

## 9.1. Information on basic physical and chemical properties

Physical State	Solid	
Appearance	White - Off-white	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	35 - 38 °C / 95 - 100.4 °F	Based on available literature
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	> 110 °C / > 230 °F	<b>Method -</b> No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	Not applicable	Solid
Water Solubility	hydrolyses	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

## 9.2. Other information

Molecular Formula	C9 H7 N O3
Molecular Weight	177.16
Evaporation Rate	Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Moisture sensitive. Stable under recommended storage conditions.

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

### 10.4. Conditions to avoid

Incompatible products. Exposure to moist air or water. Excess heat.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong bases. Alcohols. Amines. Acids. Water.

### 10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

## 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

### Product Information

**(a) acute toxicity;**

Oral	Category 4
Dermal	Category 4
Inhalation	Category 4

**(b) skin corrosion/irritation;** Category 2

**(c) serious eye damage/irritation;** Category 2

**(d) respiratory or skin sensitization;**

Respiratory	Category 1
Skin	Category 1

May cause sensitization by skin contact

**(e) germ cell mutagenicity;** No data available

**(f) carcinogenicity;** No data available

There are no known carcinogenic chemicals in this product

**(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;** Not applicable  
Solid

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

**Symptoms / effects, both acute and delayed** Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

## 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

**Ecotoxicity effects**

Reacts with water so no ecotoxicity data for the substance is available.

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

## 12.2. Persistence and degradability

<b>Persistence</b>	Persistence is unlikely, based on information available.
<b>Degradability</b>	Decomposes in contact with water.
<b>Degradation in sewage treatment plant</b>	Decomposes in contact with water.

## 12.3. Bioaccumulative potential

Product does not bioaccumulate due to reaction with water

## 12.4. Mobility in soil

Hydrolyses Is not likely mobile in the environment.

## 12.5. Results of PBT and vPvB assessment

Water reactive.

## 12.6. Endocrine disrupting properties

### **Endocrine Disruptor Information**

This product does not contain any known or suspected endocrine disruptors

## 12.7. Other adverse effects

### **Persistent Organic Pollutant Ozone Depletion Potential**

This product does not contain any known or suspected substance  
This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

#### **Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

#### **Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point.

#### **European Waste Catalogue (EWC)**

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

#### **Other Information**

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

### ADR

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

### IATA



# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

- 14.1. UN number** UN3335  
**14.2. UN proper shipping name** AVIATION REGULATED SOLID, N.O.S.  
**14.3. Transport hazard class(es)** 9  
**14.4. Packing group** III
- 14.5. Environmental hazards** No hazards identified
- 14.6. Special precautions for user** No special precautions required.
- 14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
3-Carbomethoxyphenyl isocyanate	41221-47-0	-	-	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3-Carbomethoxyphenyl isocyanate	41221-47-0	-	-	-	-	-	-	-

**Legend:** X - Listed '-' - Not Listed      **KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**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-Carbomethoxyphenyl isocyanate	41221-47-0	-	-	-

#### Seveso III Directive (2012/18/EC)

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
3-Carbomethoxyphenyl isocyanate	41221-47-0	Not applicable	Not applicable

**Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals**

Not applicable

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

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

## National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** Water endangering class = 3 (self classification)

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed  
H312 - Harmful in contact with skin  
H332 - Harmful if inhaled  
H315 - Causes skin irritation  
H317 - May cause an allergic skin reaction  
H319 - Causes serious eye irritation  
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H335 - May cause respiratory irritation

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

### Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

### Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

# SAFETY DATA SHEET

3-(Methoxycarbonyl)phenyl isocyanate

Revision Date 04-Feb-2024

---

Prepared By	Health, Safety and Environmental Department
Creation Date	22-Sep-2009
Revision Date	04-Feb-2024
Revision Summary	New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

## 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 Safety Data Sheet**