

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Revision Date 23-Jan-2024 Revision Number 3

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

1.1. Product identifier

Product Description: 4-Chlorophenyl isocyanate

Cat No. : A14966

Synonyms p-Chlorophenyl isocyanate; 1-Chloro-4-isocyanatobenzene; 4-Chloroisocyanatobenzene

 Index No
 615-044-00-1

 CAS No
 104-12-1

 Molecular Formula
 C7 H4 CI N O

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

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

ALFAAA14966

Revision Date 23-Jan-2024

4-Chlorophenyl isocyanate

Acute oral toxicity Category 3 (H301) Acute Inhalation Toxicity - Dusts and Mists Category 2 (H330) Skin Corrosion/Irritation Category 2 (H315) Serious Eye Damage/Eye Irritation Category 1 (H318) Respiratory Sensitization Category 1 (H334) Specific target organ toxicity - (single exposure) Category 3 (H335) **Environmental hazards** Acute aquatic toxicity Category 1 (H400) Chronic aquatic toxicity Category 1 (H410)

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H315 - Causes skin irritation

H410 - Very toxic to aquatic life with long lasting effects

H335 - May cause respiratory irritation

H318 - Causes serious eye damage

H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled

H330 - Fatal if inhaled

H301 - Toxic if swallowed

Precautionary Statements

P280 - Wear 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

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P342 + P311 - If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician

P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

P273 - Avoid release to the environment

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

2.3. Other hazards

Lachrymator (substance which increases the flow of tears)

Toxic to terrestrial vertebrates

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
-1					UK SI 2020/1567

4-Chlorophenyl isocyanate

		T T		
Benzene, 1-chloro-4-isocyanato-	104-12-1	EEC No. 203-176-9	98	Acute Tox. 3 (H301)
				Acute Tox. 2 (H330)
				Skin Irrit. 2 (H315)
				Eye Dam. 1 (H318)
				Resp. Sens. 1 (H334)
				STOT SE 3 (H335)
				Aquatic Acute 1 (H400)
				Aguatic Chronic 1 (H410)

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Benzene, 1-chloro-4-isocyanato-	-	10 (acute) 1 (Chronic)	-

REACH registration number	-

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

Eye Contact Immediate medical attention is required. Rinse immediately with plenty of water, also under

the eyelids, for at least 15 minutes.

Skin Contact Wash off immediately with soap and plenty of water while removing all contaminated

clothes and shoes. Immediate medical attention is required.

Ingestion Never give anything by mouth to an unconscious person. Drink plenty of water. Induce

vomiting, but only if victim is fully conscious. Call a physician immediately. Clean mouth with

Revision Date 23-Jan-2024

water.

Inhalation Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial

respiration. Immediate medical attention is required.

Self-Protection of the First Aider 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

Causes eye burns. May cause allergy or asthma symptoms or breathing difficulties if inhaled. Causes severe eye damage. 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

Carbon dioxide (CO₂). Powder. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

4-Chlorophenyl isocyanate

Revision Date 23-Jan-2024

Flammable. Combustible material. Combustible material. Containers may explode when heated. Do not allow run-off from fire-fighting to enter drains or water courses.

Hazardous Combustion Products

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen cyanide (hydrocyanic acid), nitric acid, Hydrogen chloride gas.

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

Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

6.3. Methods and material for containment and cleaning up

Avoid dust formation. Prevent product from entering drains. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Sweep up and shovel into suitable containers for disposal. Do not flush into surface water or sanitary sewer system.

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

Do not breathe dust. Do not get in eyes, on skin, or on clothing. Handle product only in closed system or provide appropriate exhaust ventilation. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Keep away from open flames, hot surfaces and sources of ignition.

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, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 6.1A 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

List source(s): UK - EH40/2005 Work Exposure Limits, Fourth edition. Published 2020.

Component	The United Kingdom	European Union	Ireland
Benzene, 1-chloro-4-isocyanato-	STEL: 0.07 mg/m ³ 15 min		
	TWA: 0.02 mg/m ³ 8 hr		
	Resp. Sens.		

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

Goggles (European standard - EN 166) **Eye Protection**

Hand Protection Protective gloves

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

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

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

4-Chlorophenyl isocyanate Revision Date 23-Jan-2024

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits Large scale/emergency use

> are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Particulates filter conforming to EN 143

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure Small scale/Laboratory use

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 Prevent product from entering drains. Do not allow material to contaminate ground water

system. Local authorities should be advised if significant spillages cannot be contained.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Solid

Light yellow **Appearance** pungent Odor

No data available **Odor Threshold**

29 - 31 °C / 84.2 - 87.8 °F Melting Point/Range

Softening Point No data available

Boiling Point/Range 203 - 204 °C / 397.4 - 399.2 °F @ 760 mmHg

Flammability (liquid) Not applicable Solid

Flammability (solid,gas) No information available

Explosion Limits Lower 2.3 Upper 6.8

Flash Point 60 °C / 140 °F

Method - No information available

450 °C / 842 °F **Autoignition Temperature Decomposition Temperature** No data available pН Not applicable

Viscosity Not applicable Solid

Water Solubility DECOMPOSES IN WATER Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

log Pow Component Benzene, 1-chloro-4-isocyanato-3.12

1.33 hPa @ 35 °C **Vapor Pressure**

Density / Specific Gravity 1.260

Bulk Density No data available

Vapor Density Not applicable Solid

Particle characteristics No data available

9.2. Other information

Molecular Formula C7 H4 CI N O **Molecular Weight** 153.57

Explosive Properties explosive air/vapour mixtures possible

Not applicable - Solid **Evaporation Rate**

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions. Moisture sensitive.

10.3. Possibility of hazardous reactions

4-Chlorophenyl isocyanate Revision Date 23-Jan-2024

Hazardous Polymerization Hazardous Reactions

No information available. No information available.

10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition. Excess heat.

Incompatible products. Exposure to moist air or water.

10.5. Incompatible materials

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

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid). nitric acid. Hydrogen chloride gas.

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information

(a) acute toxicity;

Oral Category 3
Dermal No data available
Inhalation Category 2

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, 1-chloro-4-isocyanato-	LD50 = 138 mg/kg (Rat)	LD50 > 5010 mg/kg (Rabbit)	LC50 113 - 272 mg/m ³ (Rat) 4
			h

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;

Respiratory Category 1 Skin No data available

No information available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

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

(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

4-Chlorophenyl isocyanate

Revision Date 23-Jan-2024

Solid

delayed

Symptoms / effects, both acute and 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**

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Microtox	M-Factor
Benzene, 1-chloro-4-isocyanato-	EC50 = 2.32 mg/L 30 min	10 (acute)
	EC50 = 2.49 mg/L 15 min	1 (Chronic)
	EC50 = 2.67 mg/L 5 min	, ,

12.2. Persistence and degradability Not readily biodegradable

Persistence

Degradation in sewage treatment plant

Soluble in water, Persistence is unlikely, based on information available. Contains substances known to be hazardous to the environment or not degradable in waste

water treatment plants.

12.3. Bioaccumulative potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)		
Benzene, 1-chloro-4-isocyanato-	3.12	No data available		

12.4. Mobility in soil

The product is water soluble, and may spread in water systems. Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB

assessment

No data available for assessment.

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

Should not be released into the environment. 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.

4-Chlorophenyl isocyanate Revision Date 23-Jan-2024

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but

application specific.

Other Information Do not flush to sewer. Waste codes should be assigned by the user based on the

application for which the product was used. Do not empty into drains. Do not let this

chemical enter the environment.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN2811

14.2. UN proper shipping name Toxic solid, organic, n.o.s.

14.3. Transport hazard class(es) 6.1 14.4. Packing group II

ADR

14.1. UN number UN2811

14.2. UN proper shipping name Toxic solid, organic, n.o.s.

14.3. Transport hazard class(es) 6.1 14.4. Packing group II

IATA

14.1. UN number UN2811

14.2. UN proper shipping name TOXIC SOLID, ORGANIC, N.O.S.*

14.3. Transport hazard class(es) 6.1 14.4. Packing group II

14.5. Environmental hazards Dangerous for the environment

Product is a marine pollutant according to the criteria set by IMDG/IMO

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk Not applicable, packaged goods

according to IMO instruments

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)

Benzene, 1-chloro-4-isocvanato- 104-12-1 203-176-9 - X X KE-05718 - X		Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
	Е	Benzene, 1-chloro-4-isocyanato-	104-12-1		-	-	Х	X	KE-05718	ı	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzene, 1-chloro-4-isocyanato-	104-12-1	X	ACTIVE	-	X	-	X	X

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

4-Chlorophenyl isocyanate

Revision Date 23-Jan-2024

Authorisation/Restrictions according to EU REACH

Component	CAS No		REACH (1907/2006) - Annex XVII - Restrictions	· · · · · · · · · · · · · · · · · · ·
		Subject to Authorization	on Certain Dangerous	Candidate List of
			Substances	Substances of Very High
				Concern (SVHC)
Benzene, 1-chloro-4-isocyanato-	104-12-1	-	Use restricted. See item	=
			75.	
			(see link for restriction	
			details)	

REACH links

https://echa.europa.eu/substances-restricted-under-reach

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
Benzene, 1-chloro-4-isocyanato-	104-12-1	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 .

National Regulations

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

WGK Classification See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Benzene, 1-chloro-4-isocyanato-	WGK3	

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

H301 - Toxic if swallowed

H315 - Causes skin irritation

H318 - Causes serious eye damage

H330 - Fatal if inhaled

H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled

4-Chlorophenyl isocyanate

Revision Date 23-Jan-2024

H335 - May cause respiratory irritation

H400 - Very toxic to aquatic life

H410 - Very toxic to aquatic life with long lasting effects

Legend

CAS - Chemical Abstracts Service

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

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic 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 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

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)

Key literature references and sources for data

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

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

Training Advice

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

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.

Chemical incident response training.

Prepared By Health, Safety and Environmental Department

Revision Date 23-Jan-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