

Creation Date 30-Apr-2012

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-Chlorophenylacetonitrile
Cat No. :	A15295
Synonyms	(4-Chlorophenyl)acetonitrile; PCCN
CAS No	140-53-4
Molecular Formula	C8 H6 Cl N
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
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E-mail address	begel.sdsdesk@thermofisher.com
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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

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Acute oral toxicity
Acute dermal toxicity
Acute Inhalation Toxicity - Dusts and Mists
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Specific target organ toxicity - (single exposure)

Category 2 (H300)
Category 3 (H311)
Category 3 (H331)
Category 2 (H315)
Category 2 (H319)
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

H300 - Fatal if swallowed
H319 - Causes serious eye irritation
H315 - Causes skin irritation
H335 - May cause respiratory irritation
H311 + H331 - Toxic in contact with skin or if inhaled

Precautionary Statements

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P312 - Call a POISON CENTER or doctor if you feel unwell
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

2.3. Other hazards

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 UK SI 2020/1567
Benzeneacetonitrile, 4-chloro-	140-53-4	EEC No. 205-418-9	>95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 2 (H300) Acute Tox. 3 (H311) Acute Tox. 3 (H331)

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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	Call a physician immediately. Clean mouth with 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

No information available.

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 (CO₂). Dry chemical. Chemical 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_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen cyanide (hydrocyanic 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

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Ensure adequate ventilation.

6.2. Environmental precautions

See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Wear self-contained breathing apparatus and protective suit. Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment.

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 breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Handle product only in closed system or provide appropriate exhaust ventilation.

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.

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
Benzeneacetonitrile, 4-chloro-	STEL: 15 mg/m ³ 15 min TWA: 5 mg/m ³ 8 hr Skin		

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

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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	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
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

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

9.1. Information on basic physical and chemical properties

Physical State

Low melting solid

Appearance

Clear

Odor

Odorless

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Odor Threshold	No data available	
Melting Point/Range	29 - 30 °C / 84.2 - 86 °F	
Softening Point	No data available	
Boiling Point/Range	265 - 267 °C / 509 - 512.6 °F	@ 760 mmHg
Flammability (liquid)	No data available	
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	133 °C / 271.4 °F	Method - No information available
Autoignition Temperature	500 °C / 932 °F	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	Insoluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Benzeneacetonitrile, 4-chloro-	2.47	
Vapor Pressure	0.133 mbar @ 20 °C	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	No data available	

9.2. Other information

Molecular Formula	C8 H6 Cl N
Molecular Weight	151.6

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization	No information available.
Hazardous Reactions	No information available.

10.4. Conditions to avoid

Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases. Strong reducing agents.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic 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;

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Oral Category 2
Dermal Category 3
Inhalation Category 3

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzeneacetonitrile, 4-chloro-	LD50 = 50 mg/kg (Rat)	-	-

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;
Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; 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; No data available

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

Symptoms / effects, both acute and delayed No information available.

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 Do not empty into drains.

Component	Microtox	M-Factor
Benzeneacetonitrile, 4-chloro-	EC50 = 0.30 mg/L 30 min EC50 = 0.30 mg/L 5 min EC50 = 0.31 mg/L 15 min	

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12.2. Persistence and degradability

Persistence Persistence is unlikely.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Benzeneacetonitrile, 4-chloro-	2.47	No data available

12.4. Mobility in soil

Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility.

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 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

14.1. UN number UN3439
14.2. UN proper shipping name NITRILES, SOLID, TOXIC, N.O.S.
14.3. Transport hazard class(es) 6.1
14.4. Packing group II

ADR

14.1. UN number UN3439
14.2. UN proper shipping name NITRILES, SOLID, TOXIC, N.O.S.
14.3. Transport hazard class(es) 6.1
14.4. Packing group II

IATA

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14.1. UN number	UN3439
14.2. UN proper shipping name	NITRILES, TOXIC, SOLID, N.O.S.*
14.3. Transport hazard class(es)	6.1
14.4. Packing group	II

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
Benzeneacetonitrile, 4-chloro-	140-53-4	205-418-9	-	-	X	X	-	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzeneacetonitrile, 4-chloro-	140-53-4	X	INACTIVE	-	X	X	X	X

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)
Benzeneacetonitrile, 4-chloro-	140-53-4	-	-	-

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
Benzeneacetonitrile, 4-chloro-	140-53-4	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

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

WGK Classification Water endangering class = 3 (self classification)

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
Benzeneacetonitrile, 4-chloro- 140-53-4 (>95)	Prohibited and Restricted Substances		

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

H300 - Fatal if swallowed
H311 - Toxic in contact with skin
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H331 - Toxic 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

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

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

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

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

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.

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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.

Prepared By	Health, Safety and Environmental Department
Creation Date	30-Apr-2012
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