

Creation Date 18-Mar-2010

Revision Date 28-Jan-2024

Revision Number 4

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

### 1.1. Product identifier

Product Description:	<b><u>2,3-Dichloro-5,6-dicyano-1,4-benzoquinone</u></b>
Cat No. :	<b>A11879</b>
Synonyms	4,5-Dichloro-3,6-dioxo-1,4-cyclohexadiene-1,2-carbonitrile; DDQ
CAS No	84-58-2
EC No	201-542-2
Molecular Formula	C8 Cl2 N2 O2
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

Category 3 (H301)

## 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

H301 - Toxic if swallowed

EUH029 - Contact with water liberates toxic gas

## Precautionary Statements

P264 - Wash face, hands and any exposed skin thoroughly after handling

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

P405 - Store locked up

## 2.3. Other hazards

Water reactive

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
1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-	84-58-2	EEC No. 201-542-2	>95	Acute Tox. 3 (H301) (EUH029)

REACH registration number

-

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is

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	required.
<b>Eye Contact</b>	In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
<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

None reasonably foreseeable.

## 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**

CO<sub>2</sub>, dry chemical, dry sand, alcohol-resistant foam.

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

Contact with water liberates toxic gas.

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

Contact with water liberates toxic gas.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Hydrogen cyanide (hydrocyanic acid), Nitrogen oxides (NO<sub>x</sub>), 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. Thermal decomposition can lead to release of irritating gases and vapors.

## 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. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.

### 6.2. Environmental precautions

Should not be released into the environment.

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

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Sweep up and shovel into suitable containers for disposal. Avoid dust formation. Do not expose spill to water.

## 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

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid dust formation. Use only under a chemical fume hood. Do not breathe (dust, vapor, mist, gas). Do not ingest. If swallowed then seek immediate medical assistance. Do not allow contact with water. Handle under an inert atmosphere.

### **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 away from water or moist air. Keep refrigerated. Store under an inert atmosphere. Keep container tightly closed in a dry and well-ventilated place. Protect from moisture.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 6.1C  
**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

#### **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.

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## 8.2. Exposure controls

### Engineering Measures

Use only under a chemical fume hood. 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** 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 compatibility, 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

<b>Physical State</b>	Solid	
<b>Appearance</b>	Yellow-orange	
<b>Odor</b>	Odorless	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	210 - 217 °C / 410 - 422.6 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flammability (liquid)</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	No information available	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	

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pH	No information available	
Viscosity	Not applicable	Solid
Water Solubility	Water reactive	
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	C8 Cl2 N2 O2
Molecular Weight	227.01
Evaporation Rate	Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

Yes

### 10.2. Chemical stability

Water reactive. Moisture sensitive.

### 10.3. Possibility of hazardous reactions

**Hazardous Polymerization** Hazardous polymerization does not occur.  
**Hazardous Reactions** None under normal processing.

### 10.4. Conditions to avoid

Incompatible products. Excess heat. Exposure to moist air or water. Exposure to moisture. Avoid dust formation. Temperatures above 100°C.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong reducing agents. Water. Strong acids. Strong bases. Alcohols.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen cyanide (hydrocyanic acid). Nitrogen oxides (NO<sub>x</sub>). 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	No data available

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-	82 mg/kg (Rat)	-	-

(b) skin corrosion/irritation; No data available

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(c) serious eye damage/irritation;	No data available
(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;	No data available
(i) STOT-repeated exposure;	No data available
Target Organs	None known.
(j) aspiration hazard;	Not applicable
	Solid
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. Reacts with water so no ecotoxicity data for the substance is available.

### 12.2. Persistence and degradability

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

12.3. Bioaccumulative potential Product does not bioaccumulate due to reaction with water

12.4. Mobility in soil Reacts with water Is not likely mobile in the environment.

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**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. Do not flush to sewer.

## SECTION 14: TRANSPORT INFORMATION

**IMDG/IMO**

**14.1. UN number** UN3439  
**14.2. UN proper shipping name** Nitriles, toxic, solid, n.o.s.  
**Technical Shipping Name** 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** III

**ADR**

**14.1. UN number** UN3439  
**14.2. UN proper shipping name** Nitriles, toxic, solid, n.o.s.  
**Technical Shipping Name** 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** III

**IATA**

**14.1. UN number** UN3439  
**14.2. UN proper shipping name** Nitriles, toxic, solid, n.o.s.  
**Technical Shipping Name** 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** III

**14.5. Environmental hazards** No hazards identified

**14.6. Special precautions for user** No special precautions required.



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**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
1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-	84-58-2	201-542-2	-	-	X	X	-	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-	84-58-2	X	ACTIVE	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)
1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-	84-58-2	-	-	-

#### 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
1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-	84-58-2	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

Water endangering class = 3 (self classification)

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## 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

EUH029 - Contact with water liberates toxic gas

### 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

**PNEC** - 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/MDG** - 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.

### Prepared By

Health, Safety and Environmental Department

### Creation Date

18-Mar-2010

### Revision Date

28-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,

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**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**