

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

Revision Date 13-Mar-2024 Revision Number 3

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

1.1. Product identifier

Product Description: AY 9944 dihydrochloride

Cat No.: **J65079 CAS No** 366-93-8

Molecular Formula C22 H28 Cl2 N2.2HCl

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

Recommended Use Laboratory chemicals.
Uses advised against Laboratory chemicals.
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

Acute oral toxicity Category 3 (H301)
Reproductive Toxicity Category 1A (H360)

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AY 9944 dihydrochloride

Revision Date 13-Mar-2024

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

H360 - May damage fertility or the unborn child

Precautionary Statements

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

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician

P201 - Obtain special instructions before use

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

P308 + P313 - IF exposed or concerned: Get medical advice/attention

Additional EU labelling

Restricted to professional users

2.3. Other hazards

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
AY 9944 dihydrochloride	366-93-8		<=100	Acute Tox. 3 (H301) Repr. 1A (H360)

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 required.

AY 9944 dihydrochloride Revision Date 13-Mar-2024

Eye Contact In the case of contact with eyes, rinse immediately with plenty of water and seek medical

advice.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Immediate medical

attention is required.

Ingestion Do NOT induce vomiting. Call a physician or poison control center immediately.

Inhalation 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.

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

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

Carbon dioxide (CO₂). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion.

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

Carbon monoxide (CO), Carbon dioxide (CO2), Nitrogen oxides (NOx), Hydrogen chloride.

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. See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

AY 9944 dihydrochloride

Revision Date 13-Mar-2024

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.

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 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 Storage Class (LGK) (Germany)

Class 6.1C

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.

8.2. Exposure controls

AY 9944 dihydrochloride Revision Date 13-Mar-2024

Engineering Measures

Ensure adequate ventilation, especially in confined areas.

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 Wear safety glasses with side shields (or 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 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.

Solid

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 Solid

Appearance White

Odor
Odor No information available
No data available
Melting Point/Range
No data available
No data available
No data available
No information available
No information available

Flammability (liquid) Not applicable

Flammability (solid,gas)

Explosion Limits

No information available

No data available

Flash Point No information available Method - No information available

Autoignition TemperatureNo data availableDecomposition TemperatureNo data available

No information available

Viscosity Not applicable Solid

Water Solubility No information available

AY 9944 dihydrochloride Revision Date 13-Mar-2024

Solid

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

No data available **Vapor Pressure Density / Specific Gravity** No data available **Bulk Density** No data available Not applicable **Vapor Density**

No data available

Particle characteristics

9.2. Other information

C22 H28 Cl2 N2.2HCl Molecular Formula

Molecular Weight 464.30

Not applicable - Solid **Evaporation Rate**

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability

Hygroscopic.

10.3. Possibility of hazardous reactions

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

10.4. Conditions to avoid

Exposure to moist air or water.

10.5. Incompatible materials

Oxidizing agent.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NOx). Hydrogen chloride.

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

(b) skin corrosion/irritation; No data available

No data available (c) serious eye damage/irritation;

(d) respiratory or skin sensitization;

Respiratory No data available Skin No data available

No data available (e) germ cell mutagenicity;

Revision Date 13-Mar-2024 AY 9944 dihydrochloride

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

Category 1A (g) reproductive toxicity;

No data available (h) STOT-single exposure;

(i) STOT-repeated exposure; No data available

No information available. **Target Organs**

Not applicable (j) aspiration hazard;

Solid

Symptoms / effects,both acute and No information available.

delayed

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

Contains no substances known to be hazardous to the environment or that are not **Ecotoxicity effects**

degradable in waste water treatment plants.

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

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 This product does not contain any known or suspected substance This product does not contain any known or suspected substance **Ozone Depletion Potential**

SECTION 13: DISPOSAL CONSIDERATIONS

AY 9944 dihydrochloride Revision Date 13-Mar-2024

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 UN2811

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

Technical Shipping Name (1,4-Bis(2-chlorobenzylaminomethyl)cyclohexane dihydrochloride)

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

ADR

14.1. UN number UN2811

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

Technical Shipping Name (1,4-Bis(2-chlorobenzylaminomethyl)cyclohexane dihydrochloride)

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

IATA

14.1. UN number UN2811

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

Technical Shipping Name (1,4-Bis(2-chlorobenzylaminomethyl)cyclohexane dihydrochloride)

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.

<u>14.7. Maritime transport in bulk</u> Not applicable, packaged goods <u>according to IMO instruments</u>

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
AY 9944 dihydrochloride	366-93-8	-	ı	ı	ı	1	ı	1	-

AY 9944 dihydrochloride

Revision Date 13-Mar-2024

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
AY 9944 dihydrochloride	366-93-8	ı	•	1	ı	-	1	-

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) -	REACH (1907/2006) -	REACH Regulation (EC
		Annex XIV - Substances	Annex XVII - Restrictions	1907/2006) article 59 -
		Subject to Authorization	on Certain Dangerous	Candidate List of
			Substances	Substances of Very High
				Concern (SVHC)
AY 9944 dihydrochloride	366-93-8	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident	Seveso III Directive (2012/18/EC) -
		Notification	Requirements
AY 9944 dihydrochloride	366-93-8	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

Take note of Directive 94/33/EC on the protection of young people at work

Take note of Dir 92/85/EC on the protection of pregnant and breastfeeding women 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)

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

H360 - May damage fertility or the unborn child

AY 9944 dihydrochloride Revision Date 13-Mar-2024

Inventory

CAS - Chemical Abstracts Service

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

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

Training Advice

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

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

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

Health, Safety and Environmental Department **Prepared By**

Revision Date 13-Mar-2024

New emergency telephone response service provider. **Revision Summary**

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

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

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

ENCS - Japanese Existing and New Chemical Substances AICS - Australian Inventory of Chemical Substances

Predicted No Effect Concentration (PNEC)

NZIoC - New Zealand Inventory of Chemicals

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)