SAFETY DATA SHEET

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

Revision Date 23-Feb-2024 **Revision Number** 3

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

1.1. Product identifier

Product Description: **5-[3-(Dimethylamino)propylidene]dibenzosuberane hydrochloride**
Cat No. : **J65596**
CAS No 549-18-8
Molecular Formula C20 H23 N.HCl

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

Acute oral toxicity	Category 3 (H301)
Reproductive Toxicity	Category 2 (H361d)

Specific target organ toxicity - (single exposure)	Category 1 (H370)
Environmental hazards	
Chronic aquatic toxicity	Category 1 (H410)

Full text of Hazard Statements: see section 16

2.2. Label elements

Signal Word **Danger**

Hazard Statements

H301 - Toxic if swallowed
H370 - Causes damage to organs
H361d - Suspected of damaging the unborn child
H410 - Very toxic to aquatic life with long lasting effects

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
P308 + P311 - IF exposed or concerned: Call a POISON CENTER or doctor
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

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
1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cycloheptaen-5-ylidene)-N,N-dimethyl-, hydrochloride	549-18-8	EEC No. 208-964-6	<=100	Acute Tox. 3 (H301) Repr. 2 (H361d) STOT SE 1 (H370) Aquatic Chronic 1 (H410)

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cycloheptaen-5-ylidene)-N,N-dimethyl-, hydrochloride	-	1	-

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.

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 No special precautions required.

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 (CO_2). 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

Do not allow run-off from fire-fighting to enter drains or water courses.

Hazardous Combustion Products
Carbon monoxide (CO), Carbon dioxide (CO_2), 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

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

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

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. Avoid dust formation. Do not get in eyes, on skin, or on clothing. 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.

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

Engineering Measures
None under normal use conditions.

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 Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

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 No protective equipment is needed under normal use conditions.

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: Particle filter

Small scale/Laboratory use Maintain adequate ventilation

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
Appearance	White - Off-white
Odor	No information available
Odor Threshold	No data available
Melting Point/Range	196 - 197 °C / 384.8 - 386.6 °F
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	No information available	**Method -** No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	Not applicable	Solid
Water Solubility	Soluble in water	
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	C20 H23 N.HCl
Molecular Weight	313.86
Evaporation Rate	Not applicable - Solid

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	None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat.

10.5. Incompatible materials

Oxidizing agent.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO_2). 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

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cycloheptaen-5-ylidene)-N,N-dimethyl-, hydrochloride	LD50 = 240 mg/kg (Rat)	-	-

(b) skin corrosion/irritation; No data available

(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; Category 2

(h) STOT-single exposure; Category 1

Results / Target organs Central nervous system (CNS), Cardiovascular system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Not applicable
Solid

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 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
1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cycloheptaen-5-ylidene)-N,N-dimethyl-, hydrochloride		1

12.2. Persistence and degradability
Persistence Soluble in water, Persistence is unlikely, based on information available.
Degradation in sewage treatment plant Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential Bioaccumulation is unlikely

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 This product does not contain any known or suspected substance

Ozone Depletion Potential 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.

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.
Technical Shipping Name (5-[3-(Dimethylamino)propylidene]dibenzosuberane hydrochloride)
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 (5-[3-(Dimethylamino)propylidene]dibenzosuberane hydrochloride)
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	(5-[3-(Dimethylamino)propylidene]dibenzosuberane hydrochloride)
14.3. Transport hazard class(es)	6.1
14.4. Packing group	III
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 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-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-, hydrochloride	549-18-8	208-964-6	-	-	-	X	KE-10614	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-, hydrochloride	549-18-8	X	INACTIVE	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

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-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-, hydrochloride	549-18-8	-	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
1-Propanamine, 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-, hydrochloride	549-18-8	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 work .
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
H370 - Causes damage to organs
H361d - Suspected of damaging the unborn child
H410 - Very toxic to aquatic life with long lasting effects

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
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 hygiene.
Chemical incident response training.

Prepared By	Health, Safety and Environmental Department
Revision Date	23-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. .

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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