SAFETY DATA SHEET

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

Creation Date 12-Feb-2015 **Revision Date** 28-Jan-2024 **Revision Number** 3

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

1.1. Product identifier

Product Description:	**1,4-Diazabicyclo[2.2.2]octane**
Cat No. :	**A14003**
Synonyms	Triethylenediamine; TED; BACO; Dabcº4
CAS No	280-57-9
EC No	205-999-9
Molecular Formula	C6 H12 N2
REACH registration number	-

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

Recommended Use	Laboratory chemicals.
Sector of use	SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites
Product category	PC21 - Laboratory chemicals
Process categories	PROC15 - Use as a laboratory reagent
Environmental release category	ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)
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

Flammable solids	Category 2 (H228)

Health hazards

Acute oral toxicity	Category 4 (H302)
Skin Corrosion/Irritation	Category 2 (H315)
Serious Eye Damage/Eye Irritation	Category 1 (H318)

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
H228 - Flammable solid
H302 - Harmful if swallowed
H318 - Causes serious eye damage
H315 - Causes skin irritation

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
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P273 - Avoid release to the environment
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

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-Diazabicyclo[2.2.2]octane	280-57-9	EEC No. 205-999-9	>95	Flam Sol. 2 (H228) Skin Irrit. 2 (H315) Eye Dam. 1 (H318) Acute Tox. 4 (H302)

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 Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

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

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

Inhalation Remove to fresh air. 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. Get medical attention. If not breathing, give artificial respiration.

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

Difficulty in breathing. Causes eye burns. Causes severe eye damage. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

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, alcohol-resistant foam. 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

Flammable. Risk of ignition. Dust can form an explosive mixture with air. Containers may explode when heated. Thermal decomposition can lead to release of irritating gases and vapors. Keep product and empty container away from heat and sources of ignition. Combustible material.

Hazardous Combustion Products
Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO_2), Ammonia, nitric acid.

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

Use personal protective equipment as required. Remove all sources of ignition. Avoid dust formation. Take precautionary measures against static discharges. Ensure adequate ventilation. Avoid contact with skin, eyes or clothing.

6.2. Environmental precautions

Avoid release to the environment. See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Remove all sources of ignition. Sweep up and shovel into suitable containers for disposal. Avoid dust formation. Use spark-proof tools and explosion-proof equipment.

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

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Use spark-proof tools and explosion-proof equipment. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges. Do not get in eyes, on skin, or on clothing. 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 away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place. Flammables area.

Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK) (Germany) Class 4.1B

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits
List source(s):

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)
See table for values

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
1,4-Diazabicyclo[2.2.2]octane 280-57-9 (>95)				DNEL = 1.4mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
1,4-Diazabicyclo[2.2.2]octane 280-57-9 (>95)				DNEL = 8.24mg/m³

Predicted No Effect Concentration (PNEC)
See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
1,4-Diazabicyclo[2.2.2]octane 280-57-9 (>95)	PNEC = 0.1mg/L	PNEC = 1.3mg/kg sediment dw	PNEC = 1mg/L	PNEC = 200mg/L	PNEC = 0.19mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
1,4-Diazabicyclo[2.2.2]octane 280-57-9 (>95)	PNEC = 0.01mg/L	PNEC = 0.13mg/kg sediment dw			

8.2. Exposure controls

Engineering Measures
Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. 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
Natural rubber Nitrile rubber Neoprene PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

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	Solid	
Appearance	White	
Odor	Ammonia-like	
Odor Threshold	No data available	
Melting Point/Range	155 - 160 °C / 311 - 320 °F	
Softening Point	No data available	
Boiling Point/Range	174 °C / 345.2 °F	@ 760 mmHg
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	62 °C / 143.6 °F	**Method -** No information available
Autoignition Temperature	350 °C / 662 °F	
Decomposition Temperature	No data available	
pH	10.8	10g/l aq.sol
Viscosity	Not applicable	Solid
Water Solubility	46 g/100ml (26°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	2.9 mmHg @ 50 °C	
Density / Specific Gravity	1.140	
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

9.2. Other information

Molecular Formula	C6 H12 N2
Molecular Weight	112.17
Explosive Properties	explosive air/vapour mixtures possible
Flammable solids	Burning rate or burning time = > 2.2 mm/s or < 45 secs Wetted zone passed - No
Evaporation Rate	Not applicable - Solid

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 Hazardous polymerization does not occur.
Hazardous Reactions No information available.

10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition. Avoid dust formation. Incompatible products. Exposure to moist air or water.

10.5. Incompatible materials

Strong oxidizing agents. Peroxides. Acids. sodium hypochlorite. copper. Aldehydes.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO_2). Ammonia. nitric acid.

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 4
Dermal Based on available data, the classification criteria are not met
Inhalation Based on available data, the classification criteria are not met

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
1,4-Diazabicyclo[2.2.2]octane	700 mg/kg (Rat)	>2000 mg/kg (Rabbit)	>20 mg/L/1h (Rat)

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;
Respiratory Based on available data, the classification criteria are not met
Skin Based on available data, the classification criteria are not met

(e) germ cell mutagenicity; Based on available data, the classification criteria are not met

Not mutagenic in AMES Test

(f) carcinogenicity; Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; Based on available data, the classification criteria are not met

(h) STOT-single exposure; Based on available data, the classification criteria are not met

(i) STOT-repeated exposure; Based on available data, the classification criteria are not met

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 Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

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 This product contains the following substance(s) which are hazardous for the environment. .

Component	Freshwater Fish	Water Flea	Freshwater Algae
1,4-Diazabicyclo[2.2.2]octane	LC50: 1510 - 1980 mg/L, 96h flow-through (Pimephales promelas)		

12.2. Persistence and degradability

Not readily biodegradable

Persistence Soluble in water, Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
1,4-Diazabicyclo[2.2.2]octane		<13 dimensionless

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

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB).

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 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 UN1325
14.2. UN proper shipping name Flammable solid, organic, n.o.s.
Technical Shipping Name 1,4-Diazabicyclo[2.2.2]octane
14.3. Transport hazard class(es) 4.1
14.4. Packing group II

ADR

14.1. UN number UN1325
14.2. UN proper shipping name Flammable solid, organic, n.o.s.
Technical Shipping Name 1,4-Diazabicyclo[2.2.2]octane
14.3. Transport hazard class(es) 4.1
14.4. Packing group II

IATA

14.1. UN number UN1325
14.2. UN proper shipping name Flammable solid, organic, n.o.s.
Technical Shipping Name 1,4-Diazabicyclo[2.2.2]octane
14.3. Transport hazard class(es) 4.1
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
1,4-Diazabicyclo[2.2.2]octane	280-57-9	205-999-9	-	-	X	X	KE-09862	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1,4-Diazabicyclo[2.2.2]octane	280-57-9	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) -	REACH (1907/2006) -	REACH Regulation (EC

		Annex XIV - Substances Subject to Authorization	Annex XVII - Restrictions on Certain Dangerous Substances	1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
1,4-Diazabicyclo[2.2.2]octane	280-57-9	-	-	-

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-Diazabicyclo[2.2.2]octane	280-57-9	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
1,4-Diazabicyclo[2.2.2]octane	WGK1	

Component	France - INRS (Tables of occupational diseases)
1,4-Diazabicyclo[2.2.2]octane	Tableaux des maladies professionnelles (TMP) - RG 49

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
H228 - Flammable solid
H302 - Harmful if swallowed
H315 - Causes skin irritation
H318 - Causes serious eye damage

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

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

IECSC - Chinese Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated 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.
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	12-Feb-2015
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, 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