

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

1.1. Product identifier

Product Description:	<u>N-tert-Butyl-2-benzothiazolesulfenamide</u>
Cat No. :	L13356
CAS No	95-31-8
Molecular Formula	C11 H14 N2 S2

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

Skin Sensitization

Category 1 Sub-category 1B (H317)

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Environmental hazards

Acute aquatic toxicity
Chronic aquatic toxicity

Category 1 (H400)
Category 1 (H410)

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H317 - May cause an allergic skin reaction
H410 - Very toxic to aquatic life with long lasting effects

Precautionary Statements

P280 - Wear protective gloves/protective clothing
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P333 + P313 - If skin irritation or rash occurs: Get medical advice/attention

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
N-tert-Butyl-2-benzothiazolesulfenamide	95-31-8	EEC No. 202-409-1	<=100	Skin Sens. 1B (H317) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
N-tert-Butyl-2-benzothiazolesulfenamide	-	10 (acute) 1 (Chronic)	-

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

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4.1. Description of first aid measures

General Advice	If symptoms persist, call a physician.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Self-Protection of the First Aider	No special precautions required.

4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable. May cause allergic skin reaction. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

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

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

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Sulfur oxides.

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

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent

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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. Keep in suitable, closed containers for disposal.

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. Ensure adequate ventilation. Avoid ingestion and inhalation. Avoid dust formation. Do not get in eyes, on skin, or on clothing.

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 container tightly closed in a dry and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 11
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):

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)
N-tert-Butyl-2-benzothiazolesulfenamide 95-31-8 (≤100)		DNEL = 534mg/kg bw/day		DNEL = 67mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
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N-tert-Butyl-2-benzothiazolesulfenamide 95-31-8 (<=100)	DNEL = 14mg/m ³	DNEL = 14mg/m ³	DNEL = 14mg/m ³	DNEL = 14mg/m ³
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Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
N-tert-Butyl-2-benzothiazolesulfenamide 95-31-8 (<=100)	PNEC = 0.0023mg/L	PNEC = 0.08mg/kg sediment dw	PNEC = 0.00071mg/L	PNEC = 100mg/L	PNEC = 0.796mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
N-tert-Butyl-2-benzothiazolesulfenamide 95-31-8 (<=100)	PNEC = 0.00023mg/L	PNEC = 0.008mg/kg sediment dw			

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 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

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

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Physical State	Solid	
Appearance	White - Cream	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	105 - 110 °C / 221 - 230 °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	165 °C / 329 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	Not applicable	
Viscosity	Not applicable	Solid
Water Solubility	Insoluble in water	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
N-tert-Butyl-2-benzothiazolesulfenamide	3.36	
Vapor Pressure	No data available	
Density / Specific Gravity	1.29 g/cm3	@ 20 °C
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

9.2. Other information

Molecular Formula	C11 H14 N2 S2
Molecular Weight	238.38
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 (CO₂). Nitrogen oxides (NO_x). Sulfur oxides.

SECTION 11: TOXICOLOGICAL INFORMATION

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11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

Oral

Based on available data, the classification criteria are not met

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
N-tert-Butyl-2-benzothiazolesulfenamide	LD50 = 6850 mg/kg (Rat)	LD50 > 7940 mg/kg (Rabbit)	-

(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

Sub-category 1B

May cause sensitization by skin contact

(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

No information available.

(j) aspiration hazard;

Not applicable

Solid

Symptoms / effects, both acute and delayed

Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

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

The product contains following substances which are hazardous for the environment. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

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Component	Freshwater Fish	Water Flea	Freshwater Algae
N-tert-Butyl-2-benzothiazolesulfenamide	LC50: > 0.3 mg/L, 96h static (Pimephales promelas) LC50: > 0.3 mg/L, 96h static (Oncorhynchus mykiss) LC50: > 0.3 mg/L, 96h static (Lepomis macrochirus)	EC50: > 0.3 mg/L, 48h (Daphnia magna)	EC50: > 0.3 mg/L, 96h (Pseudokirchneriella subcapitata)

Component	Microtox	M-Factor
N-tert-Butyl-2-benzothiazolesulfenamide		10 (acute) 1 (Chronic)

12.2. Persistence and degradability

Persistence

May persist.

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

Product has a high potential to bioconcentrate

Component	log Pow	Bioconcentration factor (BCF)
N-tert-Butyl-2-benzothiazolesulfenamide	3.36	No data available

12.4. Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and sinks in water Is not likely mobile in the environment due its low water solubility. Is not likely mobile in the environment due its low water solubility and propensity to bind to soil particles

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 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

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

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IMDG/IMO

14.1. UN number	UN3077
14.2. UN proper shipping name Technical Shipping Name	Environmentally hazardous substances, solid, n.o.s. (N-tert-Butyl-2-benzothiazolesulfenamide)
14.3. Transport hazard class(es)	9
14.4. Packing group	III

ADR

14.1. UN number	UN3077
14.2. UN proper shipping name Technical Shipping Name	Environmentally hazardous substances, solid, n.o.s. (N-tert-Butyl-2-benzothiazolesulfenamide)
14.3. Transport hazard class(es)	9
14.4. Packing group	III

IATA

14.1. UN number	UN3077
14.2. UN proper shipping name Technical Shipping Name	Environmentally hazardous substances, solid, n.o.s. (N-tert-Butyl-2-benzothiazolesulfenamide)
14.3. Transport hazard class(es)	9
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
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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
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SECTION 15: REGULATORY INFORMATION

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

International Inventories

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
N-tert-Butyl-2-benzothiazolesulfenamide	95-31-8	202-409-1	-	-	X	X	KE-11372	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDL	AICS	NZIoC	PICCS
N-tert-Butyl-2-benzothiazolesulfenamide	95-31-8	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)
N-tert-Butyl-2-benzothiazolesulfenamide	95-31-8	-	-	-

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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
N-tert-Butyl-2-benzothiazole sulfenamide	95-31-8	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 .

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
N-tert-Butyl-2-benzothiazolesulfenamide	WGK2	

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
N-tert-Butyl-2-benzothiazolesulfenamide 95-31-8 (<=100)	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

H317 - May cause an allergic skin reaction

H400 - Very toxic to aquatic life

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

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

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

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PICCS - Philippines Inventory of Chemicals and Chemical Substances
IECSC - Chinese Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances

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	24-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.

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