

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

Revision Date 01-Mar-2024

Revision Number 3

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

1.1. Product identifier

Product Description:	4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydrothiophene 1,1-dioxide
Cat No. :	B24153
CAS No	54714-10-2
Molecular Formula	C16 H12 O4 S
1.2. Relevant identified uses of the s	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 sat	fety 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

Skin Corrosion/Irritation Serious Eye Damage/Eye Irritation Category 2 (H315) Category 2 (H319)

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Specific target organ toxicity - (single exposure)

Category 3 (H335)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Warning

Hazard Statements

Signal Word

- H315 Causes skin irritation
- H319 Causes serious eye irritation
- H335 May cause respiratory irritation

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P332 + P313 - If skin irritation occurs: Get medical advice/attention
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P337 + P313 - If eye irritation persists: Get medical advice/attention
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P312 - Call a POISON CENTER or doctor if you feel unwell

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
4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydroth iophene 1,1-dioxide	54714-10-2		<=100	Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydrothiophene 1,1-dioxide

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	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.
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SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam.

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), 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

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. Keep in suitable, closed containers for disposal.

4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydrothiophene 1,1-dioxide

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

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

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 Ensure that eyewash stations and safety showers are close to the workstation location.

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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 equ Eye Protection		(European standard	I - EN 166)		
Hand Protection	Protectiv	e gloves			
Glove material Nitrile rubber Neoprene Natural rubber PVC	Breakthrough time See manufacturers recommendations	Glove thickness -	EU standard EN 374	Glove comments (minimum requirement)	
Skin and body prote	Skin and body protection Long sleeved clothing.				

Skin and body protection

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

No information available. Environmental exposure controls

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Solid	
Appearance Odor Odor Threshold	White - Cream No information available No data available	
Melting Point/Range Softening Point	238 - 241 °C / 460.4 - 465.8 °F No data available	
Boiling Point/Range Flammability (liquid)	No information available Not applicable	Solid
Flammability (solid,gas) Explosion Limits	No information available No data available	
Flash Point	No information available	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature pH	No data available No information available	
Viscosity Water Solubility	Not applicable No information available	Solid
Solubility in other solvents	No information available	

4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydrothiophene 1,1-dioxide

Partition Coefficient (n-octanol/	water)		
Vapor Pressure Density / Specific Gravity Bulk Density Vapor Density Particle characteristics	No data available No data available No data available Not applicable No data available	Solid	
9.2. Other information Molecular Formula Molecular Weight	C16 H12 O4 S 300.34		

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 react	ions_
Hazardous Polymerization Hazardous Reactions	No information available. None under normal processing.
10.4. Conditions to avoid	Incompatible products. Excess heat.
10.5. Incompatible materials	None known.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides.

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information

Evaporation Rate

(a) acute toxicity; Oral

- OralNo data availableDermalNo data availableInhalationNo data available
- (b) skin corrosion/irritation; Category 2
- (c) serious eye damage/irritation; Category 2
- (d) respiratory or skin sensitization; Respiratory Skin No data available No data available
- (e) germ cell mutagenicity; No data available

4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydrothiophene 1,1-dioxide

(f) carcinogenicity;	No data available
	There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	Category 3
Results / Target organs	Respiratory 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	Contains no substances known to be hazardous to the environment or that are not 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
<u>12.5. Results of PBT and vPvB</u> assessment	No data available for assessment.
<u>12.6. Endocrine disrupting</u> properties Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
<u>12.7. Other adverse effects</u> 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.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO	Not regulated
<u>14.1. UN number</u> 14.2. UN proper shipping name 14.3. Transport hazard class(es) 14.4. Packing group	
ADR	Not regulated
<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> <u>14.3. Transport hazard class(es)</u> <u>14.4. Packing group</u>	
IATA	Not regulated
<u>14.1. UN number</u> 14.2. UN proper shipping name 14.3. Transport hazard class(es) 14.4. Packing group	
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
4-Hydroxy-3-oxo-2,5-diphenyl-2,3-	54714-10-2	-	-	-	-	-	-	-	-
dihydrothiophene 1,1-dioxide									
Component	CAS No	TSCA	TSCA In	ventory	DSL	NDSL	AICS	NZIoC	PICCS

4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydrothiophene 1,1-dioxide

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			notification - Active-Inactive					
4-Hydroxy-3-oxo-2,5-diphenyl-2,3- dihydrothiophene 1,1-dioxide	54714-10-2	-	-	-	-	-	-	-

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 Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
4-Hydroxy-3-oxo-2,5-diphenyl-2,3-di hydrothiophene 1,1-dioxide	54714-10-2	-	-	

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
4-Hydroxy-3-oxo-2,5-diphen yl-2,3-dihydrothiophene 1,1-dioxide	54714-10-2	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)

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

4-Hydroxy-3-oxo-2,5-diphenyl-2,3-dihydrothiophene 1,1-dioxide

Legend

CAS - Chemical Abstracts Service	TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
EINECS/ELINCS - European Inventory of Existing Commercial Chemica Substances/EU List of Notified Chemical Substances	Substances List
PICCS - Philippines Inventory of Chemicals and Chemical Substances	ENCS - Japanese Existing and New Chemical Substances
IECSC - Chinese Inventory of Existing Chemical Substances	AICS - Australian Inventory of Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances	NZIOC - New Zealand Inventory of Chemicals
WEL - Workplace Exposure Limit	TWA - Time Weighted Average
ACGIH - American Conference of Governmental Industrial Hygienists	IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level	Predicted No Effect Concentration (PNEC)
RPE - Respiratory Protective Equipment LC50 - Lethal Concentration 50%	LD50 - Lethal Dose 50% EC50 - Effective Concentration 50%
NOEC - No Observed Effect Concentration	POW - Partition coefficient Octanol:Water
PBT - Persistent, Bioaccumulative, Toxic	vPvB - very Persistent, very Bioaccumulative
ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road	ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code	MARPOL - International Convention for the Prevention of Pollution from Ships
OECD - Organisation for Economic Co-operation and Development	ATE - Acute Toxicity Estimate
BCF - Bioconcentration factor	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, F	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
Revision Date	01-Mar-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