

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

Revision Date 18-Mar-2024 Revision Number 3

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

1.1. Product identifier

Product Description: Xanthine Cat No.: A11077

Synonyms Xanthic oxide; 3,7-dihydro-1H-Purine-2,6-dione; 2,6-dioxopurine

CAS No 69-89-6 **Molecular Formula** C5 H4 N4 O2

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

Skin Corrosion/Irritation Category 2 (H315)

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Serious Eye Damage/Eye Irritation

Specific target organ toxicity - (single exposure)

Category 2 (H319) 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



Signal Word

Warning

Hazard Statements

H335 - May cause respiratory irritation

H315 - Causes skin irritation

H319 - Causes serious eye irritation

Precautionary Statements

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P280 - Wear protective gloves/protective clothing/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

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
1H-Purine-2,6-dione, 3,7-dihydro-	69-89-6	EEC No. 200-718-6	98	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

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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 soap and plenty of water while removing all contaminated

clothes and shoes. Get medical attention.

Ingestion Clean mouth with water. Get medical attention.

Inhalation Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial

respiration. Get medical attention.

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

No information available.

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. Chemical 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

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

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.

6.2. Environmental precautions

See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Avoid dust formation. Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

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SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Avoid contact with skin and eyes. Do not breathe dust. 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 in a dry, cool and well-ventilated place. Keep container tightly closed.

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 adequate ventilation, especially in confined areas. 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

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Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Protective gloves **Hand Protection**

Breakthrough time Glove thickness EU standard Glove comments Glove material Nitrile rubber See manufacturers EN 374 (minimum requirement) recommendations

Neoprene Natural rubber

PVC

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.

No protective equipment is needed under normal use conditions. **Respiratory Protection**

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

Solid

Small scale/Laboratory use Maintain adequate ventilation

No information available. **Environmental exposure controls**

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Powder Solid

Appearance Off-white Odor Odorless

Odor Threshold No data available 300 °C / 572 °F **Melting Point/Range Softening Point** No data available **Boiling Point/Range** No information available

Flammability (liquid) Not applicable

Flammability (solid,gas) No information available

Explosion Limits No data available

No information available Method - No information available **Flash Point**

Autoignition Temperature Not applicable **Decomposition Temperature** No data available

Ha

No information available

Viscosity Not applicable Solid

1g/14.5l (16°C) Water Solubility

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure No data available No data available **Density / Specific Gravity Bulk Density** No data available

Vapor Density Not applicable Solid

Particle characteristics No data available

9.2. Other information

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Molecular Formula C5 H4 N4 O2 Molecular Weight 152.11

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 PolymerizationNo information available.Hazardous ReactionsNo information available.

10.4. Conditions to avoid

Avoid dust formation. Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

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

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product InformationNo acute toxicity information is available for this product

(a) acute toxicity;

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;

RespiratoryNo data availableSkinNo 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; No data available

(h) STOT-single exposure; Category 3

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Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Not applicable

Solid

Other Adverse Effects The toxicological properties have not been fully investigated.

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

Ecotoxicity effects Do not empty into drains.

12.2. Persistence and degradability

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

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

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.

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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

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

ADR Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

IATA Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

No hazards identified 14.5. Environmental hazards

No special precautions required. 14.6. Special precautions for user

14.7. Maritime transport in bulk

according to IMO instruments

SECTION 15: REGULATORY INFORMATION

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

Not applicable, packaged goods

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
1H-Purine-2,6-dione, 3,7-dihydro-	69-89-6	200-718-6	-	-	X	X	KE-10741	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1H-Purine-2,6-dione, 3,7-dihydro-	69-89-6	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)

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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)
1H-Purine-2,6-dione, 3,7-dihydro-	69-89-6	-	-	-

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
1H-Purine-2,6-dione, 3,7-dihydro-	69-89-6	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

Full text of H-Statements referred to under sections 2 and 3

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

Legend

CAS - Chemical Abstracts Service

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

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

Substances List **ENCS** - Japanese Existing and New Chemical Substances

PICCS - Philippines Inventory of Chemicals and 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

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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 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 18-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

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)

TWA - Time Weighted Average

EC50 - Effective Concentration 50%

LD50 - Lethal Dose 50%

IARC - International Agency for Research on Cancer

Predicted No Effect Concentration (PNEC)

POW - Partition coefficient Octanol:Water **vPvB** - very Persistent, very Bioaccumulative