

Creation Date 09-Oct-2015 Revision Date 24-Aug-2023 Revision Number 2

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

1.1. Product identifier

Product Description: 4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl}

methyl)-7-hydroxy-2H-chromen-2-one

Cat No.: HTS08006SC

CAS No N/A

Molecular Formula C21 H17 N3 O4 S

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

UK entity/business name

Thermo Fisher Scientific (Heysham),

Shore Road,

Port of Heysham Industrial Park, Heysham, Lancashire, LA3 2XY

United Kingdom

EU entity/business name Thermo Fisher Scientific Janssen Pharmaceuticalaan 3a

2440 Geel, Belgium

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 - Regulation (EC) No 1272/2008

#### Physical hazards

Based on available data, the classification criteria are not met

#### **Health hazards**

4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl} methyl)-7-hydroxy-2H-chromen-2-one

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Acute oral toxicity
Acute dermal toxicity
Acute Inhalation Toxicity - Dusts and Mists
Category 4 (H312)
Skin Corrosion/Irritation
Category 2 (H315)
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**

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

#### **Precautionary Statements**

P280 - Wear protective gloves/protective clothing/eye protection/face protection

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

P312 - Call a POISON CENTER or doctor if you feel unwell

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P332 + P313 - If skin irritation occurs: Get medical advice/attention

P337 + P313 - If eye irritation persists: Get medical advice/attention

#### 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 - Regulation (EC) No 1272/2008
Maybridge Screening Products Harmful Irritant	N/A		90-100	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)

4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl} methyl)-7-hydroxy-2H-chromen-2-one

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Full text of Hazard Statements: see section 16

## **SECTION 4: FIRST AID MEASURES**

## 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 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.

#### **SECTION 5: FIREFIGHTING MEASURES**

#### 5.1. Extinguishing media

#### Suitable Extinguishing Media

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 (CO<sub>2</sub>), Nitrogen oxides (NOx), 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.

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## **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.

#### 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. 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.

## 7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. To maintain product quality. Keep at temperature not exceeding 25°C.

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

4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl} methyl)-7-hydroxy-2H-chromen-2-one

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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.

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

		EU standard	Glove comments (minimum requirement)
recommendations	-	EN 374	(minimum requirement)
	See manufacturers	See manufacturers -	See manufacturers - EN 374

**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 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**

Solid

Solid

4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl} methyl)-7-hydroxy-2H-chromen-2-one

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9.1. Information on basic physical and chemical properties

Physical State Solid

**Appearance** 

Odor No information available
Odor Threshold No data available
Melting Point/Range No data available
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

Flash Point Not applicable Method - No information available

Autoignition Temperature
Decomposition Temperature
pH

Not applicable
No data available
No information available

Viscosity Not applicable

Water Solubility No information available

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure

Density / Specific Gravity

Bulk Density

Vapor Density

No data available
No data available
No data available

Vapor Density Not applicable Solid

Particle characteristics No data available

9.2. Other information

Molecular Formula C21 H17 N3 O4 S

Molecular Weight 407.44

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 Hazardous polymerization does not occur.

**Hazardous Reactions** None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

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

## **SECTION 11: TOXICOLOGICAL INFORMATION**

4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl} methyl)-7-hydroxy-2H-chromen-2-one

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

#### **Product Information**

(a) acute toxicity;

OralCategory 4DermalCategory 4InhalationCategory 4

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(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; No data available

(h) STOT-single exposure; Category 3

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Not applicable

Solid

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**Contains no substances known to be hazardous to the environment or that are not

degradable in waste water treatment plants.

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4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl} methyl)-7-hydroxy-2H-chromen-2-one

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

No information available 12.4. Mobility in soil

No data available for assessment. 12.5. Results of PBT and vPvB

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 Waste is classified as hazardous. Dispose of in accordance with the European Directives **Products** 

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

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

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4-({ [4-(2,3-Dihydro-1H-inden-2-yl)-5-hydroxy-4H-1,2,4-triazol-3-yl]sulfanyl} methyl)-7-hydroxy-2H-chromen-2-one

IATA Not regulated

14.1. UN number

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
Maybridge Screening Products	N/A	-	-	-	-	-	-	-	-
Harmful Irritant									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Maybridge Screening Products Harmful Irritant	N/A	-	-	-	-	-	-	-

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)
Maybridge Screening Products Harmful Irritant	N/A	-	-	-

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
Maybridge Screening Products Harmful Irritant	N/A	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

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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

#### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) is not required (< 10 t/y)

## **SECTION 16: OTHER INFORMATION**

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

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H332 - Harmful if inhaled

H315 - Causes skin irritation

H319 - Causes serious eve irritation

H335 - May cause respiratory irritation

#### Legend

**CAS** - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic 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

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

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

Substances List

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

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

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

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Shins

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

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#### **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.

**Creation Date** 09-Oct-2015 **Revision Date** 24-Aug-2023

Revision Summary SDS sections updated, 1, 2, 15, 9, 11, 12, 16.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No. 1907/2006

#### **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**