

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Smoc-L-Thr(tBu)-OH

Revision date: 06.06.2024

Product code: SAA1160

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Smoc-L-Thr(tBu)-OH

Further trade names

O-(tert-butyl)-N-(((2,7-disulfo-9H-fluoren-9-yl)methoxy)carbonyl)-L-threonine potassium salt potassium 9-(((1S,2R)-2-(tert-butoxy)-1-carboxypropyl)carbonyloxy)methyl)-9H-fluorene-2,7-disulfonate, Smoc-Thr(tBu)-OH

Substance name: Smoc-L-Thr(tBu)-OH
CAS No: 2442552-94-3**1.2. Relevant identified uses of the substance or mixture and uses advised against****Use of the substance/mixture**

Laboratory chemical. Manufacture of the substance.

Uses advised against

Do not use for private purposes (household).

Restrictions on use: Pharmaceutical substance

1.3. Details of the supplier of the safety data sheet

Company name:	Iris Biotech GmbH	
Street:	Adalbert-Zoellner-Straße 1	
Place:	D-95615 Marktredwitz, Germany	
Post-office box:	568	
	D-95605 Marktredwitz, Germany	
Telephone:	+49 9231 97121 0	Telefax: +49 9231 97121 99
E-mail:	info@iris-biotech.de	
Contact person:	Health & Safety Department	Telephone: +49 9231 97121 0
E-mail:	sds@iris-biotech.de	
Internet:	www.iris-biotech.de	
Responsible Department:	Only available during office hours.	

1.4. Emergency telephone number: +49 (0)89 19240 (POISON CENTER Munich: 24 h)**Further Information**

The substance is classified as not hazardous according to regulation (EC) No 1272/2008 [CLP].

Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Regulation (EC) No 1272/2008**

This substance is not classified as hazardous in accordance with Regulation (EC) No 1272/2008.

2.2. Label elements**Regulation (EC) No 1272/2008****Precautionary statements**

P202	Do not handle until all safety precautions have been read and understood.
P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P262	Do not get in eyes, on skin, or on clothing.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

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Additional advice on labelling

Labelling according to Regulation (EC) No. 1272/2008 [CLP]: none (GHS/CLP criteria are not met.)

Warning - substance not yet tested completely.

2.3. Other hazards

Product is not dust explosive in its original delivery form. The addition of particulate matter, however, results in a dust explosion risk.

SECTION 3: Composition/information on ingredients**3.1. Substances****Chemical characterization**

O-(tert-butyl)-N-(((2,7-disulfo-9H-fluoren-9-yl)methoxy)carbonyl)-L-threonine potassium salt

Sum formula: C₂₃H₂₅K₂NO₁₁S₂

Molecular weight: 633,77 g/mol

Relevant ingredients

none (according to Regulation (EC) No 1907/2006 (REACH))

SECTION 4: First aid measures**4.1. Description of first aid measures****General information**

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

In all cases of doubt, or when symptoms persist, seek medical advice.

After inhalation

Provide fresh air. Remove casualty to fresh air and keep warm and at rest. In case of irregular breathing or respiratory arrest provide artificial respiration.

After contact with skin

Wash with plenty of water. Take off contaminated clothing and wash it before reuse. After contact with skin, wash immediately with plenty of water and soap.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water. If product gets into the eye, keep eyelid open and rinse immediately with large quantities of water, for at least 5 minutes. Subsequently consult an ophthalmologist.

After ingestion

Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

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

Treat symptomatically.

SECTION 5: Firefighting measures**5.1. Extinguishing media****Suitable extinguishing media**

Co-ordinate fire-fighting measures to the fire surroundings. Water spray. alcohol resistant foam. Dry extinguishing powder. Sand.

Unsuitable extinguishing media

High power water jet.

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5.2. Special hazards arising from the substance or mixture

Non-flammable. Thermal decomposition can lead to the escape of irritating gases and vapours.
In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

Additional information

Usual measures for fire prevention.

SECTION 6: Accidental release measures**6.1. Personal precautions, protective equipment and emergency procedures****General advice**

Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid contact with skin, eyes and clothes.
Wear personal protection equipment.
In case of fire: Evacuate area.

For non-emergency personnel

Remove all sources of ignition. Provide adequate ventilation.
Use personal protection equipment.

For emergency responders

Wear personal protection equipment (refer to section 8).
Take up mechanically, placing in appropriate containers for disposal. Take up dust-free and set down dust-free.

6.2. Environmental precautions

Do not allow to enter into soil/subsoil.
Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up**For containment**

Avoid dust formation.

For cleaning up

Take up mechanically.

Other information

Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation.
Clear contaminated areas thoroughly.

6.4. Reference to other sections

Safe handling: see section 7
Personal protection equipment: see section 8
Disposal: see section 13

Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

Provide adequate ventilation.
Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid contact with skin, eyes and clothes.

Advice on protection against fire and explosion

Usual measures for fire prevention.

Advice on general occupational hygiene

Take off contaminated clothing. Wash hands before breaks and after work. When using do not eat, drink,

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smoke, sniff. Avoid contact with skin, eyes and clothes. Provide adequate ventilation.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container tightly closed in a cool, well-ventilated place.
Handle and store contents under inert gas. Protect from moisture.
storage temperature: +2°C - 8°C

Hints on joint storage

No special measures are necessary.

7.3. Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8: Exposure controls/personal protection**8.1. Control parameters****Additional advice on limit values**

To date, no national critical limit values exist.

8.2. Exposure controls**Appropriate engineering controls**

The receiver of our product is singularly responsible for adhering to existing laws and regulations.

Individual protection measures, such as personal protective equipment**Eye/face protection**

Wear eye protection/face protection.
Tightly fitting safety goggles. Face shield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. Wear suitable gloves.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Skin protection

Use of protective clothing.

Respiratory protection

In case of inadequate ventilation wear respiratory protection. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Thermal hazards

No data available

Environmental exposure controls

Discharge into the environment must be avoided.

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SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state:	solid	
Colour:	white/ whitish	
Odour:	No data available	
Odour threshold:	No data available	
Melting point/freezing point:		No data available
Boiling point or initial boiling point and boiling range:		No data available
Flammability:		not determined
Lower explosion limits:		No data available
Upper explosion limits:		No data available
Flash point:		No data available
Auto-ignition temperature:		No data available
Decomposition temperature:		No data available
pH-Value:		No data available
Viscosity / kinematic:		not applicable
Water solubility:		No data available
Solubility in other solvents		
not determined		
Dissolution rate:		No data available
Partition coefficient n-octanol/water:		No data available
Dispersion stability:		No data available
Vapour pressure:		No data available
Density:		No data available
Relative density:		No data available
Bulk density:		No data available
Relative vapour density:		No data available
Particle characteristics:		No data available

9.2. Other information**Information with regard to physical hazard classes**

Explosive properties

Product is not dust explosive in its original delivery form. The addition of particulate matter, however, results in a dust explosion risk.

Sustaining combustion: No data available

Self-ignition temperature

Solid: No data available

Gas: not applicable

Oxidizing properties

No data available

Other safety characteristics

Solvent content: No data available

Viscosity / dynamic: not applicable

Flow time: not applicable

SECTION 10: Stability and reactivity**10.1. Reactivity**

No data available

10.2. Chemical stability

Stable under recommended storage conditions.

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10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoidProtect from moisture.
Keep away from heat.**10.5. Incompatible materials**

Oxidizing agents, strong.

10.6. Hazardous decomposition productsThermal decomposition can lead to the escape of irritating gases and vapours.
In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).**Further information**

In case of fire: See chapter 5.

SECTION 11: Toxicological information**11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008****Toxicokinetics, metabolism and distribution**

No data available

Acute toxicity

Based on available data, the classification criteria are not met.

Irritation and corrosivitySkin corrosion/irritation: Based on available data, the classification criteria are not met.
Serious eye damage/eye irritation: Based on available data, the classification criteria are not met.**Sensitising effects**

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproductionGerm cell mutagenicity: Based on available data, the classification criteria are not met.
Carcinogenicity: Based on available data, the classification criteria are not met.
Reproductive toxicity: Based on available data, the classification criteria are not met.
IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.**STOT-single exposure**

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

The substance is classified as not hazardous according to regulation (EC) No 1272/2008 [CLP].

Practical experience

No data available

11.2. Information on other hazards**Endocrine disrupting properties**

No data available

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Further information

RTECS: No data available

To our knowledge, the chemical, physical and toxicological properties have not been extensively studied. Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information**12.1. Toxicity**

Based on available data, the classification criteria are not met.

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No data available

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Warning - substance not yet tested completely.

Further information

Avoid release to the environment.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

Handle contaminated packages in the same way as the substance itself.

Contaminated packaging

Wash with plenty of water. Completely emptied packages can be recycled.

SECTION 14: Transport information**Land transport (ADR/RID)****14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

Inland waterways transport (ADN)**14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

Marine transport (IMDG)**14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

Air transport (ICAO-TI/IATA-DGR)**14.2. UN proper shipping name:**

No dangerous good in sense of these transport regulations.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No information available.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

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SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**Information according to Directive
2012/18/EU (SEVESO III):

Not subject to 2012/18/EU (SEVESO III)

Additional information

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH)

National regulatory information

Water hazard class (D):

3 - highly hazardous to water

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

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Abbreviations and acronyms

ADR: Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road).
IMDG: International Maritime Code for Dangerous Goods
IATA: International Air Transport Association
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service
LC50: Lethal concentration, 50%
LD50: Lethal dose, 50%
CLP: Classification, labelling and Packaging
REACH: Registration, Evaluation and Authorization of Chemicals
GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals
UN: United Nations
CAS: Chemical Abstracts Service
DNEL: Derived No Effect Level
DMEL: Derived Minimal Effect Level
PNEC: Predicted No Effect Concentration
ATE: Acute toxicity estimate
LL50: Lethal loading, 50%
EL50: Effect loading, 50%
EC50: Effective Concentration 50%
ErC50: Effective Concentration 50%, growth rate
NOEC: No Observed Effect Concentration
BCF: Bio-concentration factor
PBT: persistent, bioaccumulative, toxic
vPvB: very persistent, very bioaccumulative
RID: Regulations concerning the international carriage of dangerous goods by rail
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures)
EmS: Emergency Schedules
MFAG: Medical First Aid Guide
IATA: International Air Transport Association
ICAO: International Civil Aviation Organization
MARPOL: International Convention for the Prevention of Marine Pollution from Ships
IBC: Intermediate Bulk Container
SVHC: Substance of Very High Concern
For abbreviations and acronyms, see table at <http://abbrev.esdscom.eu>

Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.