

# Safety data sheet

according to 1907/2006/EC, Article 31

Printing date 18.07.2021

Revision: 18.07.2021

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### · 1.1 Product identifier

· **Trade name:** (S)-2-[[3,5-Bis(trifluoromethyl)phenyl]thioureido]-N-benzyl-N,3,3-trimethylbutanamide, 98%, (99% ee)

· **Item number:** 07-1417

· **CAS Number:**  
959979-30-7

· **1.2 Relevant identified uses of the substance or mixture and uses advised against**  
No further relevant information available.

### · 1.3 Details of the supplier of the safety data sheet

#### · **Manufacturer/Supplier:**

Strem Chemicals, Inc.  
7 Mulliken Way  
NEWBURYPORT, MA 01950  
USA  
info@strem.com

· **Further information obtainable from:** Technical Department

#### · 1.4 Emergency telephone number:

EMERGENCY: CHEMTREC: + 1 (800) 424-9300  
During normal opening times: +1 (978) 499-1600

## SECTION 2: Hazards identification

### · 2.1 Classification of the substance or mixture

· **Classification according to Regulation (EC) No 1272/2008**  
The substance is not classified according to the CLP regulation.

### · 2.2 Label elements

· **Labelling according to Regulation (EC) No 1272/2008** Void

· **Hazard pictograms** Void

· **Signal word** Void

· **Hazard statements** Void

· **Precautionary statements**

P262 Do not get in eyes, on skin, or on clothing.

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.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

### · 2.3 Other hazards

· **Results of PBT and vPvB assessment**

· **PBT:** Not applicable.

· **vPvB:** Not applicable.

## SECTION 3: Composition/information on ingredients

### · 3.1 Chemical characterisation: Substances

#### · **CAS No. Description**

959979-30-7 (R)-2-[[3,5-Bis(trifluoromethyl)phenyl]thioureido]-N-benzyl-N,3,3-trimethylbutanamide, 98%, (99% ee)

GB

(Contd. on page 2)

**Safety data sheet**  
according to 1907/2006/EC, Article 31

Printing date 18.07.2021

Revision: 18.07.2021

**Trade name:** (S)-2-[[3,5-Bis(trifluoromethyl)phenyl]thioureido]-N-benzyl-N,3,3-trimethylbutanamide, 98%, (99% ee)

(Contd. of page 1)

**SECTION 4: First aid measures**

- **4.1 Description of first aid measures**
- **General information:** No special measures required.
- **After inhalation:** Supply fresh air; consult doctor in case of complaints.
- **After skin contact:** Generally the product does not irritate the skin.
- **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
- **After swallowing:** If symptoms persist consult doctor.
- **4.2 Most important symptoms and effects, both acute and delayed** No further relevant information available.
- **4.3 Indication of any immediate medical attention and special treatment needed**  
No further relevant information available.

**SECTION 5: Firefighting measures**

- **5.1 Extinguishing media**
- **Suitable extinguishing agents:** Use fire extinguishing methods suitable to surrounding conditions.
- **5.2 Special hazards arising from the substance or mixture** No further relevant information available.
- **5.3 Advice for firefighters**
- **Protective equipment:** No special measures required.

**SECTION 6: Accidental release measures**

- **6.1 Personal precautions, protective equipment and emergency procedures** Not required.
- **6.2 Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **6.3 Methods and material for containment and cleaning up:**  
Dispose contaminated material as waste according to item 13.
- **6.4 Reference to other sections**  
See Section 7 for information on safe handling.  
See Section 8 for information on personal protection equipment.  
See Section 13 for disposal information.

**SECTION 7: Handling and storage**

- **7.1 Precautions for safe handling** No special measures required.
- **Information about fire - and explosion protection:** No special measures required.
- **7.2 Conditions for safe storage, including any incompatibilities**
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** None.
- **7.3 Specific end use(s)** No further relevant information available.

**SECTION 8: Exposure controls/personal protection**

- **Additional information about design of technical facilities:** No further data; see item 7.
- **8.1 Control parameters**
- **Ingredients with limit values that require monitoring at the workplace:** Not required.

(Contd. on page 3)

**Safety data sheet**  
according to 1907/2006/EC, Article 31

Printing date 18.07.2021

Revision: 18.07.2021

**Trade name:** (S)-2-[[3,5-Bis(trifluoromethyl)phenyl]thioureido]-N-benzyl-N,3,3-trimethylbutanamide, 98%, (99% ee)

(Contd. of page 2)

- **Additional information:** The lists valid during the making were used as basis.
- **8.2 Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**  
The usual precautionary measures are to be adhered to when handling chemicals.
- **Respiratory protection:** Not required.
- **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.  
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

- **Material of gloves**  
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material**  
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
- **Eye protection:** Safety glasses

· **9.1 Information on basic physical and chemical properties**

· **General Information**

· **Appearance:**

<b>Form:</b>	Powder
<b>Colour:</b>	Whitish
<b>Odour:</b>	Characteristic
<b>Odour threshold:</b>	Not determined.

· **pH-value:** Not applicable.

· **Change in condition**

<b>Melting point/freezing point:</b>	Undetermined.
<b>Initial boiling point and boiling range:</b>	Undetermined.

· **Flash point:** Not applicable.

· **Flammability (solid, gas):** Product is not flammable.

· **Ignition temperature:**

**Decomposition temperature:** Not determined.

· **Auto-ignition temperature:** Not determined.

· **Explosive properties:** Product does not present an explosion hazard.

· **Explosion limits:**

<b>Lower:</b>	Not determined.
<b>Upper:</b>	Not determined.

· **Vapour pressure:** Not applicable.

· **Density:** Not determined.

· **Relative density** Not determined.

· **Vapour density** Not applicable.

(Contd. on page 4)

**Safety data sheet**  
according to 1907/2006/EC, Article 31

Printing date 18.07.2021

Revision: 18.07.2021

**Trade name:** (S)-2-[[3,5-Bis(trifluoromethyl)phenyl]thioureido]-N-benzyl-N,3,3-trimethylbutanamide, 98%, (99% ee)

(Contd. of page 3)

· <b>Evaporation rate</b>	Not applicable.
· <b>Solubility in / Miscibility with water:</b>	Insoluble.
· <b>Partition coefficient: n-octanol/water:</b>	Not determined.
· <b>Viscosity:</b>	
<b>Dynamic:</b>	Not applicable.
<b>Kinematic:</b>	Not applicable.
· <b>Solvent content:</b>	
<b>Organic solvents:</b>	0.0 %
<b>VOC (EC)</b>	0.00 %
· <b>9.2 Other information</b>	No further relevant information available.

### SECTION 10: Stability and reactivity

- **10.1 Reactivity** No further relevant information available.
- **10.2 Chemical stability**
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- **10.3 Possibility of hazardous reactions** No dangerous reactions known.
- **10.4 Conditions to avoid** No further relevant information available.
- **10.5 Incompatible materials:** No further relevant information available.
- **10.6 Hazardous decomposition products:** No dangerous decomposition products known.

### SECTION 11: Toxicological information

- **11.1 Information on toxicological effects**
- **Acute toxicity** Based on available data, the classification criteria are not met.
- **Primary irritant effect:**
- **Skin corrosion/irritation** Based on available data, the classification criteria are not met.
- **Serious eye damage/irritation** Based on available data, the classification criteria are not met.
- **Respiratory or skin sensitisation** Based on available data, the classification criteria are not met.
- **CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)**
- **Germ 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.
- **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.

### SECTION 12: Ecological information

- **12.1 Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **12.2 Persistence and degradability** No further relevant information available.
- **12.3 Bioaccumulative potential** No further relevant information available.
- **12.4 Mobility in soil** No further relevant information available.

(Contd. on page 5)

**Safety data sheet**  
according to 1907/2006/EC, Article 31

Printing date 18.07.2021

Revision: 18.07.2021

**Trade name:** (S)-2-[[3,5-Bis(trifluoromethyl)phenyl]thioureido]-N-benzyl-N,3,3-trimethylbutanamide, 98%, (99% ee)

(Contd. of page 4)

- **Additional ecological information:**
- **General notes:**  
Water hazard class 1 (German Regulation) (Self-assessment): slightly hazardous for water  
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.
- **12.5 Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **12.6 Other adverse effects** No further relevant information available.

**SECTION 13: Disposal considerations**

- **13.1 Waste treatment methods**
- **Recommendation** Disposal must be made according to official regulations.
- **Uncleaned packaging:**
- **Recommendation:** Disposal must be made according to official regulations.

**SECTION 14: Transport information**

- |  |                 |
|--|-----------------|
| · <b>14.1 UN-Number</b>  |                 |
| · <b>ADR, ADN, IMDG, IATA</b>  | not regulated   |
| · <b>14.2 UN proper shipping name</b>  |                 |
| · <b>ADR, ADN, IMDG, IATA</b>  | not regulated   |
| · <b>14.3 Transport hazard class(es)</b>   |                 |
| · <b>ADR, ADN, IMDG, IATA</b>  |                 |
| · <b>Class</b>   | not regulated   |
| · <b>14.4 Packing group</b>  |                 |
| · <b>ADR, IMDG, IATA</b>   | not regulated   |
| · <b>14.5 Environmental hazards:</b>   | Not applicable. |
| · <b>14.6 Special precautions for user</b>                                       | Not applicable. |
| · <b>14.7 Transport in bulk according to Annex II of Marpol and the IBC Code</b> | Not applicable. |
| · <b>UN "Model Regulation":</b>  | not regulated   |

**SECTION 15: Regulatory information**

- **15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
- **Directive 2012/18/EU**
- **Named dangerous substances - ANNEX I** Substance is not listed.
- **National regulations:**
- **Waterhazard class:** Water hazard class 1 (Self-assessment): slightly hazardous for water.
- **15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

GB

(Contd. on page 6)

**Safety data sheet**  
according to 1907/2006/EC, Article 31

Printing date 18.07.2021

Revision: 18.07.2021

**Trade name: (S)-2-[[3,5-Bis(trifluoromethyl)phenyl]thioureido]-N-benzyl-N,3,3-trimethylbutanamide, 98%, (99% ee)**

(Contd. of page 5)

**SECTION 16: Other information**

*This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.*

· **Department issuing SDS:** Technical Department.

· **Contact:** Technical Director

· **Abbreviations and acronyms:**

*ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)*

*IMDG: International Maritime Code for Dangerous Goods*

*IATA: International Air Transport Association*

*GHS: Globally Harmonised System of Classification and Labelling of Chemicals*

*CAS: Chemical Abstracts Service (division of the American Chemical Society)*

*VOC: Volatile Organic Compounds (USA, EU)*

*PBT: Persistent, Bioaccumulative and Toxic*

*vPvB: very Persistent and very Bioaccumulative*

GB