SAFETY DATA SHEET

According to JIS Z 7253:2019
Revision date 27-Feb-2024
Revision Number 13.04

Section 1: PRODUCT AND COMPANY IDENTIFICATION

Product Name	(S,S)-3,4,5-Trifluorophenyl-NAS Bromide)
Product Code	201-16401,207-16403

Supplier
FUJIFILM Wako Pure Chemical Corporation
1-2 Doshomachi 3-Chome, Chuo-ku, Osaka 540-8605, Japan
Phone: +81-6-6203-3741
Fax: +81-6-6203-2029

Emergency telephone number +81-6-6203-3741 / +81-3-3270-8571
Recommended uses For research use only
Restrictions on use Seek expert judgment when using for purposes other than those recommended.

Section 2: HAZARDS IDENTIFICATION

GHS classification
Classification of the substance or mixture

Carcinogenicity	Category 1A
Reproductive Toxicity	Category 1A
Specific target organ toxicity (repeated exposure)	Category 2

Pictograms

Signal word Danger

Hazard statements
H350 - May cause cancer
H360 - May damage fertility or the unborn child
H373 - May cause damage to organs through prolonged or repeated exposure

Precautionary statements-(Prevention)
- Obtain special instructions before use
- Do not handle until all safety precautions have been read and understood
- Use personal protective equipment as required
- Do not breathe dust/fume/gas/mist/vapors/spray

Precautionary statements-(Response)
- IF exposed or concerned: Get medical advice/attention

Precautionary statements-(Storage)
- Store locked up

Precautionary statements-(Disposal)
- Dispose of contents/container to an approved waste disposal plant

Others
Other hazards Not available

Section 3: COMPOSITION/INFORMATION ON INGREDIENTS

Single Substance or Mixture Substance

Formula C56H34BrF6N

Chemical Name	Weight-%	Molecular weight	ENCS	ISHL No.	CAS RN
(S,S)-3,4,5-Trifluorophenyl-NAS Bromide)	=<100	914.77	N/A	N/A	287384-12-7
Hexane	<2	86.18	(2)-6	*	110-54-3
Methanol	<1	32.04	(2)-201	*	67-56-1

Note on ISHL No.: * in the table means announced chemical substances.

Impurities and/or Additives： Impurities :, Hexane, Methanol

Section 4: FIRST AID MEASURES

Inhalation
Remove to fresh air. If symptoms persist, call a physician.
Skin contact
Wash off immediately with soap and plenty of water. If symptoms persist, call a physician.
Eye contact
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediate medical attention is required.
Ingestion
Rinse mouth. Never give anything by mouth to an unconscious person. Call a physician or poison control center immediately. Do not induce vomiting without medical advice.
Protection of first-aiders
Use personal protective equipment as required.

Section 5: FIRE FIGHTING MEASURES

Suitable extinguishing media
Water spray (fog), Carbon dioxide (CO2), Foam, Extinguishing powder, Sand
Unsuitable extinguishing media
No information available
Specific hazards arising from the chemical product
Thermal decomposition can lead to release of irritating and toxic gases and vapors.
Special extinguishing method
No information available
Special protective actions for fire-fighters
Use personal protective equipment as required. Firefighters should wear self-contained breathing apparatus and full firefighting turnout gear.

Section 6: ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures
For indoor, provide adequate ventilation process until the end of working. Deny unnecessary entry other than the people involved by, for example, using a rope. While working, wear appropriate protective equipments to avoid adhering it on skin, or inhaling the gas. Work from windward, and retract the people downwind.
Environmental precautions
To be careful not discharged to the environment without being properly handled waste water contaminated.
Methods and materials for contaminent and methods and materials for cleaning up
Sweep up and gather scattered particles, and collect it in an empty airtight container.
Recoverly, neutralization
No information available

Secondary disaster prevention measures

Clean contaminated objects and areas thoroughly observing environmental regulations.

Section 7: HANDLING AND STORAGE

Handling

Technical measures

Avoid contact with strong oxidizing agents. Use with local exhaust ventilation.

Precautions

Do not rough handling containers, such as upsetting, falling, giving a shock, and dragging. Prevent leakage, overflow, and scattering. Not to generate steam and dust in vain. Seal the container after use. After handling, wash hands and face, and then gargle. In places other than those specified, should not be smoking or eating and drinking. Should not be brought contaminated protective equipment and gloves to rest stops. Deny unnecessary entry of non-emergency personnel to the handling area.

Safety handling precautions

Avoid contact with skin, eyes or clothing. Use personal protective equipment as required.

Storage

Safe storage conditions

Storage conditions Keep container protect from light, store in well-ventilated place at room temperature (preferably cool). Keep container tightly closed.

Safe packaging material Glass

Incompatible substances Strong oxidizing agents

Section 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

Engineering controls

In case of indoor workplace, seal the source or use a local exhaust system. Provide the safety shower facility, and hand- and eye-wash facility. And display their position clearly.

Exposure limits

Chemical Name	JSOH (Japan)	ISHL (Japan)	ACGIH
Hexane 110-54-3	TWA: 40 ppm OEL TWA: 140 mg/m³ OEL Skin ISHL/ACL: 40 ppm	ISHL/ACL: 40 ppm	TWA: 50 ppm Skin
Methanol 67-56-1	TWA: 200 ppm OEL TWA: 260 mg/m³ OEL Skin ISHL/ACL: 200 ppm	200ppm	TWA 200ppm(260mg/m³) STEL 250ppm

Personal protective equipment

Respiratory protection Dust mask (JIS T 8151)

Hand protection chemical protective gloves (JIS T 8116)

Eye protection protective eyeglasses or chemical safety goggles (JIS T 8147)

Skin and body protection Long-sleeved work clothes

General hygiene considerations

Handle in accordance with good industrial hygiene and safety practice.

If this product is classified as ”Chemical Substances Hazardous to Skin, etc.”, use appropriate protective equipment to them.

Section 9: PHYSICAL AND CHEMICAL PROPERTIES

Form

Color White - brown

Appearance crystals - powder

Odor	no data available
Melting point/freezing point	no data available
Boiling point, initial boiling point and boiling range	no data available
Flammability	no data available
Evaporation rate:	no data available
Flammability (solid, gas):	no data available
Upper/lower flammability or explosive limits	
Upper:	no data available
Lower:	no data available
Flash point	no data available
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH	no data available
Viscosity (coefficient of viscosity)	no data available
Dynamic viscosity	no data available
Solubilities	chloroform : soluble .
n-Octanol/water partition coefficient:(log Pow)	no data available
Vapour pressure	no data available
Specific Gravity / Relative density	no data available
Vapour density	no data available
Particle characteristics	no data available

Section 10: STABILITY AND REACTIVITY

Stability

Reactivity	no data available
Chemical stability	May be altered by light.

Hazardous reactions

None under normal processing

Conditions to avoid

Extremes of temperature and direct sunlight

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

Carbon monooxide (CO), Carbon dioxide (CO_2), Nitrogen oxides (NOx), Halides

Section 11: TOXICOLOGICAL INFORMATION

Described about residual hazardous components.

Acute toxicity

Chemical Name	Oral LD50	Dermal LD50	Inhalation LC50
Hexane	15800 mg/kg (Rat)	3297 mg/kg (Rabbit)	48000 ppm (Rat) 4 h
Methanol	1400 mg/kg (Human)	15800 mg/kg (Rabbit)	>31500 ppm (Rat) 4 h (vapor)

Chemical Name	Acute toxicity -oral- source information	Acute toxicity -dermal- source information	Acute toxicity -inhalation gas- source information
Hexane	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.

Chemical Name	Acute toxicity -inhalation vapor- source information	Acute toxicity -inhalation dust- source information	Acute toxicity -inhalation mist- source information
Hexane	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS	Based on the NITE GHS	Based on the NITE GHS

	Classification results.	classification results.	classification results.

Skin irritation/corrosion

Chemical Name	Skin corrosion/irritation source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

Serious eye damage/ irritation

Chemical Name	Serious eye damage/irritation source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

Respiratory or skin sensitization

Chemical Name	Respiratory or Skin sensitization source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

Reproductive cell mutagenicity

Chemical Name	germ cell mutagencity source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

Carcinogenicity

Chemical Name	Carcinogenicity source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

Reproductive toxicity

Chemical Name	Reproductive toxicity source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

STOT-single exposure

Chemical Name	STOT -single exposure- source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

STOT-repeated exposure

Chemical Name	STOT -repeated exposure- source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

Aspiration hazard

Chemical Name	Aspiration Hazard source information
Hexane	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification results.

Section 12: ECOLOGICAL INFORMATION

Described about residual hazardous components.

Ecotoxicity

Chemical Name	Algae/aquatic plants	Fish	Crustacea
Hexane	*N/A*	*LC50:Pimephales promelas 2.1 - 2.98 mg/L 96 h*	*LC50 : Daphnia magna 3.88 mg/L 48 h*
Methanol	*N/A*	*LC50 : Lepomis macrochirus 15400 mg/L 96 h*	*LC50 : Artemia 1340 mg/L 96 h*

Other data

Chemical Name	Short-term (acute) hazardous to the aquatic environment source information	Long-term (chronic) hazardous to the aquatic environment source information
Hexane	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.
Methanol	Based on the NITE GHS classification	Based on the NITE GHS classification

	results.	results.

Persistence and degradability No information available
Bioaccumulative potential No information available
Mobility in soil No information available
Hazard to the ozone layer No information available

Section 13: DISPOSAL CONSIDERATIONS

Waste from residues
Disposal should be in accordance with applicable regional, national and local laws and regulations.
Contaminated container and contaminated packaging
Disposal should be in accordance with applicable regional, national and local laws and regulations.

Section 14: TRANSPORT INFORMATION

ADR/RID Not regulated
UN number -
Proper shipping name:
UN classfication
Subsidiary hazard class
Packing group
Marine pollutant Not applicable

IMDG Not regulated
UN number -
Proper shipping name:
UN classfication
Subsidiary hazard class
Packing group
Marine pollutant (Sea) Not applicable
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code No information available

IATA Not regulated
UN number -
Proper shipping name:
UN classfication
Subsidiary hazard class
Packing group
Environmentally Hazardous Substance Not applicable

Section 15: REGULATORY INFORMATION

Japanese regulations
Fire Service Act Not applicable
Poisonous and Deleterious Substances Control Law Not applicable
Industrial Safety and Health Act Harmful Substances Whose Names Are to be Indicated on the Label (Law Art.57)
Notifiable Substances (Law Art.57-2)
Industrial Safety and Health Act (2024~) 【2024.4.1~】Chemical Substances Hazardous to Skin, etc.(Regulations Article 594-2 Paragraph 1)
Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc Priority Assessment Chemical Substances (Law Article 2, Para.5)
Regulations for the carriage Not applicable

and storage of dangerous goods in ship	
Civil Aeronautics Law	Not applicable
Pollutant Release and Transfer Register Law (2023.4.1-)	Class 1
Class 1 - No.	392
Export Trade Control Order	Not applicable

Chemical Name	Poisonous and Deleterious Substances Control Law	Industrial Safety and Health Act Substances (Law Art.57-2)	Pollutant Release and Transfer Register Law (2023.4.1-)
Hexane 110-54-3 (<2)	-	Applicable	Applicable
Methanol 67-56-1 (<1)	-	Applicable	-

Section 16: OTHER INFORMATION

Key literature references and sources for data etc.

NITE: National Institute of Technology and Evaluation (JAPAN)
http://www.safe.nite.go.jp/japan/db.html
IATA dangerous Goods Regulations
RTECS:Registry of Toxic Effects of Chemical Substances
Japan Industrial Safety and Health Association GHS Model SDS
Dictionary of Synthetic Oraganic Chemistry , SSOCJ, Koudansha Scientific Co.Ltd.
Chemical Dictionary, Kyouritsu Publishing Co., Ltd.
etc

Record of SDS revisions

The following contents were revised. Regulatory information.

Disclaimer

This SDS is according to JIS Z 7253: 2019. 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, 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.
GHS Classification is according to JIS Z 7252:2019. *JIS: Japanese Industrial Standards

End of Safety Data Sheet