

SAFETY DATA SHEET

According to JIS Z 7253:2019
Revision date 04-Apr-2022
 Revision Number 2.02

Section 1: PRODUCT AND COMPANY IDENTIFICATION

Product Name	(R,R)-3,4,5-Trifluorophenyl-NAS Bromide
Product Code	201-15921,207-15923

Manufacturer	FUJIFILM Wako Pure Chemical Corporation 1-2 Doshomachi 3-Chome Chuo-ku, Osaka 540-8605, Japan Phone: +81-6-6203-3741 Fax: +81-6-6203-5964
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 and restrictions on use	For research use only

Section 2: HAZARDS IDENTIFICATION

GHS classification

Classification of the substance or mixture**Specific target organ toxicity (repeated exposure)**

Category 2

Category 2 nervous system, central nervous system, ears

Acute aquatic toxicity

Category 2

Chronic aquatic toxicity

Category 2

Pictograms



Signal word

Warning

Hazard statements

H401 - Toxic to aquatic life

H411 - Toxic to aquatic life with long lasting effects

H373 - May cause damage to the following organs through prolonged or repeated exposure: nervous system, central nervous system, ears

Precautionary statements-(Prevention)

- Do not breathe dust/fume/gas/mist/vapors/spray
- Avoid release to the environment

Precautionary statements-(Response)

- Get medical advice/attention if you feel unwell
- Collect spillage

Precautionary statements-(Storage)

- Not applicable

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
(R,R)-3,4,5-Trifluorophenyl-NAS Bromide	=<96	914.77	N/A	N/A	534570-50-8
n-Heptane	=<3	100.20	(2)-7	*	142-82-5
1-Butanol	=<1	74.12	(2)-3049	2-(8)-299	71-36-3

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

Impurities and/or Additives: residue, Heptane =<3%, 1-Butanol =<1%

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 contaminant and methods and materials for cleaning up

Sweep up and gather scattered particles, and collect it in an empty airtight container.

Recovery, 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

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

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
n-Heptane 142-82-5	TWA: 200 ppm OEL TWA: 820 mg/m ³ OEL	N/A	STEL: 500 ppm TWA: 400 ppm
1-Butanol 71-36-3	50ppm(150mg/m ³)	ISHL/ACL: 25 ppm	TWA: 20 ppm

Personal protective equipment**Respiratory protection**

Dust mask

Hand protection

Protection gloves

Eye protection

protective eyeglasses or chemical safety goggles

Skin and body protection

Long-sleeved work clothes

General hygiene considerations

Handle in accordance with good industrial hygiene and safety practice.

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 monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Halides

Section 11: TOXICOLOGICAL INFORMATION

Acute toxicity

Chemical Name	Oral LD50	Dermal LD50	Inhalation LC50
n-Heptane	5,000 mg/kg (Mouse)	3,000 mg/kg (Rabbit)	103 g/m ³ (Rat)
1-Butanol	700 mg/kg (Rat) 790 mg/kg (Rat)	3400 mg/kg (Rabbit) 3402 mg/kg (Rabbit)	> 8000 ppm (Rat) 4 h

Chemical Name	Acute toxicity -oral- source information	Acute toxicity -dermal- source information	Acute toxicity -inhalation gas-source information
n-Heptane	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.
1-Butanol	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
n-Heptane	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS Classification results.

Skin irritation/corrosion

Chemical Name	Skin corrosion/irritation source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

Serious eye damage/ irritation

Chemical Name	Serious eye damage/irritation source information
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n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

Respiratory or skin sensitization

Chemical Name	Respiratory or Skin sensitization source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

Reproductive cell mutagenicity

Chemical Name	germ cell mutagenicity source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

Carcinogenicity

Chemical Name	Carcinogenicity source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

Reproductive toxicity

Chemical Name	Reproductive toxicity source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

STOT-single exposure

Chemical Name	STOT -single exposure- source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

STOT-repeated exposure

Chemical Name	STOT -repeated exposure- source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

Aspiration hazard

Chemical Name	Aspiration Hazard source information
n-Heptane	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.

Section 12: ECOLOGICAL INFORMATION

Ecotoxicity

Chemical Name	Algae/aquatic plants	Fish	Crustacea
n-Heptane	N/A	LC50 : Cichlid Fish 375.0 mg/L 96 h	LC50 : Mysidopsis bahia 0.1 mg/L 96 h
1-Butanol	ErC50 : Pseudokirchneriella subcapitata >1,000 mg/L 72 h	LC50 : Oryzias latipes > 1,000 mg/L 96 h	EC50 : Daphnia magna > 1,000 mg/L 48 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
n-Heptane	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.
1-Butanol	Based on the NITE GHS classification results.	Based on the NITE GHS classification 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
Mobility	

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

UN number	UN3077
Proper shipping name:	Environmentally hazardous substance, solid, n.o.s. (Mixture of n-Heptane and (R,R)-3,4,5-Trifluorophenyl-NAS Bromide)
UN classification	9
Subsidiary hazard class	
Packing group	III
Marine pollutant	Yes

IMDG

UN number	UN3077
Proper shipping name:	Environmentally hazardous substance, solid, n.o.s. (Mixture of n-Heptane and (R,R)-3,4,5-Trifluorophenyl-NAS Bromide)
UN classification	9
Subsidiary hazard class	
Packing group	III
Marine pollutant (Sea)	Yes
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	No information available

IATA

UN number	UN3077
Proper shipping name:	Environmentally hazardous substance, solid, n.o.s. (Mixture of n-Heptane and (R,R)-3,4,5-Trifluorophenyl-NAS Bromide)
UN classification	9
Subsidiary hazard class	
Packing group	III
Environmentally Hazardous Substance	Yes

Section 15: REGULATORY INFORMATION

International Inventories

EINECS/ELINCS	Listed
TSCA	Listed

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, Para.1, Enforcement Order Art.18) Notifiable Substances (Law Art.57-2, Enforcement Order Art.18-2 Attached Table No.9)No.477,526
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 and storage of dangerous goods in ship	Noxious Substances (Ordinance Art.3, Ministry of Transportation Ordinance Regarding Transport by Ship and Storage, Attached Table 1)
Civil Aeronautics Law	Misellaneous Dangerous Substances and Articles (Ordinance Art.194, MITL Notification for Air Transportation of Explosives etc., Attached Table 1)

Marine Pollution Prevention Law	Enforcement ordinance Appendix No. 1 Noxious liquid substance	Category X
Pollutant Release and Transfer Register Law (~2023.3.31)	Enforcement ordinance Appendix No. 1 Noxious liquid substance	Category Z
Pollutant Release and Transfer Register Law (2023/4/1~)	Class 1	
Class 1 - No.	731	
Export Trade Control Order	Not applicable	

Chemical Name	Poisonous and Deleterious Substances Control Law	Industrial Safety and Health Act Substances (Law Art.57-2) (~2024.3.31)	Pollutant Release and Transfer Register Law (~2023.3.31)
n-Heptane 142-82-5 (=<3)	-	Applicable	-
1-Butanol 71-36-3 (=<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 Organic Chemistry , SSOCJ, Koudansha Scientific Co.Ltd.
 Chemical Dictionary, Kyouritsu Publishing Co., Ltd.
 etc

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 Z7252(2019). *JIS: Japanese Industrial Standards

End of Safety Data Sheet