

Safety Data Sheet

1. CHEMICALS AND COMPANY IDENTIFICATION

Company name : National Institute of Advanced Industrial Science and Technology (AIST)

Address : 1-3-1 Kasumigaseki, Chiyoda-ku, Tokyo

Department in charge : Reference Material Office, Center for Quality Management of Metrology, The National Metrology Institute of Japan

Person responsible : Person in charge of certified reference materials

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Arrangement number : 4601001

Name of chemical : Reference material NMIJ CRM 4601-a 3,5-Bis (trifluoromethyl) benzoic acid
(3,5-Bis (trifluoromethyl) benzoic acid)

Recommended applications and limitations of use : This reference material is used for the calibration of signal intensity of ^1H and ^{19}F in quantitative assay using the nuclear magnetic resonance (NMR) method; it can be used for the validation of an assay method or assay device. This material shall not be used for purposes other than testing and research.

2. HAZARDS IDENTIFICATION

GHS classification: Skin corrosivity/irritation : Classification 2
Severe eye damage/irritation : Classification 2A

GHS-labeling element:



Signal word: Warning
Hazard and toxicity information: Skin irritation
Severe eye irritation

Other toxicity information: -

Cautionary statement: [Safety Measures]
Wash hands thoroughly after using.
Wear protective glasses/protective mask/protective gloves.
[Emergency Measures]

If in contact with eyes: Rinse with water carefully for several minutes. Then, if using contact lenses, take them off if possible, and continue rinsing. If eye irritation persists, seek medical attention and treatment.

If in contact with skin: Wash with plenty of water using soap. In case of skin irritation, seek medical attention and treatment.

Take off any contaminated clothes and wash them well before reuse.

[Storage]

Store in the dark at room temperature (15 °C to 25 °C) in a clean desiccator.

[Disposal]

Follow the related regulations and ordinances of the local government.

Use a waste-treatment firm certified by prefectural governor.

Classification is impossible or not applicable for hazards not mentioned above.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Single substance or compound	: Single substance
Chemical name	: 3,5-Bis (trifluoromethyl) benzoic acid
Synonyms	: 3,5-Di (trifluoromethyl) benzoic acid
Concentration	: 99 % or higher
Chemical or structural formula	: $C_9H_4F_6O_2$
Molecular weight	: 258.12
Reference number in the gazetted list in Japan	: Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc.: Not applicable Industrial Safety and Health Act: 4- (4) -1097
CAS number	: 725-89-3
Hazardous component	: None

4. FIRST-AID MEASURES

Eye contact	: Wash with clean water for at least 15 minutes, and then seek medical attention.
Skin contact	: Wash with clean water thoroughly. Take off any contaminated clothes and shoes. Immediately seek medical attention.
Inhalation	: Move to a place with fresh air. Rest and keep warm. Seek medical attention.
Ingestion	: Wash the mouth well with a lot of water to attenuate the effects. If the person is unconscious, do not give anything; Contact a physician.
Estimated acute and late symptom	: -

- Most important symptoms and effects : -
- Protection of first-aiders : Persons administering first-aid should wear rubber gloves and safety goggles.

5. FIRE-FIGHTING MEASURES

- Extinguishing media : Dry extinguishing agent, foam, water spray, carbonic anhydride, and dried sand.
- Specific hazards with regard to firefighting : Irritating or toxic fumes (or gas) may be generated in the event of fire.
- Specific methods of firefighting : Eliminate the origin of fire and put the fire out with extinguishing media. If possible, move containers to a safe place. If not, cool the peripheral areas with water spray.
- Protection for firefighters : Work from the windward side to prevent the inhalation of toxic gas. Use fire-prevention clothing, fireproof clothing, fire-protection clothing, respirator, circulating oxygen breathing apparatus, rubber gloves, and rubber boots.

6. ACCIDENTAL RELEASE MEASURES

- Personal precautions : Promptly remove all potential ignition sources from peripheral areas. In case of ignition, prepare the equipment for firefighting.
- Protective equipment and emergency measures : When accidental release takes place indoors, thoroughly clear the air until the emergency measures are complete. Before the operation, wear appropriate protective equipment to protect skin from droplets and to prevent inhalation of dust and gas.
- Environmental precautions : Prevent the released product from being drained into a river or other area that might cause environmental damage. Prevent the polluted discharge from being drained into the environment without being processed properly.
- Recovery and neutralization : Sweep and collect the leaked material and store it in an empty, sealable container. Wash and clean the spilled area with plenty of water.
- Prevention of the second accident : Surround the area with a rope, etc., to prevent unauthorized people from entering the area. Work from the windward side and evacuate people to the leeward side.

7. HANDLING AND STORAGE

- Handling
- Technical measures : Avoid contact with strong oxidants.
- Local ventilation and general ventilation : In case steam, mist, or powdered dust is generated, seal the source and provide local exhaust ventilation.
- Precautions for safe handling : Avoid rough handling such as dropping, shocking, dragging, or otherwise agitating the container.
Do not cause the substance to leak, overflow, or drift, and prevent powdered dust or steam from being generated.



Seal the container after use.

Wash hands, face, and other necessary parts thoroughly, and gargle after handling.

Do not eat, drink, or smoke in places other than the designated areas.

Do not bring gloves and other contaminated protective equipment into the break area.

Only authorized people should be allowed in the handling area.

Wear appropriate protective equipment to prevent inhalation, or contact with eyes, skin, or clothing.

When handling indoors, provide local exhaust ventilation.

Storage

- Appropriate storage conditions : Avoid direct sunlight and store in a well-ventilated, cool place.
- Incompatible materials : Do not store with oxidants or materials with a strong oxidizing nature.
- Safe packaging materials : Glass

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Standard control concentration

N/A

Threshold limit values

- ACGIH TLV-TWA : N/A
- Value recommended by Japanese Society of Occupational Health : N/A

Society of Occupational Health

- OSHA PEL TWA : N/A

Engineering controls

Ventilation and emission : Local ventilation equipment or general ventilation equipment

Safety management and gas detection : Measuring device, detection tube

Storage precautions : Ventilate along the floor surface and seal the container. Keep away from combustible/reducing materials and strong oxidants.

Protective equipment

Respiratory protection : Dust mask

Hand protection : Protective gloves

Eye protection : Protective glasses with side wall (goggle type as needed)

Skin and body protection : Long-sleeve protective clothing

Hygiene measures

Install facilities to wash the eyes and other body parts close to the site of use; install guide signs clearly indicating such facilities.

9. PHYSICAL AND CHEMICAL PROPERTIES

• Appearance	:	Powder
• Color	:	White
• Smell	:	No data
• pH	:	No data
• Melting point	:	142 °C to 143 °C
• Boiling point	:	No data
• Flashpoint	:	No data
• Explosion range	:	No data
• Steam pressure	:	No data
• Relative vapor density (air = 1)	:	No data
• Gravity (relative density)	:	1.71 g/cm ³
• Solubility	:	Soluble in ethanol and acetone; barely soluble in water
• n-octanol/water partition coefficient log P _{o/w}	:	No data
• Spontaneous ignition temperature	:	No data
• Decomposition temperature	:	No data
• Combustibility	:	No data

10. STABILITY AND REACTIVITY

- ◇ Stability
 - Stable under normal conditions
- ◇ Reactivity
 - Contact with strong oxidant causes the risk of ignition.
- ◇ Conditions to avoid
 - Sunlight, heat
- ◇ Hazardous decomposition products
 - Carbon monoxide, carbon dioxide, halides

11. TOXICOLOGICAL INFORMATION

Acute toxicity	Abdominal cavity mouse LD ₅₀ :100 mg/kg
Skin corrosivity/irritation	No data
Serious eye damage/eye irritation	No data
Germ-cell mutagenicity	No data
Carcinogenicity	No data

12. ECOLOGICAL INFORMATION

Degradability/Concentration

- No data

Bioaccumulation

- No data



Ecotoxicity
• No data

13. DISPOSAL CONSIDERATIONS

Residues : Comply with local, national, and on-site rules.
Contaminated containers and packaging : Comply with local, national, and on-site rules.

14. TRANSPORTATION INFORMATION

UN Dangerous Goods Number : Not applicable
UN classification : Not applicable
Product name : -
Packing group : -
ICAO/IATA : -
Marine pollutant : Not applicable
Matters to be attended to : Avoid direct sunlight. Prevent leakage and fires caused by shock or agitation to the container, and transport with caution.

15. REGULATORY INFORMATION

Not applicable

16. OTHER INFORMATION

Others

The information in this Safety Data Sheet is not intended to be exhaustive and is based on currently-available information and data. The precautions given in this data sheet are applicable only to normal handling conditions. When handling this reference material under special conditions etc., it is recommended to take safety precautions appropriate to each specific application and context of use. This Safety Data Sheet (SDS) is intended to provide information and not intended to guarantee anything in handling the reference material. This Safety Data Sheet (SDS) is prepared based on JIS Z7253, and presents identical information to Material Safety Data Sheet (MSDS) prepared based on JIS Z7250:2010.
