

Safety Data Sheet



1. Identification of the Substance/Mixture and the Supplier

Supplier : National Institute of Advanced Industrial Science and Technology (AIST)
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 Emergency Contact : Same as above

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ID Number : 4601002

Identity of Substance/Mixture : Certified reference material: NMIJ CRM 4601-b
 3,5-Bis (trifluoromethyl) benzoic acid
 Recommended Use of the Chemical and Restriction on Use : This reference material is used for the calibration of signal intensity of ¹H and ¹⁹F in quantitative assay using the nuclear magnetic resonance (NMR) method; it can be used for the validation of an assay method or assay device. Do not use this reference material for other purposes than testing/research. This CRM is a reference material (specified in the Japanese Industrial Standard (JIS) Q 0030).

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
 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

Substance or mixture	: 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

4. First-aid Measures

Inhalation	: Move to a place with fresh air. Rest and keep warm. Seek medical attention.
Skin contact	: Wash with clean water thoroughly. Take off any contaminated clothes and shoes. Immediately seek medical attention.
Eye contact	: Wash with clean water for at least 15 minutes, and then 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.
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, carbon dioxide, and dried sand.
Specific hazards with	: Irritating or toxic fumes (or gas) may be generated in the event of

- regard to firefighting : 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

※ Refer to the reference material certificate for the precaution statement regarding the appropriate condition of the storage and usage of the reference material.

8. Exposure Controls/Personal Protection

Standard control concentration

N/A

Threshold limit values

- ACGIH TLV-TWA : N/A
- Value recommended : N/A

by Japanese 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

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, etc. : Powder
- Color : White
- Odor : No data

- pH : No data
- Melting point : 142 °C to 143 °C
- Boiling point : No data
- Flashing point : No data
- Explosive range : No data
- Vapor pressure : No data
- Relative vapor density(Air=1) : No data
- Specific gravity or bulk specific gravity : 1.71 g/cm³
- Solubility : Soluble in ethanol and acetone; barely soluble in water
- *n*-Octanol/water partition coefficient (Log Po/w) : No data
- Auto-ignition temperature : No data
- Decomposition temperature : No data
- Flammability : No data

10. Stability and Reactivity

- Stability : Stable under recommended storage conditions
- Reactivity : Contact with strong oxidant causes the risk of ignition.
- Possibility of hazardous reaction : No data
- Conditions to avoid : Sunlight, heat
- Incompatible materials : No data
- Hazardous decomposition products : Carbon monoxide, carbon dioxide, halides

11. Toxicological Information

- Acute toxicity : Abdominal cavity mouse LD₅₀:100 mg/kg

12. Ecological Information

- Ecotoxicity : No data
- Persistence and Degradability : No data
- Bioaccumulative Potential : No data
- Mobility in soil : No data
- Influence to the ozone layer : No data

13. Disposal Considerations

- Residues : Dispose of in accordance with relevant laws and regulations of the country in which the material will be used.
Entrust disposal of this reference material to a professional waste disposal company licensed by prefectural government.
When entrusting waste disposal, entrust residues after adequately announcing the danger and hazard.
- Contaminated containers and packaging : To dispose of an empty container, completely remove the contents.
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14. Transport Information

- UN Dangerous Goods Number : Not applicable
UN classification : Not applicable
Product name : -
Packing group : -
ICAO/IATA : Not applicable
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.
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15. Regulatory Information

Not applicable

- © This SDS is originally prepared for the use of the material in Japan, thus the stated laws and regulations are stipulated and carried out in Japan. The use of the material in other countries should be referred to and by application of the relevant laws and regulations of the country in which the material will be used.
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16. Other Information

Others

The information in this document is not intended to be exhaustive and is based on currently available information and data. The measures given in this document are applicable only to normal handling conditions. When handling this reference material under special conditions etc., it is recommended to take safety measures appropriate to each specific application and context of use. This document is intended to provide information and not intended to guarantee anything in handling this reference material.
