

SAFETY DATA SHEET

According to JIS Z 7253:2019
Revision date 05-Mar-2024
 Revision Number 6.04

Section 1: PRODUCT AND COMPANY IDENTIFICATION

Product Name	Theobromine
Product Code	205-13562,209-13565

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**

Acute toxicity - Oral

Category 4

Germ cell mutagenicity

Category 2

Reproductive Toxicity

Category 1B

Specific target organ toxicity (single exposure)

Category 1

Pictograms**Signal word**

Danger

Hazard statements

- H302 - Harmful if swallowed
- H341 - Suspected of causing genetic defects
- H360 - May damage fertility or the unborn child
- H370 - Causes damage to organs

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
- Wash face, hands and any exposed skin thoroughly after handling
- Do not eat, drink or smoke when using this product
- Do not breathe dust/fume/gas/mist/vapors/spray

Precautionary statements-(Response)

- IF exposed: Call a POISON CENTER or doctor/physician
- IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
- Rinse mouth

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 C7H8N4O2

Chemical Name	Weight-%	Molecular weight	ENCS	ISHL No.	CAS RN
Theobromine	98.0	180.16	(9)-847	8-(2)-851	83-67-0

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

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

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

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

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

Appearance

powder

Odor

characteristic odor

Melting point/freezing point

347 °C

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	water , Ethanol and acetone : Very slightly 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 (CO ₂), Nitrogen oxides (NO _x)

Section 11: TOXICOLOGICAL INFORMATION

Acute toxicity

Chemical Name	Oral LD50	Dermal LD50	Inhalation LC50
Theobromine	950 mg/kg (Rat)	N/A	N/A

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

Serious eye damage/ irritation

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

Respiratory or skin sensitization

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

Reproductive cell mutagenicity

Chemical Name	germ cell mutagenicity source information

Theobromine	Based on the NITE GHS classification results.
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Carcinogenicity

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

Chemical Name	NTP	IARC	ACGIH	JSOH (Japan)
Theobromine 83-67-0		Group 3		

Reproductive toxicity

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

STOT-single exposure

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

STOT-repeated exposure

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

Aspiration hazard

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

Section 12: ECOLOGICAL INFORMATION

Ecotoxicity No information available

Other data

Chemical Name	Short-term (acute) hazardous to the aquatic environment source information	Long-term (chronic) hazardous to the aquatic environment source information
Theobromine	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

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 classification
Subsidiary hazard class
Packing group
Marine pollutant Not applicable

IMDG Not regulated
UN number -
Proper shipping name:

UN classification	
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 classification	
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	Not applicable
Industrial Safety and Health Act (2024-)	【2024.4.1~】 Harmful Substances Whose Names Are to be Indicated on the Label (Law Art.57) 【2024.4.1~】 Notifiable Substances (Law Art.57-2)
Regulations for the carriage and storage of dangerous goods in ship	Not applicable
Civil Aeronautics Law	Not applicable
Pollutant Release and Transfer Register Law (2023.4.1-)	Not applicable
Export Trade Control Order	Not applicable

Industrial Safety and Health Law

Law Name	Chemical Name in Regulation	Weight %	
Notifiable Substances (Law Art.57-2)	3,7-dimethylxanthine (alias: theobromine)	98.0	2024/4/1

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

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