

Safety Data Sheet

Theobromine

Version : V2.0.0.1

Report No. : BWJ4719-2016-MSDS-US

Creation Date : 2025/11/11

Revision Date : -



*Prepared according to American OSHA HCS-2024 (29 CFR 1910.1200)

1 Identification

Product identifier

Product Name	Theobromine
Cat No.	BWJ4719-2016
CAS No.	83-67-0
EC No.	201-494-2
Molecular Formula	C7H8N4O2

Recommended use of the product and restrictions on use

Relevant identified uses	Please consult manufacturer.
Uses advised against	Please consult manufacturer.

Details of the supplier of the Safety Data Sheet

Name of the company	Weiyel Inc
Address of the company	Hedian Light Industrial Park, Chengguan Town, Shangcheng County, Xinyang City, Henan Province, China
Post code	465350
Telephone number	010-58103678
Fax number	010-84840368
E-mail address	info@weiyel.com

Emergency phone number

Emergency phone number	010-58103678
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2 Hazard(s) identification

Hazard classification according to 29 CFR 1910.1200

Acute Toxicity - Oral	Category 4
Germ cell mutagenicity	Category 2
Reproductive Toxicity	Category 1B
Specific target organ toxicity - single exposure	Category 1

Label elements

Hazard pictograms	 
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Signal word	Danger
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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(thymus)

Precautionary statements

◆ Prevention

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P260	Do not breathe dust/fume.
P264	Wash hands and other parts of the body (if related) thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

◆ Response

P321	Specific treatment (see related instructions on the label).
P330	Rinse mouth.

◆ Storage

P405	Store locked up.
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◆ Disposal

P501	Dispose of contents/container in accordance with local/regional/national/international regulations.
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Other hazards

	Not applicable.
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Hazard description

◆ Physical and chemical hazards

	No information available
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◆ Health hazards

Inhaled	Inhalation of the product may produce adverse health effects or irritation of the respiratory tract following discomfort.
Ingestion	Accidental ingestion of the product may be harmful.
Skin Contact	Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.
Eye	This product may cause temporary discomfort following direct contact with the eye.

◆ Environmental hazards

	Please refer to 12th chapter of SDS.
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3 Composition/information on ingredients

Substance/mixture

Substance			
Component	CAS No.	EC No.	Concentration (wt, %)
Theobromine	83-67-0	201-494-2	99.2

4 First-aid measures

Description of first aid measures

General advice	Immediate medical attention is required. Show this safety data sheet (SDS) to the doctor in attendance.
Eye contact	Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician if feel uncomfortable.
Skin contact	Take off contaminated clothing and shoes immediately. Wash off with plenty of soap and water for at least 15 minutes and consult a physician if feel uncomfortable.
Ingestion	Never give anything by mouth to an unconscious person. Call a physician or Poison Control Center immediately.
Inhalation	Move victim into fresh air. If breathing is difficult, give oxygen. Do not use mouth to mouth resuscitation if victim ingested or inhaled the substance. If not breathing, give artificial respiration and consult a physician immediately.
Protecting of first-aiders	Ensure that medical personnel are aware of the substance involved. Take precautions to protect themselves and prevent spread of contamination.

Most important symptoms/effects, acute and delayed

1	Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.
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Indication of any immediate medical attention and special treatment needed

1	Treat symptomatically.
2	Symptoms may be delayed.

5 Fire-fighting measures

Extinguishing media

Suitable extinguishing media	Use extinguishing media suitable for surrounding area.
Unsuitable extinguishing media	There is no restriction on the type of extinguisher which may be used.

Specific hazards arising from the substance or mixture

1	Development of hazardous combustion gases or vapor possible in the event of fire.
2	May expansion or decompose explosively when heated or involved in fire.

Special protective equipment and precautions for fire-fighters

1	As in any fire, wear self-contained breathing apparatus (MSHA/NIOSH approved or equivalent) and full protective gear.
2	Fight fire from a safe distance, with adequate cover.
3	Prevent fire extinguishing water from contaminating surface water or the ground water system.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

1	Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.
2	Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.
3	Use personal protective equipment, do not breathe dust/fume.

Environmental precautions

1	Prevent further leakage or spillage if safe to do so.
2	Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

1	Cut off the source of the leak as much as possible.
2	Keep leaks in a ventilated place.
3	Isolation of contaminated areas and restrictions on access.
4	It is recommended that emergency personnel wear dust masks.
5	Collect the spill with a clean shovel and place it in a clean, dry, loosely closed container and move the container away from the leak.
6	Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

7 Handling and storage

Precautions for safe handling

1	Handling is performed in a well ventilated place.
2	Wear suitable protective equipment.
3	Avoid contact with skin and eyes.
4	Keep away from heat/sparks/open flames/ hot surfaces.

Conditions for safe storage, including any incompatibilities

1	Keep containers tightly closed.
2	Keep containers in a dry, cool and well-ventilated place.
3	Keep away from heat/sparks/open flames/hot surfaces.
4	Store away from incompatible materials and foodstuff containers.

8 Exposure controls/personal protection

Control parameters

◆ Occupational exposure limit values

Occupational Exposure limit values	No relevant regulations
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Engineering controls

1	Ensure adequate ventilation, especially in confined areas.
2	Ensure that eyewash stations and safety showers are close to the workstation location.
3	Use explosion-proof electrical/ventilating/lighting/equipment.
4	Set up emergency exit and necessary risk-elimination area.

Personal protection equipment

General requirement	
Eye protection	Must wear appropriate safety goggles.
Hand protection	Must wear appropriate chemical protective gloves.
Respiratory protection	Must wear appropriate personal respiratory protective equipment.
Skin and body protection	Must wear appropriate chemical protective clothing and chemical resistant shoes.

9 Physical and chemical properties and safety characteristics

Physical and chemical properties

Appearance (physical state, color, etc.)	white powder
Odor	No information available
Odor threshold	No information available
pH	No information available
Melting point/freezing point(°C)	351
Initial boiling point and boiling range(°C)	290 (1 atm)
Flash point(Closed cup, °C)	Not applicable
Evaporation rate	Not applicable
Flammability	No information available
Upper/lower explosive limits[%(v/v)]	Upper limit : No information available ; Lower limit : No information available
Vapor pressure	Not applicable
Vapor density(Air = 1)	Not applicable
Relative density(Water=1)	1.522 (20 °C)
Solubility	0.5g/L
n-octanol/water partition coefficient	-0.78
Auto-ignition temperature(°C)	No information available
Decomposition temperature(°C)	No information available
Kinematic viscosity	Not applicable

10 Stability and reactivity

Stability and reactivity

Reactivity	Contact with incompatible substances can cause decomposition or other chemical reactions.
Chemical stability	Stable under proper operation and storage conditions.
Possibility of hazardous reactions	No information available.
Conditions to avoid	Incompatible materials, heat, flame and spark.
Incompatible materials	No information available.
Hazardous decomposition products	Under normal conditions of storage and use, hazardous decomposition products should not be produced.

11 Toxicological information

Acute toxicity

Component	LD ₅₀ (oral)	LD ₅₀ (dermal)	LC ₅₀ (inhalation,4h)
Theobromine	1265mg/kg(Rat)	No information available	No information available

Carcinogenicity

Component	List of carcinogens by the IARC Monographs	Report on Carcinogens by NTP	OSHA Carcinogen List
Theobromine	Category 3	Not Listed	Not Listed

Others

Theobromine(Component)	
Skin corrosion/irritation	Based on available data, the classification criteria are not met
Serious eye damage/irritation	Based on available data, the classification criteria are not met
Skin sensitization	Based on available data, the classification criteria are not met
Respiratory sensitization	Based on available data, the classification criteria are not met
Reproductive toxicity	May damage fertility or the unborn child(Category 1B)
STOT-single exposure	Causes damage to organs(thymus)(Category 1)
STOT-repeated exposure	Based on available data, the classification criteria are not met
Aspiration hazard	Based on available data, the classification criteria are not met
Germ cell mutagenicity	Suspected of causing genetic defects(Category 2)

12 Ecological information

Acute aquatic toxicity

Component	Fish	Crustaceans	Algae or other aquatic plants
Theobromine	LC ₅₀ : 150.4mg/L (96h)(Fish)	EC ₅₀ : > 100mg/L (48h)(Crustaceans)	ErC ₅₀ : > 100mg/L (72h)(Algae)

Chronic aquatic toxicity

Chronic aquatic toxicity	No information available
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Persistence and degradability

Component	Persistence (water/soil)	Persistence (air)
Theobromine	High	High

Bioaccumulative potential

Component	Bioaccumulative potential	Comments
Theobromine	Low	Log Kow=-0.78

Mobility in soil

Component	log Koc	Remark
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Theobromine	1.000	
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13 Disposal considerations

Disposal considerations

Waste chemicals	Before disposal should refer to the relevant national and local laws and regulation. Recommend the use of incineration disposal.
Contaminated packaging	Containers may still present chemical hazard when empty. Keep away from hot and ignition source of fire. Return to supplier for recycling if possible.
Disposal recommendations	Refer to section waste chemicals and contaminated packaging.

14 Transport information

Label and Mark

Transporting Label	Not applicable
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IMDG-CODE

IMDG-CODE	NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS
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IATA-DGR

IATA-DGR	NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS
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UN-ADR

UN-ADR	NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS
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Transport in bulk according to IMO instruments

- ◆ Transport in bulk according to Annex II of MARPOL and the IBC code

	Not Available
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- ◆ Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

	Not Available
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- ◆ Transport in bulk in accordance with the IGC Code

	Not Available
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Others

Precautions for transport	Transport vehicles should be equipped with the appropriate variety and quantity of fire equipment and emergency equipment leakage during transport. Before transport, should be preceded by checking whether container integrity, sealing. The transport unit must be placarded and marked in accordance with relevant transporting requirements.
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15 Regulatory information

International chemical inventory

Component	A	B	C	D	E	F	G	H	I	J	K	L	M
Theobromine	√	√	√	×	√	√	×	√	√	×	×	√	√

- [A] China Inventory of Existing Chemical Substances(IECSC)
 [B] European Inventory of Existing Commercial Chemical Substances(EC inventory)
 [C] United States Toxic Substances Control Act Inventory(TSCA)
 [D] Canadian Domestic Substances List(DSL)

- [E] New Zealand Inventory of Chemicals(NZIoC)
- [F] Philippines Inventory of Chemicals and Chemical Substances(PICCS)
- [G] Korea Existing Chemicals Inventory(KECL)
- [H] Australian. Inventory of Industrial Chemical (AIICS)
- [I] Japan Inventory of Existing & New Chemical Substances(ENCS)
- [J] Thailand Existing Chemicals Inventory(TECI)
- [K] Mexico National Inventory of Chemical Substances (INSQ)
- [L] Russia Inventory of Existing Substances(DRAFT)
- [M] Inventory of Existing Chemical Substances in Taiwan, China (TCSI)

List of Chemical Substances under International Conventions

Component	A	B	C
Theobromine	x	x	x

- [A] The Montreal Protocol on Substances that Deplete the Ozone Layer
- [B] Stockholm Convention on Persistent Organic Pollutants (POPs)
- [C] Rotterdam Convention on the prior informed consent procedure for certain hazardous chemicals and pesticides in international trade

US chemical inventory

Component	A	B	C	D	E	F	G	H
Theobromine	x	x	x	x	x	x	x	x

- [A] US Clean Air Act (CAA)- Section 112, Hazardous Air Pollutants
- [B] US SARA 302- Extremely Hazardous Substance List
- [C] US CERCLA- Hazardous Substances List
- [D] US Massachusetts Right-to-Know Substance List
- [E] US New Jersey Right to Know Hazardous Substance List
- [F] US Pennsylvania Right to Know Hazardous Substance List
- [G] US New York City Right-to-Know Hazardous Substance List
- [H] US California Proposition 65 List

Note:

“√” Indicates that the substance included in the regulations.

“x” No data or not included in the regulations.

16 Other information

Information on revision

Creation Date	2025/11/11
Revision Date	-
Reason for revision	-

Reference

- [1] IPCS: The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>.
- [2] IARC, website: <http://www.iarc.fr/>.
- [3] OECD: The Global Portal to Information on Chemical Substances, website: <https://www.echemportal.org/echemportal/>.
- [4] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>.
- [5] NLM: ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>.
- [6] EPA: Integrated Risk Information System, website: <http://cfpub.epa.gov/iris/>.
- [7] U.S. Department of Transportation: ERG, website: <http://www.phmsa.dot.gov/hazmat/library/erg>.
- [8] Germany GESTIS-database on hazard substance, website: <http://gestis-en.itrust.de/>.

Abbreviations and acronyms

CAS Chemical Abstracts Service
PC-STEL Short term exposure limit

UN The United Nations
OECD Organization for Economic Co-operation and Development

PC-TWA	Time Weighted Average	IMDG-CODE	International Maritime Dangerous Goods CODE
MAC	Maximum Allowable Concentration	IARC	International Agency for Research on Cancer
DNEL	Derived No Effect Level	ICAO	International Civil Aviation Organization
PNEC	Predicted No Effect Concentration	IATA	International Air Transportation Association
NOEC	No Observed Effect Concentration	ACGIH	American Conference of Governmental Industrial Hygienists
LC ₅₀	Lethal Concentration 50%	NFPA	National Fire Protection Association
LD ₅₀	Lethal Dose 50%	NTP	National Toxicology Program
EC ₅₀	Effective Concentration 50%	PBT	Persistent, Bioaccumulative, Toxic
EC _x	Effective Concentration X%	vPvB	very Persistent, very Bioaccumulative
P _{OW}	Partition coefficient Octanol: Water	CMR	Carcinogens, mutagens or substances toxic to reproduction
BCF	Bioconcentration factor	RPE	Respiratory Protective Equipment
ED	Endocrine disruptor	HCS	Hazard Communication Standard

Disclaimer

This Safety Data Sheet (SDS) was prepared according to OSHA HCS-2024. The data included was derived from international authoritative database and provided by the enterprise. Other information was based on the present state of our knowledge. We try to ensure the correctness of all information. However, due to the diversity of information sources and the limitations of our knowledge, this document is only for user's reference. Users should make their independent judgment of suitability of this information for their particular purposes. We do not assume responsibility for loss, damage or expense arising out of or in any way connected with the handling, storage, use or disposal of the product.