

SAFETY DATA SHEET

Revision Date 14-Feb-2020

Revision Number 2

1. Identification

Product Name 7-(2-Chloroethyl)theophylline

Cat No. : J65111

CAS-No 5878-61-5
Synonyms 7-(2-Chloroethyl)-1,3-dimethyl-2,6(1H,3H)-purinedione

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.
Details of the supplier of the safety data sheet

Company

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Emergency Telephone Number

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660.
After normal business hours, call Carechem 24 at (866) 928-0789.

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity	Category 4
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Label Elements

Signal Word

Warning

Hazard Statements

Harmful if swallowed

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product

Ingestion

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

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
7-(2-Chloroethyl)-1,3-dimethyl-(1H,3H)-purine-2,6-dione	5878-61-5	97

4. First-aid measures

Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.
Skin Contact	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.
Inhalation	Remove from exposure, lie down. Remove to fresh air.
Ingestion	Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. If possible drink milk afterwards.
Most important symptoms and effects	No information available.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray. Carbon dioxide (CO ₂). Dry chemical. Alcohol resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	No information available
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available

Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required.

Environmental Precautions

See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Sweep up and shovel into suitable containers for disposal.

7. Handling and storage

Handling

Avoid contact with skin and eyes. Avoid contact with skin and clothing. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Avoid breathing vapors or mists. Do not ingest. If swallowed then seek immediate medical assistance. Wash thoroughly after handling.

Storage

Keep in a dry, cool and well-ventilated place. Refer product specification and/or product label for specific storage temperature requirement. Keep container tightly closed.

8. Exposure controls / personal protection

Exposure Guidelines

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

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ventilation systems.

Personal Protective Equipment

Eye/face Protection

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

No protective equipment is needed under normal use conditions.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State

Powder Solid

Appearance

White

Odor

Odorless

Odor Threshold

No information available

pH

No information available

Melting Point/Range	122 - 127 °C / 251.6 - 260.6 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	Not applicable
Molecular Formula	C9 H11 Cl N4 O2
Molecular Weight	242.66

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products.
Incompatible Materials	Strong oxidizing agents, Oxidizing agent
Hazardous Decomposition Products	Thermal decomposition can lead to release of irritating gases and vapors
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Toxicologically Synergistic Products	No information available
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Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
7-(2-Chloroethyl)-1,3-dimethyl-(1H,3H)-purine-2,6-dione	5878-61-5	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects	No information available
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Reproductive Effects	No information available.
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Developmental Effects	No information available.
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Teratogenicity	No information available.
STOT - single exposure	None known
STOT - repeated exposure	None known
Aspiration hazard	No information available
Symptoms / effects, both acute and delayed	No information available
Endocrine Disruptor Information	No information available
Other Adverse Effects	The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability	No information available
Bioaccumulation/ Accumulation	No information available.
Mobility	No information available.

13. Disposal considerations

Waste Disposal Methods	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
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14. Transport information

DOT	Not regulated
TDG	Not regulated
IATA	Not regulated
IMDG/IMO	Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS-No	TSCA	TSCA Inventory notification - Active/Inactive	TSCA - EPA Regulatory Flags
7-(2-Chloroethyl)-1,3-dimethyl-(1H,3H)-purine-2,6-dione	5878-61-5	-	-	-

Legend:

TSCA - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export	Not applicable
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International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Australia (AICS), China (IECSC), Korea (ECL).

Component	CAS-No	DSL	NDSL	EINECS	PICCS	ENCS	AICS	IECSC	KECL
7-(2-Chloroethyl)-1,3-dimethyl-(1H,3H)-purine-2,6-dione	5878-61-5	-	-	227-553-2	-	-	-	-	-

U.S. Federal Regulations

SARA 313	Not applicable
SARA 311/312 Hazard Categories	See section 2 for more information
CWA (Clean Water Act)	Not applicable
Clean Air Act	Not applicable
OSHA - Occupational Safety and Health Administration	Not applicable
CERCLA	Not applicable
California Proposition 65	This product does not contain any Proposition 65 chemicals.
U.S. State Right-to-Know Regulations	Not applicable
U.S. Department of Transportation	
Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N
U.S. Department of Homeland Security	This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade	No information available
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16. Other information

Prepared By	Health, Safety and Environmental Department Email: tech@alfa.com www.alfa.com
Revision Date	14-Feb-2020
Print Date	14-Feb-2020
Revision Summary	SDS authoring systems update, replaces ChemGes SDS No. 5878-61-5.

Disclaimer

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, use, processing, storage, transportation, disposal and release 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

End of SDS