

Material Safety Data Sheet

7-(2-Chloroethyl)-Theophylline, 97%

ACC# 29116

Section 1 - Chemical Product and Company Identification

MSDS Name: 7-(2-Chloroethyl)-Theophylline, 97%

Catalog Numbers: AC155750000, AC155750050

Synonyms: 7-(2-Chloroethyl)-1,3-Dimethyl-2,6(1H,3H)-Purinedione; Benaphyllin.

Company Identification:

Acros Organics N.V.

One Reagent Lane

Fair Lawn, NJ 07410

For information in North America, call: 800-ACROS-01

For emergencies in the US, call CHEMTREC: 800-424-9300

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
5878-61-5	7-(2-Chloroethyl)Theophylline	97	227-553-2

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: white solid.

Caution! May cause eye and skin irritation. May cause respiratory and digestive tract irritation. The toxicological properties of this material have not been fully investigated.

Target Organs: None known.

Potential Health Effects

Eye: May cause eye irritation. The toxicological properties of this material have not been fully investigated.

Skin: May cause skin irritation. The toxicological properties of this material have not been fully investigated.

Ingestion: May cause gastrointestinal irritation with nausea, vomiting and diarrhea. The toxicological properties of this substance have not been fully investigated.

Inhalation: May cause respiratory tract irritation. The toxicological properties of this substance have not been fully investigated.

Chronic: No information found.

Section 4 - First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.

Skin: Get medical aid. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse.

Ingestion: Never give anything by mouth to an unconscious person. Get medical aid immediately. Do NOT induce vomiting. If conscious and alert, rinse mouth and drink 2-4 cupfuls of milk or water.

Inhalation: Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.

Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas.

Extinguishing Media: Use agent most appropriate to extinguish fire. Use water spray, dry chemical, carbon dioxide, or appropriate foam.

Flash Point: Not available.

Autoignition Temperature: Not available.

Explosion Limits, Lower:N/A

Upper: N/A

NFPA Rating: (estimated) Health: ; Flammability: ; Instability:

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.

Spills/Leaks: Clean up spills immediately, observing precautions in the Protective Equipment section. Sweep up, then place into a suitable container for disposal. Avoid generating dusty conditions. Provide ventilation.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Use with adequate ventilation. Avoid contact with eyes, skin, and clothing. Keep container tightly closed. Avoid ingestion and inhalation.

Storage: Keep container closed when not in use. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits.

Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
7-(2-Chloroethyl)Theophylline	none listed	none listed	none listed

OSHA Vacated PELs: 7-(2-Chloroethyl)Theophylline: No OSHA Vacated PELs are listed for this chemical.

Personal Protective Equipment

Eyes: 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: Wear appropriate protective gloves to prevent skin exposure.

Clothing: Wear appropriate protective clothing to prevent skin exposure.

Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Solid

Appearance: white

Odor: odorless

pH: Not available.

Vapor Pressure: Not available.

Vapor Density: 8.4

Evaporation Rate:Not available.

Viscosity: Not available.

Boiling Point: Not available.

Freezing/Melting Point:124.00 - 125.00 deg C

Decomposition Temperature:Not available.

Solubility: Not available.

Specific Gravity/Density:Not available.

Molecular Formula:C9H11ClN4O2

Molecular Weight:242.66

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.

Conditions to Avoid: Incompatible materials, strong oxidants.

Incompatibilities with Other Materials: Oxidizing agents.

Hazardous Decomposition Products: Nitrogen oxides, carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, nitrogen, chloride fumes.

Hazardous Polymerization: Has not been reported.

Section 11 - Toxicological Information

RTECS#:

CAS# 5878-61-5: XH5090000

LD50/LC50:

CAS# 5878-61-5:

Oral, mouse: LD50 = 374 mg/kg;

Carcinogenicity:

CAS# 5878-61-5: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information available.

Teratogenicity: No information available.

Reproductive Effects: No information available.

Mutagenicity: No information available.

Neurotoxicity: No information available.

Other Studies:

Section 12 - Ecological Information

No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

RCRA P-Series: None listed.

RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	Not regulated as a hazardous material	No information available.
Hazard Class:		
UN Number:		
Packing Group:		

Section 15 - Regulatory Information

US FEDERAL

TSCA

CAS# 5878-61-5 is not listed on the TSCA inventory. It is for research and development use only.

Health & Safety Reporting List

None of the chemicals are on the Health & Safety Reporting List.

Chemical Test Rules

None of the chemicals in this product are under a Chemical Test Rule.

Section 12b

None of the chemicals are listed under TSCA Section 12b.

TSCA Significant New Use Rule

None of the chemicals in this material have a SNUR under TSCA.

CERCLA Hazardous Substances and corresponding RQs

None of the chemicals in this material have an RQ.

SARA Section 302 Extremely Hazardous Substances

None of the chemicals in this product have a TPQ.

Section 313

No chemicals are reportable under Section 313.

Clean Air Act:

This material does not contain any hazardous air pollutants.

This material does not contain any Class 1 Ozone depleters.

This material does not contain any Class 2 Ozone depleters.

Clean Water Act:

None of the chemicals in this product are listed as Hazardous Substances under the CWA.

None of the chemicals in this product are listed as Priority Pollutants under the CWA.

None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:

None of the chemicals in this product are considered highly hazardous by OSHA.

STATE

CAS# 5878-61-5 is not present on state lists from CA, PA, MN, MA, FL, or NJ.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

Not available.

Risk Phrases:

Safety Phrases:

S 37 Wear suitable gloves.

S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

S 28A After contact with skin, wash immediately with plenty of water

WGK (Water Danger/Protection)

CAS# 5878-61-5: No information available.

Canada - DSL/NDSL

None of the chemicals in this product are listed on the DSL or NDSL list.

Canada - WHMIS

WHMIS: Not available.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

Section 16 - Additional Information

MSDS Creation Date: 7/06/1998

Revision #3 Date: 10/03/2005

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall Fisher be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if Fisher has been advised of the possibility of such damages.