
SAFETY DATA SHEET

SECTION 1. CHEMICAL IDENTIFICATION

CATALOG #: 32460

NAME: 1-(3-Chloropropyl)theobromine

SYNONYMS: 1-(3-Chloropropyl)-3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione; 1-(3-Chloropropyl)-3,7-dimethylxanthine;

24 HR EMERGENCY TELEPHONE: (800) 535-5053 (USA)
352-323-3500 (INTERNATIONAL)

TO REQUEST AN SDS: (800) 869-9290

CUSTOMER SERVICE: (630) 766-2112

SECTION 2. HAZARD IDENTIFICATION

CLASSIFICATION OF THE SUBSTANCE OR MIXTURE
NOT A HAZARDOUS SUBSTANCE OR MIXTURE

GHA LABEL ELEMENTS, INCLUDING PRECAUTIONARY STATEMENTS
NOT A HAZARDOUS SUBSTANCE OR MIXTURE

HAZARDS NOT OTHERWISE CLASSIFIED (HNOC) OR NOT COVERED BY GHS NONE

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

MF: C10H13ClN4O2

MW: 256.69

CAS RN: 74409-52-2

PURITY: $\geq 98\%$ (HPLC, AT)

SECTION 4. FIRST-AID MEASURES

DESCRIPTION OF FIRST AID MEASURES

GENERAL ADVICE	IMMEDIATELY REMOVE ANY CLOTHING CONTAMINATED BY THE PRODUCT. MOVE OUT OF DANGEROUS AREA. CONSULT A PHYSICIAN AND SHOW THIS SAFETY DATA SHEET
IF INHALED	MOVE PERSON TO FRESH AIR. IF NOT BREATHING, GIVE ARTIFICIAL RESPIRATION. IF BREATHING IS DIFFICULT, GIVE OXYGEN AND CONSULT A PHYSICIAN
IN CASE OF SKIN CONTACT	IMMEDIATELY FLUSH SKIN WITH RUNNING WATER FOR AT LEAST 15 MINUTES WHILE REMOVING CONTAMINATED CLOTHING AND SHOES. WASH CLOTHING BEFORE REUSE. CONSULT A PHYSICIAN IMMEDIATELY
IN CASE OF EYE CONTACT	IMMEDIATELY WASH SKIN WITH COPIOUS AMOUNTS OF WATER FOR AT LEAST 15 MINUTES. ASSURE ADEQUATE FLUSHING OF THE EYES BY SEPARATING THE EYELIDS WITH FINGERS. IF IRRITATION PERSISTS, CONSULT A PHYSICIAN.
IF SWALLOWED	DO NOT INDUCE VOMITING. NEVER GIVE ANYTHING BY MOUTH TO AN UNCONSCIOUS PERSON. RINSE MOUTH WITH WATER. CONSULT A PHYSICIAN.
MOST IMPORTANT SYMPTOMS AND EFFECTS, BOTH ACUTE AND DELAYED	THE MOST IMPORTANT KNOWN SYMPTOMS AND EFFECTS ARE DESCRIBED IN THE LABELLING (SEE SECTION 2) AND/OR IN SECTION 11
INDICATION OF ANY IMMEDIATE MEDICAL ATTENTION AND SPECIAL TREATMENT NEEDED	NO DATA AVAILABLE

SECTION 5. FIRE AND EXPLOSION DATA

EXTINGUISHING MEDIA

SUITABLE EXTINGUISHING MEDIA	USE WATER SPRAY, DRY CHEMICAL, CARBON DIOXIDE OR CHEMICAL FOAM.
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**SPECIAL HAZARDS
ARISING FROM THE
SUBSTANCE OR MIXTURE**

CARBON OXIDES, NITROGEN OXIDES (NOX), SULPHUR OXIDES,
POTASSIUM OXIDES

**ADVICE FOR
FIREFIGHTERS**

WEAR SELF CONTAINED BREATHING APPARATUS FOR FIRE
FIGHTING IF NECESSARY.

FURTHER INFORMATION

NO DATA AVAILABLE

SECTION 6. ACCIDENTAL RELEASE MEASURES

**PERSONAL
PRECAUTIONS,
PROTECTIVE EQUIPMENT
AND EMERGENCY
PROCEDURES**

WEAR PROTECTIVE EQUIPMENT AND KEEP UNPROTECTED
PERSONNEL AWAY. ENSURE ADEQUATE VENTILATION. REMOVE ALL
SOURCES OF IGNITION. PREVENT FURTHER LEAK OR SPILL IF SAFE
TO DO SO.

FOR PERSONAL PROTECTION SEE SECTION 8.

**ENVIRONMENTAL
PRECAUTIONS**

PREVENT FURTHER LEAKAGE OR SPILLAGE IF SAFE TO DO SO. DO
NOT LET PRODUCT ENTER DRAINS. DISCHARGE INTO THE
ENVIRONMENT MUST BE AVOIDED.

**METHODS AND
MATERIALS FOR
CONTAINMENT AND
CLEANING UP**

PREVENT FURTHER LEAK OR SPILL IF SAFE TO DO SO. VACUUM,
SWEEP UP, OR ABSORB WITH INERT MATERIAL AND PLACE INTO A
SUITABLE DISPOSAL CONTAINER. CONSULT LOCAL REGULATIONS
FOR DISPOSAL

**REFERENCE TO OTHER
SECTIONS**

FOR DISPOSAL SEE SECTION 13.

SECTION 7. HANDLING AND STORAGE

**PRECAUTIONS FOR SAFE
HANDLING**

AVOID CONTACT WITH SKIN, EYES, AND PERSONAL CLOTHING.
WASH HANDS THOROUGHLY AFTER HANDLING. AVOID BREATHING
FUMES. USE ONLY WITH ADEQUATE VENTILATION. WEAR SUITABLE
PROTECTIVE CLOTHING, GLOVES, AND EYE/FACE PROTECTION.
KEEP AWAY FROM SOURCES OF IGNITION. MINIMIZE DUST
GENERATION AND ACCUMULATION. KEEP CONTAINER TIGHTLY
CLOSED. OPEN AND HANDLE CONTAINER WITH CARE. DO NOT EAT,
DRINK, OR SMOKE WHILE HANDLING.
FOR PRECAUTIONS SEE SECTION 2.

**CONDITIONS FOR SAFE
STORAGE, INCLUDING
ANY INCOMPATIBILITIES**

STORE IN A TIGHTLY CLOSED CONTAINER WHEN NOT IN USE. STORE
IN A COOL, DRY, WELL-VENTILATED AREA AWAY FROM
INCOMPATIBLE SUBSTANCES. KEEP AWAY FROM SOURCES OF
IGNITION.

**RECOMMENDED
STORAGE TEMPERATURE**

Store at RT

SPECIFIC END USE(S)

FOR LABORATORY USE ONLY

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

CONTROL PARAMETERS

**COMPONENTS WITH
WORKPLACE CONTROL
PARAMETERS**

CONTAINS NO SUBSTANCES WITH OCCUPATIONAL EXPOSURE LIMIT VALUES.

EXPOSURE CONTROLS

**APPROPRIATE
ENGINEERING CONTROLS**

AVOID CONTACT WITH SKIN, EYES, AND CLOTHING. WASH HANDS BEFORE BREAKS AND IMMEDIATELY AFTER HANDLING THE PRODUCT. FACILITIES STORING OR UTILIZING THIS MATERIAL SHOULD BE EQUIPPED WITH AN EYEWASH FOUNTAIN. USE ADEQUATE VENTILATION TO KEEP AIRBORNE CONCENTRATIONS LOW.

PERSONAL PROTECTIVE EQUIPMENT

EYE/FACE PROTECTION

SAFETY GLASSES WITH SIDE-SHIELDS CONFORMING TO EN166 USE EQUIPMENT FOR EYE PROTECTION TESTED AND APPROVED UNDER APPROPRIATE GOVERNMENT STANDARDS SUCH AS NIOSH (US) OR EN166 (EU).

SKIN PROTECTION

HANDLE WITH GLOVES. GLOVES MUST BE INSPECTED PRIOR TO USE. USE PROPER GLOVE REMOVAL TECHNIQUE (WITHOUT TOUCHING GLOVE'S OUTER SURFACE) TO AVOID SKIN CONTACT WITH THIS PRODUCT. DISPOSE OF CONTAMINATED GLOVES AFTER USE IN ACCORDANCE WITH APPLICABLE LAWS AND GOOD LABORATORY PRACTICES. WASH AND DRY HANDS.

BODY PROTECTION

IMPERVIOUS CLOTHING, THE TYPE OF PROTECTIVE EQUIPMENT MUST BE SELECTED ACCORDING TO THE CONCENTRATION AND AMOUNT OF THE DANGEROUS SUBSTANCE AT THE SPECIFIC WORKPLACE.

**RESPIRATORY
PROTECTION**

WHERE RISK ASSESSMENT INDICATES AIR-PURIFYING RESPIRATORS ARE REQUIRED USE A DUST MASK TYPE N95 (US) OR TYPE P1 (EN 143) RESPIRATOR. RESPIRATORS AND COMPONENTS MUST TESTED AND APPROVED UNDER APPROPRIATE GOVERNMENT STANDARDS - NIOSH (US) OR CEN (EU).

CONTROL OF ENVIRONMENTAL EXPOSURE

PREVENT FURTHER LEAKAGE OR SPILLAGE IF SAFE TO DO SO. DO NOT LET PRODUCT ENTER DRAINS. DISCHARGE INTO THE ENVIRONMENT MUST BE AVOIDED.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

INFORMATION ON BASIC PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE	White to light yellow crystalline powder
ODOR	NO DATA AVAILABLE
ODOR THRESHOLD	NO DATA AVAILABLE
pH	NO DATA AVAILABLE
MELTING/FREEZING POINT	144 - 146 °C

INITIAL BOILING POINT AND BOILING RANGE

FLASH POINT

EVAPORATION RATE NO DATA AVAILABLE

FLAMMABILITY (SOLID, GAS) NO DATA AVAILABLE

UPPER/LOWER FLAMMABILITY OR EXPLOSIVE LIMITS NO DATA AVAILABLE

VAPOR PRESSURE NO DATA AVAILABLE

VAPOR DENSITY NO DATA AVAILABLE

RELATIVE DENSITY

WATER SOLUBILITY NO DATA AVAILABLE

PARTITION COEFFICIENT: N- OCTANOL/ WATER NO DATA AVAILABLE

AUTO-IGNITION TEMPERATURE NO DATA AVAILABLE

DECOMPOSITION TEMPERATURE NO DATA AVAILABLE

VISCOSITY NO DATA AVAILABLE

EXPLOSIVE PROPERTIES NO DATA AVAILABLE

OXIDIZING PROPERTIES NO DATA AVAILABLE

OTHER SAFETY INFORMATION NO DATA AVAILABLE

SECTION 10. STABILITY AND REACTIVITY

REACTIVITY NO DATA AVAILABLE

CHEMICAL STABILITY STABLE UNDER RECOMMENDED STORAGE CONDITIONS.

POSSIBILITY OF HAZARDOUS REACTIONS	NO DATA AVAILABLE
CONDITIONS TO AVOID	HEAT, FLAMES AND SPARKS
INCOMPATIBLE MATERIALS	STRONG OXIDIZING AGENTS
HAZARDOUS DECOMPOSITION PRODUCTS	CARBON MONOXIDE, NITROGEN OXIDES, HYDROGEN CHLORIDE IN THE EVENT OF FIRE: SEE SECTION 5

SECTION 11. TOXICOLOGICAL INFORMATION

INFORMATION ON TOXICOLOGICAL EFFECTS

ACUTE TOXICITY NO DATA AVAILABLE

SKIN CORROSION/ IRRITATION NO DATA AVAILABLE

SERIOUS EYE DAMAGE/ EYE IRRITATION NO DATA AVAILABLE

RESPIRATORY OR SKIN SENSITISATION NO DATA AVAILABLE

GERM CELL MUTAGENICITY NO DATA AVAILABLE

CARCINOGENICITY

IARC: NO COMPONENT OF THIS PRODUCT PRESENT AT LEVELS GREATER THAN OR EQUAL TO 0.1% IS IDENTIFIED AS PROBABLE, POSSIBLE OR CONFIRMED HUMAN CARCINOGEN BY IARC.

ACGIH: NO COMPONENT OF THIS PRODUCT PRESENT AT LEVELS GREATER THAN OR EQUAL TO 0.1% IS IDENTIFIED AS A CARCINOGEN OR POTENTIAL CARCINOGEN BY ACGIH.

NTP: NO COMPONENT OF THIS PRODUCT PRESENT AT LEVELS GREATER THAN OR EQUAL TO 0.1% IS IDENTIFIED AS A KNOWN OR ANTICIPATED CARCINOGEN BY NTP.

OSHA: NO COMPONENT OF THIS PRODUCT PRESENT AT LEVELS GREATER THAN OR EQUAL TO 0.1% IS IDENTIFIED AS A CARCINOGEN OR POTENTIAL CARCINOGEN BY OSHA.

REPRODUCTIVE TOXICITY	NO DATA AVAILABLE
SPECIFIC TARGET ORGAN TOXICITY - SINGLE EXPOSURE	NO DATA AVAILABLE
SPECIFIC TARGET ORGAN TOXICITY - REPEATED EXPOSURE	NO DATA AVAILABLE
ASPIRATION HAZARD	NO DATA AVAILABLE
ADDITIONAL INFORMATION	RTECS: NOT AVAILABLE TO THE BEST OF OUR KNOWLEDGE, THE CHEMICAL, PHYSICAL AND TOXICOLOGICAL PROPERTIES OF THIS SUBSTANCE HAVE NOT BEEN THOROUGHLY INVESTIGATED.

SECTION 12. ECOLOGICAL INFORMATION

TOXICITY	NO DATA AVAILABLE
PERSISTENCE AND DEGRADABILITY	NO DATA AVAILABLE
BIOACCUMULATIVE POTENTIAL	NO DATA AVAILABLE
MOBILITY IN SOIL	NO DATA AVAILABLE
RESULTS OF PBT AND VPVB ASSESSMENT	PBT/VPVB ASSESSMENT NOT AVAILABLE AS CHEMICAL SAFETY ASSESSMENT NOT REQUIRED/NOT CONDUCTED
OTHER ADVERSE EFFECTS	NO DATA AVAILABLE

SECTION 13. DISPOSAL CONSIDERATIONS

WASTE TREATMENT METHODS

PRODUCT	OFFER SURPLUS AND NON-RECYCLABLE CHEMICAL TO A LICENSED DISPOSAL COMPANY. CONTACT A LICENSED PROFESSIONAL WASTE DISPOSAL SERVICE TO DISPOSE OF THIS MATERIAL.
CONTAMINATED PACKAGING	DISPOSE OF AS UNUSED PRODUCT.

SECTION 14. TRANSPORT INFORMATION

DOT (US)

NOT DANGEROUS GOODS

IMDG

NOT DANGEROUS GOODS

IATA

NOT DANGEROUS GOODS

SECTION 15. REGULATORY INFORMATION

SARA 302 COMPONENTS

SARA 302: NO CHEMICALS IN THIS MATERIAL ARE SUBJECT TO THE REPORTING REQUIREMENTS OF SARA TITLE III, SECTION 302.

SARA 313 COMPONENTS

SARA 313: THIS MATERIAL DOES NOT CONTAIN ANY CHEMICAL COMPONENTS WITH KNOWN CAS NUMBERS THAT EXCEED THE THRESHOLD (DE MINIMIS) REPORTING LEVELS ESTABLISHED BY SARA TITLE III, SECTION 313.

MASSACHUSETTS RIGHT TO KNOW COMPONENTS

NO COMPONENTS ARE SUBJECT TO THE MASSACHUSETTS RIGHT TO KNOW ACT.

PENNSYLVANIA RIGHT TO KNOW COMPONENTS

	CAS RN	REVISION DATE
1-(3-Chloropropyl)theobromine	74409-52-2	

NEW JERSEY RIGHT TO KNOW COMPONENTS

	CAS RN	REVISION DATE
1-(3-Chloropropyl)theobromine	74409-52-2	

CALIFORNIA PROP. 65 COMPONENTS

THIS PRODUCT DOES NOT CONTAIN ANY CHEMICALS KNOWN TO STATE OF CALIFORNIA TO CAUSE CANCER, BIRTH DEFECTS, OR ANY OTHER REPRODUCTIVE HARM.

SECTION 16. OTHER INFORMATION

SDS LEGEND

MW:	MOLECULAR WEIGHT
MF:	MOLECULAR FORMULA
VOC:	VOLATILE ORGANIC COMPOUNDS
ACGIH:	AMERICAN CONFERENCE OF GOVERNMENTAL INDUSTRIAL HYGINISTS
CAS RN:	CHEMICAL ABSTRACTS SERVICE REGISTRY NUMBER
OSHA:	OCCUPATIONAL SAFETY AND HEALTH ADMINISTRATION
PEL:	PERMISSIBLE EXPOSURE LIMIT (OSHA)
TLV:	THRESHOLD LIMIT VALUE (ACGIH)

IMPORTANT:

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