2-Chloro-5-(trifluoromethyl)benzonitrile

sc-230147

Material Safety Data Sheet

Hazard Alert Code Key:	EXTREME	HIGH	MODERATE	LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME
2-Chloro-5-(trifluoromethyl)benzonitrile

STATEMENT OF HAZARDOUS NATURE
CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA

SUPPLIER
Santa Cruz Biotechnology, Inc.
2145 Delaware Avenue
Santa Cruz, California 95060
800.457.3801 or 831.457.3800

EMERGENCY
ChemWatch
Within the US & Canada: 877-715-9305
Outside the US & Canada: +800 2436 2255
(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS
C8-H3-Cl-F3-N, F3CC6H3(Cl)CN

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability	1		
Toxicity	3		
Body Contact	2		
Reactivity	1		
Chronic	2		

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4

CANADIAN WHMIS SYMBOLS

EMERGENCY OVERVIEW

RISK

Toxic if swallowed.
Contact with acids liberates very toxic gas.
Harmful by inhalation and in contact with skin.
Irritating to eyes, respiratory system and skin.
Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ Aromatic nitriles, unlike aliphatic nitriles, do not appear to liberatecyanide within the body.
■ Nitrile poisoning exhibits similar symptoms to poisoning due to hydrogen cyanide.
The substances irritate the eyes and skin, and are absorbed quickly and completely through the skin.

EYE

■ This material can cause eye irritation and damage in some persons.

SKIN

■ Skin contact with the material may be harmful; systemic effects may result following absorption.
■ This material can cause inflammation of the skin oncontact in some persons.
■ The material may accentuate any pre-existing dermatitis condition.
■ Open cuts, abraded or irritated skin should not be exposed to this material.
■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.
Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

■ Inhalation of vapors, aerosols (mists, fumes) or dusts, generated by the material during the course of normal handling, may be harmful.
■ The material can cause respiratory irritation in some persons.
The body's response to such irritation can cause further lung damage.
■ Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.
If prior damage to the circulatory or nervous systems has occurred or if kidney damage has been sustained, proper screenings should be conducted on individuals who may be exposed to further risk if handling and use of the material result in excessive exposures.

CHRONIC HEALTH EFFECTS

■ Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.
Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.
Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung. Prime symptom is breathlessness; lung shadows show on X-ray.
Chronic exposure to cyanides and certain nitriles may result in interference to iodine uptake by thyroid gland and its consequent enlargement. This occurs following metabolic conversion of the cyanide moiety to thiocyanate. Thyroid insufficiency may also occur as a result of metabolic conversion of cyanides to the corresponding thiocyanate. Exposure to small amounts of cyanide compounds over long periods are reported to cause loss of appetite, headache, weakness, nausea, dizziness, abdominal pain, changes in taste and smell, muscle cramps, weight loss, flushing of the face, persistent runny nose and irritation of the upper respiratory tract and eyes. These symptoms are not specific to cyanide exposure and therefore the existence of a chronic cyanide toxicity remains speculative. Repeated minor contact with cyanides produce a characteristic rash with itching, papules (small, superficial raised spots on the skin) and possible sensitization. Concerns have been expressed that low-level, long term exposures may result in damage to the nerves of the eye.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
2-chloro-5-(trifluoromethyl)benzonitrile	328-87-0	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

- Give a slurry of activated charcoal in water to drink. NEVER GIVE AN UNCONSCIOUS PATIENT WATER TO DRINK.
- At least 3 tablespoons in a glass of water should be given.
- Although induction of vomiting may be recommended (IN CONSCIOUS PERSONS ONLY), such a first aid measure is dissuaded due to the risk of aspiration of stomach contents. (i) It is better to take the patient to a doctor who can decide on the necessity and method of emptying the stomach. (ii) Special circumstances may however exist; these include non- availability of charcoal and the ready availability of the doctor.

NOTE If vomiting is induced, lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.

EYE

If this product comes in contact with the eyes

- Immediately hold eyelids apart and flush the eye continuously with running water.
- Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.
- Continue flushing until advised to stop by the Poisons Information Centre or a doctor, or for at least 15 minutes.
- Transport to hospital or doctor without delay.

SKIN

If skin contact occurs

- Immediately remove all contaminated clothing, including footwear.
- Flush skin and hair with running water (and soap if available).
- Seek medical attention in event of irritation.

INHALED

- If fumes or combustion products are inhaled remove from contaminated area.
- Lay patient down. Keep warm and rested.
- Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.
- Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary.

NOTES TO PHYSICIAN

■ Treat symptomatically.
for poisons (where specific treatment regime is absent)

BASIC TREATMENT

- Establish a patent airway with suction where necessary.
- Watch for signs of respiratory insufficiency and assist ventilation as necessary.
- Administer oxygen by non-rebreather mask at 10 to 15 L/min.
- Monitor and treat, where necessary, for pulmonary oedema .

Section 5 - FIRE FIGHTING MEASURES

Vapor Pressure (mmHG)	Negligible
Upper Explosive Limit (%)	Not available.
Specific Gravity (water=1)	1.481
Lower Explosive Limit (%)	Not available

EXTINGUISHING MEDIA

- Foam.
- Dry chemical powder.
- BCF (where regulations permit).
- Carbon dioxide.

FIRE FIGHTING

- Alert Fire Brigade and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.
- Prevent, by any means available, spillage from entering drains or water course.
- Use fire fighting procedures suitable for surrounding area.

When any large container (including road and rail tankers) is involved in a fire,
consider evacuation by 800 metres in all directions.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- Combustible solid which burns but propagates flame with difficulty; it is estimated that most organic dusts are combustible (circa

70%) - according to the circumstances under which the combustion process occurs, such materials may cause fires and / or dust explosions.
- Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust (420 micron or less) may burn rapidly and fiercely if ignited - particles exceeding this limit will generally not form flammable dust clouds.; once initiated, however, larger particles up to 1400 microns diameter will contribute to the propagation of an explosion.
- In the same way as gases and vapors, dusts in the form of a cloud are only ignitable over a range of concentrations; in principle, the concepts of lower explosive limit (LEL) and upper explosive limit (UEL).are applicable to dust clouds but only the LEL is of practical use; - this is because of the inherent difficulty of achieving homogeneous dust clouds at high temperatures (for dusts the LEL is often called the "Minimum Explosible Concentration", MEC)
- A dust explosion may release of large quantities of gaseous products; this in turn creates a subsequent pressure rise of explosive force capable of damaging plant and buildings and injuring people.

Combustion products include carbon monoxide (CO), carbon dioxide (CO_2), hydrogen chloride, phosgene, hydrogen fluoride, nitrogen oxides (NOx), other pyrolysis products typical of burning organic material.
May emit poisonous fumes.

FIRE INCOMPATIBILITY

- Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine etc. as ignition may result

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.
- Avoid contact with skin and eyes.
- Control personal contact by using protective equipment.

MAJOR SPILLS

- Clear area of personnel and move upwind.
- Alert Fire Brigade and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.
- Prevent, by any means available, spillage from entering drains or water course.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.

Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source.

- Do NOT cut, drill, grind or weld such containers.
- In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorization or permit.

RECOMMENDED STORAGE METHODS

- Lined metal can, lined metal pail/ can.
- Plastic pail.
- Polyliner drum.
- Packing as recommended by manufacturer.

For low viscosity materials

- Drums and jerricans must be of the non-removable head type.
- Where a can is to be used as an inner package, the can must have a screwed enclosure.

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STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m³	STEL ppm	STEL mg/m³	Peak ppm	Peak mg/m³	TWA F/CC	Notes
US ACGIH Threshold Limit Values (TLV)	2-chloro-5-(trifluoromethyl)benzonitrile (Fluorides, as F)		2.5						TLV® Basis Bone dam; fluorosis ; BEI
Canada - Prince Edward Island Occupational Exposure Limits	2-chloro-5-(trifluoromethyl)benzonitrile (Fluorides, as F)		2.5						TLV® Basis Bone dam; fluorosis ; BEI
US - Hawaii Air Contaminant Limits	2-chloro-5-(trifluoromethyl)benzonitrile (Fluorides (as F))		2.5						(CAS (Varies with compound))

PERSONAL PROTECTION




RESPIRATOR

- Particulate. (AS/NZS 1716 & 1715, EN 1432000 & 1492001, ANSI Z88 or national equivalent)

EYE

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lens or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience. Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59], [AS/NZS 1336 or national equivalent]

HANDS/FEET

- Wear chemical protective gloves, eg. PVC.
- Wear safety footwear or safety gumboots, eg. Rubber

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and
- dexterity

OTHER

- Overalls.
- Eyewash unit.
- Barrier cream.
- Skin cleansing cream.

ENGINEERING CONTROLS

■ Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.

The basic types of engineering controls are

Process controls which involve changing the way a job activity or process is done to reduce the risk.
Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Solid.
Does not mix with water.
Sinks in water.
Contact with acids liberates very toxic gas.

State	Divided solid	Molecular Weight	205.56
Melting Range (°F)	102- 106	Viscosity	Not Applicable
Boiling Range (°F)	410- 414	Solubility in water (g/L)	Immiscible
Flash Point (°F)	215	pH (1% solution)	Not applicable
Decomposition Temp (°F)	Not available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapor Pressure (mmHG)	Negligible
Upper Explosive Limit (%)	Not available.	Specific Gravity (water=1)	1.481
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	>1
Volatile Component (%vol)	Negligible	Evaporation Rate	Not available

APPEARANCE

Solid; does not mix well with water.

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerisation will not occur.

STORAGE INCOMPATIBILITY

- Avoid strong acids, acid chlorides, acid anhydrides and chloroformates.
- Nitriles may polymerise in the presence of metals and some metal compounds.
- They are incompatible with acids; mixing nitriles with strong oxidizing acids can lead to extremely violent reactions.
- Nitriles are generally incompatible with other oxidizing agents such as peroxides and epoxides.
- The combination of bases and nitriles can produce hydrogen cyanide. Nitriles are hydrolysed exothermally in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids).
- The covalent cyano group is endothermic and many organic nitriles are reactive under certain conditions; N-cyano derivatives are reactive or unstable.
- The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation.
- Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds.

BRETHERICK L. Handbook of Reactive Chemical Hazards.

- Avoid reaction with oxidizing agents, bases and strong reducing agents.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

2-chloro-5-(trifluoromethyl)benzonitrile

TOXICITY AND IRRITATION

■ Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound.

No significant acute toxicological data identified in literature search.

CARCINOGEN

Fluorides, as F	US ACGIH Threshold Limit Values (TLV) - Carcinogens	Carcinogen Category	A4
2-chloro-5-(trifluoromethyl)benzonitrile	US - Maine Chemicals of High Concern List	Carcinogen	A4
2-chloro-5-(trifluoromethyl)benzonitrile	Canada - Prince Edward Island Occupational Exposure Limits - Carcinogens	Notes	TLV® Basis Bone dam; fluorosis ; BEI

Section 12 - ECOLOGICAL INFORMATION

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
This material and its container must be disposed of as hazardous waste.
Avoid release to the environment.
Refer to special instructions/ safety data sheets.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
2-chloro-5-(trifluoromethyl)benzonitrile	HIGH	No Data Available	LOW	MED

Section 13 - DISPOSAL CONSIDERATIONS

US EPA Waste Number & Descriptions

A. General Product Information
Reactivity characteristic: use EPA hazardous waste number D003 (waste code R).

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

- Containers may still present a chemical hazard/ danger when empty.
- Return to supplier for reuse/ recycling if possible.

Otherwise:

- If container can not be cleaned sufficiently well to ensure that residuals do not remain or if the container cannot be used to store the same product, then puncture containers, to prevent re-use, and bury at an authorized landfill.
- Where possible retain label warnings and MSDS and observe all notices pertaining to the product.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.
A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate. In most instances the supplier of the material should be consulted.

- DO NOT allow wash water from cleaning or process equipment to enter drains.
- It may be necessary to collect all wash water for treatment before disposal.
- In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first.
- Where in doubt contact the responsible authority.
- Recycle wherever possible.
- Consult manufacturer for recycling options or consult local or regional waste management authority for disposal if no suitable treatment or disposal facility can be identified.
- Dispose of by: burial in a land-fill specifically licenced to accept chemical and / or pharmaceutical wastes or Incineration in a licenced apparatus (after admixture with suitable combustible material)
- Decontaminate empty containers. Observe all label safeguards until containers are cleaned and destroyed.

Section 14 - TRANSPORTATION INFORMATION

DOT:

Symbols:	None	Hazard class or Division:	6.1
Identification Numbers:	UN2811	PG:	III
Label Codes:	6.1	Special provisions:	IB8, IP3, T1, TP33
Packaging: Exceptions:	153	Packaging: Non-bulk:	213
Packaging: Exceptions:	153	Quantity limitations: Passenger aircraft/rail:	100 kg
Quantity Limitations: Cargo aircraft only:	200 kg	Vessel stowage: Location:	A
Vessel stowage: Other:	None		

Hazardous materials descriptions and proper shipping names:
Toxic solids, organic, n.o.s.

Air Transport IATA:

ICAO/IATA Class:	6.1	ICAO/IATA Subrisk:	None
UN/ID Number:	2811	Packing Group:	III
Special provisions:	A3		
Cargo Only			
Packing Instructions:	677	Maximum Qty/Pack:	200 kg
Passenger and Cargo		Passenger and Cargo	
Packing Instructions:	670	Maximum Qty/Pack:	100 kg
Passenger and Cargo Limited Quantity		Passenger and Cargo Limited Quantity	
Packing Instructions:	Y645	Maximum Qty/Pack:	10 kg

Shipping name:TOXIC SOLID, ORGANIC, N.O.S.(contains 2-chloro-5-(trifluoromethyl)benzonitrile)

Maritime Transport IMDG:

IMDG Class:	6.1	IMDG Subrisk:	None
UN Number:	2811	Packing Group:	III
EMS Number:	F-A,S-A	Special provisions:	223 274
Limited Quantities:	5 kg	Marine Pollutant:	Yes

Shipping name:TOXIC SOLID, ORGANIC, N.O.S.(contains 2-chloro-5-(trifluoromethyl)benzonitrile)

Section 15 - REGULATORY INFORMATION

2-chloro-5-(trifluoromethyl)benzonitrile (CAS: 328-87-0) is found on the following regulatory lists;
"Canada Non-Domestic Substances List (NDSL)","US Toxic Substances Control Act (TSCA) - Chemical Substance Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE
■ Cumulative effects may result following exposure*.
* (limited evidence).

Denmark Advisory list for selfclassification of dangerous substances

Substance	CAS	Suggested codes
2- chloro- 5- (trifluoromethyl)benzonitrile	328- 87- 0	N; R51/53

■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.
A list of reference resources used to assist the committee may be found at:
www.chemwatch.net/references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings.

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