

(S)-(-)-N-(Trifluoroacetyl)pyrrolidine-2-carbonyl solution: sc-396745



MATERIAL SAFETY DATA SHEET

1. PRODUCT AND COMPANY IDENTIFICATION

Product Name: (S)-(-)-N-(Trifluoroacetyl)pyrrolidine-2-carbonyl solution
Product Number: sc-396745
Supplier: Santa Cruz Biotechnology, Inc.
2145 Delaware Avenue
Santa Cruz, CA 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

2. COMPOSITION, INFORMATION ON INGREDIENTS

Molecular Formula:	C7H7ClF3NO2	
Molecular Weight:	229.58	
CAS-No.		Concentration
TPC; N-Trifluoroacetyl-(S)-(-)-prolyl chloride	36724-68-2	5%
N-TFA-D-prolyl chloride; (R)-1-(trifluoroacetyl)-2-pyrrolidinecarbonyl chloride	71890-93-2	0.1%
Chloroform	356-42-3	98.4%

3. HAZARDS IDENTIFICATION

Precautionary Statements

See Sections 8 and 11 for further details.

Harmful. Causes drowsiness and dizziness.

Emergency Overview

NFPA Ratings

Health	2
Fire	0
Reactivity	1W

Hazards

Harmful volatile liquid and vapor.

Causes dizziness and drowsiness.

Readily absorbed through skin and lungs. General anesthetic—central nervous system depressant.

Delayed effects possible.

Water sensitive—Contact with moist air or water may produce small amounts of HCl.

The properties of this material have not been fully investigated. Use due caution in handling and use of this material.

Potential health effects

May cause irritation to skin, eyes, mucous membranes, and respiratory tract.

May harm unborn and newborn.

Possible Cancer Hazard--based on animal data.

Emits Harmful fumes under fire conditions

Potential chemical or thermal decomposition products: carbon oxides, hydrochloric acid, chlorine, phosgene, hydrogen fluoride

Standard chemical handling precautions:

Avoid ingestion or breathing mists. Avoid contact with eyes, skin, and clothing. Wash thoroughly after handling.

Target organs:

Central nervous system, cardiovascular, blood, kidneys, liver, heart, GI, reproductive system

See Sections 4, 5, 6, 8, 9, and 10.

Other Hazard Information

This compound has not fully been tested for Toxicological, irritation, or similar tendencies.

Primary Route(s) of Entry:

Inhalation, Ingestion, Eye, Skin-- Readily absorbed through skin and lungs.

Water sensitive—Contact with moist air or water may produce small amounts of hydrochloric acid.

Eye: Can cause severe irritation with burning, itching, tearing, and redness.

Skin: Can cause severe irritation with itchiness and possible dryness, cracking and dermatitis.

Readily absorbed through skin with harmful systemic effects similar to inhalation and ingestion.

Inhalation: Harmful. Can cause respiratory tract irritation with severe burning in mouth, throat, and chest, depending on amount of exposure. High concentrations may cause central nervous system (CNS) effects characterized by headache, nausea, drowsiness, and dizziness, and burns to mucous membranes. Prolonged high exposures may cause heart, liver, and kidney damage. Chloroform may cause cancer—dependent on level and duration of exposure. Delayed effects possible.

Ingestion: Harmful. Can cause severe gastrointestinal irritation with severe burning in mouth and throat, pain in chest and nervous system depression as described under inhalation. Chloroform may pass through the placenta or be excreted in breast milk and cause harm to the unborn or newborn. The mean lethal dose in humans is about 1 ounce.

Acute/Chronic: See above route.

Pre-existing conditions that may be aggravated:

Pregnancy, alcoholism, liver, heart, kidney, nerves, GI tract, Use adrenergic agents such as epinephrine or pseudoepinephrine might enhance irregular heartbeat effect. Chloroform toxicity may be increased by exposure to alcohol, steroids, and ketones.

See Section 11 for additional Toxicological data

4. FIRST AID MEASURES

Eye contact:

Immediately flush eyes with copious amounts of water or eyewash solution for at least 15 minutes. If irritation persists, consult physician.

Skin contact:

Immediately remove contaminated clothing and shoes, then wash skin with soap and copious amounts of water. If irritation persists, consult physician.

Inhalation:

Remove to fresh air. If not breathing, give artificial respiration and keep person warm and at rest. If breathing is difficult, give oxygen; consult physician.

Ingestion:

Wash out mouth with water provided person is conscious; give large amounts of water or milk (2-4 cups). DO NOT induce vomiting; consult physician.

Physician note:

Symptomatic and supportive care. Chloroform causes cardiac sensitization to endogenous catecholamines that may lead to heart arrhythmias. DO NOT use adrenergic agents such as epinephrine or pseudoepinephrine. Effects may be delayed.

5. FIRE FIGHTING MEASURES

Flash Point: None

Autoignition: NE

OSHA Flammability Class: NA

Explosion Limits: upper: NE

lower: NE

NFPA: See Section 3

Extinguishing Media

Water spray, carbon dioxide, dry chemical powder, or appropriate foam for surrounding fire.

Special Fire Fighting Procedures

Protective clothing to prevent inhalation and contact with skin and eyes should be worn.

Standard Fire and Explosion Hazards

Avoid inhalation of material or combustion by-products. Use any means suitable for extinguishing surrounding fire.

Unusual Fire and Explosion Hazards

Slight fire hazard when exposed to high heat, otherwise practically non-flammable.

Harmful volatile liquid and vapor. Causes dizziness and drowsiness. Readily absorbed through skin and lungs.

General anesthetic--central nervous system depressant.

Contact with water may produce small amounts of hydrochloric acid, that in contact with metals may form flammable or explosive hydrogen gas.

Containers may build pressure or rupture when heated. Water spray may be used to cool fire-exposed containers.

Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas.

Emits Harmful fumes under fire conditions.

Hazardous Combustion or Decomposition Products

carbon oxides, hydrochloric acid, chlorine, phosgene, hydrogen fluoride

6. ACCIDENTAL RELEASE MEASURES

Eliminate all ignition sources/slight fire hazard. Evacuate unnecessary people from area.

Isolate spilled material. Use spark proof tools. Ventilate area.

Respiratory Protection:

Wear NIOSH/MSHA approved respirator for halogenated organic gas, dust, and mists if above exposure limits.

Skin:

Wear protective clothing to prevent contact with skin and eyes (lab coat, gloves, and safety glasses).

Proper methods for cleaning:

Contain and recover material when possible. Use chemically compatible spill pillows, or similar adsorbent material.

Sweep up, seal in appropriate hazardous waste container, and hold for proper waste disposal.

Avoid raising contaminated dust. Wash spill site after material pickup is complete.

Standard chemical precautions:

Keep out of water supplies and sewers.

7. HANDLING AND STORAGE

General Handling Measures

See Section 8 Below.

General Storage Measures

Store tightly closed in a cool, dry place with adequate ventilation, in an area suitable for halogenated solvents.

Store at 4 °C.

Special Storage Instructions

Empty containers retain product residue, (liquid/vapor), and can be dangerous.

Special Handling Instructions

Use appropriate precautions for handling Harmful, volatile halogenated organic liquids.

Light and moisture sensitive--prolonged exposure decreases pH due to the formation of hydrochloric acid.

Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas.

Wash thoroughly after handling. Avoid breathing vapors and mists. Immediately remove contaminated clothing.

8. EXPOSURE CONTROLS, PERSONAL PROTECTION

Airborne Exposure Limits		TWA (8H)/VPEL		STEL		Ceiling Limit		Ceiling (skin)	
		ppm	mg/m ³	ppm	mg/m ³	ppm	mg/m ³	ppm	mg/m ³
N-TFA-L-prolyl chloride 36724-68-2	OSHA PEL	NE	NE	NE	NE	NE	NE	NE	NE
	ACGIH - TLV	NE	NE	NE	NE	NE	NE	NE	NE
N-TFA-D-prolyl chloride 71890-93-2	OSHA PEL/VPEL	NE	NE	NE	NE	NE	NE	NE	NE
	ACGIH - TLV	NE	NE	NE	NE	NE	NE	NE	NE
Chloroform 356-42-3	OSHA PEL/VPEL	2	9.78	NE	NE	50	240	NE	NE
	ACGIH - TLV	10	49	NE	NE	NE	NE	NE	NE
Hydrochloric Acid* 7647-01-0	OSHA PEL	NE	NE	NE	NE	5	7	NE	NE
	ACGIH - TLV	NE	NE	5	7.5	5	7.5	NE	NE

*Hydrochloric acid may be formed on contact with water, moist air, or prolonged exposure to light.

Chloroform Exposure Notations

Acute

1,000-2,000 ppm may cause dizziness, headache, fatigue, salivation, and nausea.

Chronic Repeated exposure

To 77-237 ppm has caused fatigue, dullness, urinary frequency, and GI disturbances

Special/Other Control Measures

Odor threshold: 85 ppm (chloroform); 1-5 ppm (hydrochloric acid)

Personal Protective Equipment (PPE)

OSHA/ANSI approved chemical safety eyewear or goggles

Compatible chemical-resistant gloves: PVC and rubber are not suitable for PPE

Wear NIOSH/MSHA approved respirator for organic/acid gas, dust, and mists to prevent inhalation.

Protective Clothing (e.g., lab coat)

Other Standard Safety Equipment and Engineering Preventive Measures

Safety shower and eye wash

Mechanical exhaust required. Hood recommended. Use adequate general and/or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits.

Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas.

General Precautions and Handling Measures

Avoid ingestion, inhalation and contact with eyes, skin, and clothing.

Avoid prolonged or repeated exposure. Wash thoroughly after handling.

Wash contaminated clothing before reuse. Discard contaminated footwear.

Chloroform is readily absorbed through skin and lungs.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance, Odor, and Other Properties

Form:	liquid	Odor:	sweet, fruity odor
Freeze/MP:	-63.5°C	Water Reactive:	no
Boiling Point (1atm):	61-62°C	Water Solubility:	slightly
Specific Gravity (H ₂ O = 1.0):	1.483	VP (mmHg):	160mm @ 20°C
Vapor Density (air=1):	4.12	% Volatiles:	98%
Evap. Rate (BuAc = 1.0):	11.6	pH:	NE
Refractive Index (nD ₂₀):	1.4476	Critical Temp:	263.2°C
Critical Press:	54 atm	Octanol Water Dist. Coeff:	1.97
Soluble in Organic Solvents:	NE	Henry's Law Const:	3.6x10-13 atm-m ³ /mol at 24°C

10. STABILITY AND REACTIVITY

Stability

Stable if stored tightly sealed and refrigerated--protected from light, air, and heat.

Incompatibilities

Acids, Acetone, Strong oxidizers, and Aluminum, magnesium

Alkalies and caustics (ammonium hydroxide, sodium methoxide, potassium hydroxide, etc.)

Dinitrogen tetroxide, Disilane, Fluorine, Triisopropylphosphine

Water or moist air— Contact with moist air or water may produce small amounts of hydrochloric acid, that in contact with metals may form flammable or explosive hydrogen gas.

Will attack some forms of plastic, rubber, and coatings

Precautions

Avoid incompatibilities. Protect from heat, flames, sparks, and ignition sources.

Keep out of water supplies and sewers.

Hazardous Combustion or Decomposition Products

carbon oxides, hydrochloric acid, chlorine, phosgene, hydrogen fluoride

Hazardous Polymerization

None

11. TOXICOLOGICAL INFORMATION

RTECS #

CAS #

not assigned	N-TFA-L-prolyl chloride	36724-68-2
not assigned	N-TFA-D-prolyl chloride	71890-93-2
FS9100000	Chloroform	356-42-3
MW4025000	Hydrogen Chloride*	7647-01-0

Irritation Data	eye	skin
N-TFA-L-prolyl chloride	NDA	NDA
N-TFA-D-prolyl chloride	NDA	NDA
Chloroform	eye rbt 148 mg; eye rbt 20 mg/24H mod	skin rbt 10 mg/24H open mld; skin rbt 500 mg/24H mld
Hydrogen Chloride*	eye rbt 5 mg/30S rinse mld	NDA

*Small amounts of HCl may be produced on contact with water.

Toxicity Data	oral	inhalation	dermal
N-TFA-L-prolyl Cl	NDA	NDA	NDA
N-TFA-D-prolyl Cl	NDA	NDA	NDA
Chloroform	orl rat LD50 695 mg/kg	ihl rat LC50 47,702 mg/m3/4H	skin rbt LD50:>20 gm/kg
Hydrogen Chloride*	orl rbt LD50 900 mg/kg	ihl rat LC50 3124ppm/1H	NDA

*Small amounts of HCl may be produced on contact with water.

Carcinogenicity	OSHA	IARC	NTP	ACGIH	NIOSH	Notes
N-TFA-L-prolyl Cl	NL	NL	NL	NL	NL	None
N-TFA-D-prolyl Cl	NL	NL	NL	NL	NL	None
Chloroform	Y	Y	Y	Y	Y	May cause cancer based on animal studies; possible cancer hazard; ACGIH-A3-Animal Carcinogen; California-carcinogen; initial date 10/01/1987; NIOSH--occupational carcinogen; NTP-Suspect carcinogen; OSHA--Possible select carcinogen; IARC--Group 2B carcinogen
Hydrogen Chloride*	NL	NL	NL	NL	NL	IARC Group 3-Not classifiable as a carcinogen

NL = Not Listed as a carcinogen; Lab studies indicate that chloroform causes cancer in animals and may cause cancer in humans. The risk depends on level and duration of exposure. *Small amounts of HCl may be produced on contact with water.

Only selected Registry of Harmful effects of Chemical Substance data (RTECS) is presented here.

Teratogenicity and Reproductive Effects

Lab studies reported in RTECS indicate that chloroform may cause adverse fetal effects, newborn harm, and reproductive effects. RTECS also reports laboratory studies that indicate that hydrochloride acid may cause adverse fetal effects.

Neurotoxicity

No data available.

Mutagenicity

RTECS reports mutation data on chloroform and hydrogen chloride.

Acute and Chronic Effects

See specific route responses in Section 3 Hazards Identification above.

Miscellaneous

No data available.

To the best of our knowledge, the chemical, physical, and Toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

Environmental Fate

N-TFA-L-prolyl chloride and N-TFA-D-prolyl chloride:

No data available.

Chloroform:

When released into the soil, this material is expected to leach into groundwater where it will reside for long periods of time. Releases to water and land will quickly evaporate. When released into the water, this material is expected to have a half-life between 1-10 days. This material has a log octanol-water partition coefficient of less than 3.0. This material is not expected to significantly bioaccumulate. When released into the air it may be transported long distances and will moderately photodegrade with a half-life of a few months. When released into the air, this material may be removed from the atmosphere to a moderate extent by wet deposition.

Hydrochloric Acid:

Rapidly hydrolyzes when exposed to water. Will exhibit extensive evaporation from soil surfaces. Upon transport through the soil, hydrochloric acid will dissolve some of the soil materials (especially those with carbonate bases) and the acid will neutralize to some degree.

Environmental Toxicity

Chloroform:

It will not be expected to bioconcentrate into the food chain but contamination of food is likely due to its use as an extractant and its presence in drinking water. It is not expected to be toxic to aquatic life in small quantities.

N-TFA-L-prolyl chloride, N-TFA-D-prolyl chloride, and Hydrochloric Acid:

No data available.

EcoToxicity Data

Chloroform:

Fish Toxicity: 66,800 ug/L 96H LC50 (Mortality) Rainbow trout, donaldson trout (*Oncorhynchus mykiss*)

Invertebrate Toxicity: 32,000 ug/L 96H NOEC (Mortality) Pink shrimp (america) (*Penaeus duorarum*)

Algal Toxicity: >3,200,000 ug/L 48H (Population Growth) Cryptomonad (*Chilomonas paramecium*)

Other Toxicity: 270 ug/L 7H EC50 (Teratogenesis) Spring peeper (*Hyla crucifer*)

N-TFA-L-prolyl chloride, N-TFA-D-prolyl chloride, and Hydrochloric Acid:

No data available.

Fate and Transport

Chloroform: Bioconcentration: 690 Ci/mol 6H BCF (Residue) Green algae (*Selenastrum capricornutum*) 13.9 Ci/mol

N-TFA-L-prolyl chloride, N-TFA-D-prolyl chloride, and Hydrochloric Acid:

No data available.

Standard Chemical Precautions

Keep out of air, water, and soil

13. DISPOSAL CONSIDERATIONS

That which cannot be recovered or recycled, should be disposed of in accordance with all applicable Federal, State, and local environmental regulations.

RCRA waste code(s):

D022 RCRA Hazard Class (40CFR 261): Toxic--chloroform

14. TRANSPORT INFORMATION

Ship in accordance with all applicable local, State, Federal, and International transportation regulations. The following is a summary only. Check regulations for complete information:

U. S. Department of Transportation (49CFR171.101)

Shipping Name: Chloroform
 Hazard Class : 6.1, Subsidiary
 Class: none
 ID Number: UN1888
 Packing Group: III
 Labeling: 6.1; Poison PG III

15. REGULATORY INFORMATION

Reviews, Standards, and Regulations

.....	N-TFA-L-prolyl ..N-TFA-D-prolyl . Chloroform	Hydrogen			
.....	Chloride	Chloride	Chloride**	
CAS number	36724-68-2	71890-93-2	356-42-3	7647-01-0	
TSCA:.....	NL*	NL*	Y.....Y
*This compound is sold strictly for FDA or research and development use.					
**Under EPA Hydrochloric acid, aq/Hydrogen chloride, gas may be regulated differently.					
EINECS:.....	NL.....	NL.....	Y.....	Y.....	
Number	NA	NA	206-604-2	231-595-7	
OSHA Process Safety [29 CFR 1910.119]:.....	NL.....	NL.....	NL.....	Y/NL	
TQ (lbs)	NA	NA	NA	5,000/NA	
CERCLA [Section 103 (40 CFR 302.4)]:.....	NL.....	NL.....	Y.....		
RQ (lbs)	NA	NA	10	5,000	
RCRA Waste Code.....	NA	NA	U044 [pure only].....	NA	
Clean Air Act					
[Section 112r (40 CFR 68)]:.....	NL.....	NL.....	Y.....	Y.....	
TQ (lbs)	NA	NA	20,000	15,000/5,000	
Contains Ozone Depleters (Class I or Class II)	N.....	N	N	N.....	
SARA Title III Notification [40 CFR 302.4]:					
Section 302/304 (EHS) Ingredient					
[40 CFR 355.3]	NL.....	NL.....	Y.....	NL/Y	
TPQ (lbs)	NA	NA	10,000	NA/500	
RQ (lbs)	NA	NA	10,000	NA/500	
Section 313 Ingredient [40 CFR 372.65]	NL.....	NL.....	Y.....	NL/Y	
State Lists:.....					
States.....	NA	NA	CA, FL, MA.....	NA	
			MN, NJ, PA		
On CA 65 Significant Risk Level.....	NA	NA	Y.....	NA	

**WARNING: This product contains a chemical(s) known to the State of California to cause cancer.
 (Chloroform)**

Sara	Acute	Chronic	Fire	Pressure	Reactivity
Title III	Y	Y	N	N	N
	Health	Flammability	Reactivity	Special Hazards	
NFPA	2	0	1	W	
HMIS	2*	0	1	None	

European Labeling (67/548/EEC or 1999/45/EC) Symbol(s)

Xn..... Harmful

Risk Phrases:

Caution: The properties of this material have not been fully investigated.

R22 Harmful if swallowed

R36/37/38 Irritating to eyes, respiratory system, and skin

R40 Possible risk of irreversible effects

R48/20/22 Harmful: Danger of serious damage to health by prolonged exposure through inhalation and if swallowed

R64 Vapors cause drowsiness and dizziness

Safety Phrases:

S23/24/25 Do not breath vapors. Avoid contact with skin and eyes

S26/28 In case of contact with eyes or skin, rinse immediately with plenty of water and seek medical advice

S36/37/39 Wear suitable protective clothing, gloves, and eye/face protection

16. OTHER INFORMATION

The above information is believed to be correct but does not purport to be complete and should be used only as a guide. The burden of safe use of this material rests entirely with the user.

04/18/2014