

4-(Trifluoromethyl)phenylacetonitrile: sc-226445



The Power to Question

MATERIAL SAFETY DATA SHEET

1 Identification of substance:

Product Name: 4-(Trifluoromethyl)phenylacetonitrile
Catalog Number: sc-226445
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

2 Hazard(s) identification

Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008



GHS06 Skull and crossbones

Acute Tox. 3 H331 Toxic if inhaled.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.
Acute Tox. 4 H312 Harmful in contact with skin.
Skin Irrit. 2 H315 Causes skin irritation.
Eye Irrit. 2A H319 Causes serious eye irritation.
STOT SE 3 H335 May cause respiratory irritation.

Classification according to Directive 67/548/EEC or Directive 1999/45/EC



Xn; Harmful

R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.



Xi; Irritant

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

Information concerning particular hazards for human and environment: Not applicable

Hazards not otherwise classified No information known.

Label elements

Labelling according to Regulation (EC) No 1272/2008

The substance is classified and labeled according to the CLP regulation.

Hazard pictograms



GHS06

Signal word Danger

Hazard statements

H302+H312 Harmful if swallowed or in contact with skin.

H331 Toxic if inhaled.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see on this label).

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

D1B - Toxic material causing immediate and serious toxic effects

D2B - Toxic material causing other toxic effects



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH	2	Health (acute effects) = 2
FIRE	1	Flammability = 1
REACTIVITY	1	Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

2338-75-2 4-(Trifluoromethyl)phenylacetone nitrile

Identification number(s):

EC number: 219-052-2

4 First-aid measures

Description of first aid measures

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

After eye contact

Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Seek medical treatment.

Information for doctor

Most important symptoms and effects, both acute and delayed

No further relevant information available.

Indication of any immediate medical attention and special treatment needed

No further relevant information available.

5 Fire-fighting measures

Extinguishing media

Suitable extinguishing agents

Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Nitrogen oxides (NOx)

Hydrogen fluoride (HF)

Hydrogen cyanide (HCN)

Advice for firefighters

Protective equipment:

Wear self-contained respirator.

Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Environmental precautions:

Do not allow material to be released to the environment without proper governmental permits.

Do not allow product to reach sewage system or any water course.

Do not allow to penetrate the ground/soil.

Methods and material for containment and cleaning up:

Dispose contaminated material as waste according to item 13.

Ensure adequate ventilation.

Prevention of secondary hazards: No special measures required.

Reference to other sections

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

7 Handling and storage

Handling

Precautions for safe handling

Keep container tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation at the workplace.

Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities

Storage Store at room temperature.

Requirements to be met by storerooms and receptacles: No special requirements.

Information about storage in one common storage facility: Store away from oxidizing agents.

Further information about storage conditions:

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace: Not required.

Additional information: No data

Exposure controls

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

Breathing equipment: Use suitable respirator when high concentrations are present.

Protection of hands:

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality.

Quality will vary from manufacturer to manufacturer.

Eye protection: Safety glasses

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties	
General Information	
Appearance:	
Form:	Crystalline
Formula:	C ₉ H ₆ F ₃ N
Weight:	185.15
pH-value:	
Not applicable.	
Change in condition	
Melting point/Melting range:	43-47 °C (109-117 °F)
Boiling point/Boiling range:	131-132 °C (268-270 °F) (20mm Hg)
Sublimation temperature / start:	Not determined
Flash point:	
> 110 °C (> 230 °F)	
Flammability (solid, gaseous)	
Not determined.	
Ignition temperature:	
Not determined	
Decomposition temperature:	
Not determined	
Auto igniting:	
Not determined.	
Danger of explosion:	
Product does not present an explosion hazard.	
Explosion limits:	
Lower:	Not determined
Upper:	Not determined
Vapor pressure:	
Not applicable.	
Density at 20 °C (68 °F):	
1.23 g/cm ³ (10.264 lbs/gal)	
Relative density	
Not determined.	
Vapor density	
Not applicable.	
Evaporation rate	
Not applicable.	
Solubility in / Miscibility with	
Water:	Insoluble
Partition coefficient (n-octanol/water):	
Not determined.	
Viscosity:	
dynamic:	Not applicable.
kinematic:	Not applicable.
Other information	
No further relevant information available.	

10 Stability and reactivity

Reactivity No information known.

Chemical stability Stable under recommended storage conditions.

Thermal decomposition / conditions to be avoided:

Decomposition will not occur if used and stored according to specifications.

Possibility of hazardous reactions No dangerous reactions known

Incompatible materials: Oxidizing agents

Hazardous decomposition products:

Carbon monoxide and carbon dioxide

Nitrogen oxides

Hydrogen fluoride

Hydrogen cyanide

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful if inhaled.

Harmful in contact with skin.

Harmful if swallowed.

Danger through skin absorption.

LD/LC50 values that are relevant for classification: No data

Skin irritation or corrosion: Causes skin irritation.

Eye irritation or corrosion: Causes serious eye irritation.

Sensitization: No sensitizing effects known.

Germ cell mutagenicity: No effects known.

Carcinogenicity:

No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

Reproductive toxicity: No effects known.

Specific target organ system toxicity - repeated exposure: No effects known.

Specific target organ system toxicity - single exposure: May cause respiratory irritation.

Aspiration hazard: No effects known.

Subacute to chronic toxicity:

Nitriles may resemble cyanides in toxicity. Exposure to nitriles may cause increased salivation, flushing of the face, eye and respiratory tract irritation, shallow respiration, nausea, vomiting, weakness, headache and diarrhea. Jaundice, anemia, and leucocytosis has been reported in some cases.

Additional toxicological information:

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity

Aquatic toxicity: No further relevant information available.

Persistence and degradability No further relevant information available.

Behavior in environmental systems:

Bioaccumulative potential No further relevant information available.

Mobility in soil No further relevant information available.

Additional ecological information:

General notes:

Do not allow material to be released to the environment without proper governmental permits. Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

Avoid transfer into the environment.

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

Other adverse effects No further relevant information available.

13 Disposal considerations



Waste treatment methods


Recommendation Consult state, local or national regulations to ensure proper disposal.

Uncleaned packagings:

Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, ADR, IMDG, IATA	UN3439
UN proper shipping name DOT ADR IMDG, IATA	Nitriles, solid, toxic, n.o.s. (4-(Trifluoromethyl)phenylacetonitrile) 3439 Nitriles, solid, toxic, n.o.s. (4-(Trifluoromethyl)phenylacetonitrile) NITRILES, SOLID, TOXIC, N.O.S. (4-(Trifluoromethyl)phenylacetonitrile)
Transport hazard class(es) DOT  Class Label ADR  Class	6.1 Toxic substances. 6.1 6.1 (T2) Toxic substances

Label IMDG, IATA	6.1
	
Class Label	6.1 Toxic substances. 6.1
Packing group DOT, ADR, IMDG, IATA	III
Environmental hazards:	Not applicable.
Special precautions for user Danger code (Kemler):	Warning: Toxic substances 60
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information: DOT Marine Pollutant (DOT):	 No
UN "Model Regulation":	UN3439, Nitriles, solid, toxic, n.o.s. (4-Trifluoromethyl)phenylacetonitrile), 6.1, III

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations

This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.

SARA Section 313 (specific toxic chemical listings) Substance is not listed.

California Proposition 65

Prop 65 - Chemicals known to cause cancer Substance is not listed.

Prop 65 - Developmental toxicity Substance is not listed.

Prop 65 - Developmental toxicity, female Substance is not listed.

Prop 65 - Developmental toxicity, male Substance is not listed.

Information about limitation of use: For use only by technically qualified individuals.

Other regulations, limitations and prohibitive regulations

Substances of very high concern (SVHC) according to REACH, Article 57

Substance is not listed.

REACH - Pre-registered substances Substance is listed.

Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

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.