

3-Hydroxybutyric acid

sc-231749

Material Safety Data Sheet



The Power to Question

Hazard Alert Code Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

3-Hydroxybutyric acid

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

C4-H8-O3, CH₃CHOHCH₂COOH, "3-hydroxy-butanoic acid", "beta-hydroxybutyric acid", "d-hydroxybutyric acid", "l-hydroxybutyric acid", "dl-hydroxybutyric acid", "dl-beta-hydroxybutyric acid", "(+/-)-3-hydroxybutanoic acid wrongly named as", "gamma-hydroxybutyric acid"

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

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

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



CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

Irritating to eyes, respiratory system and skin.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ The material has NOT been classified as "harmful by ingestion".
This is because of the lack of corroborating animal or human evidence.

EYE

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

SKIN

■ This material can cause inflammation of the skin on contact in some persons.
■ The material may accentuate any pre-existing dermatitis condition.
■ Skin contact with the material may damage the health of the individual; systemic effects may result following absorption.
■ 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

■ The material can cause respiratory irritation in some persons.
The body's response to such irritation can cause further lung damage.
■ Inhalation hazard is increased at higher temperatures.

CHRONIC HEALTH EFFECTS

■ Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.
Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
3-hydroxybutyric acid	300-85-6	>98
on distillation decomposes to		
crotonic acid	107-93-7	

Section 4 - FIRST AID MEASURES

SWALLOWED

· Immediately give a glass of water. · First aid is not generally required. If in doubt, contact a Poisons Information Center or a doctor.

EYE

■ If this product comes in contact with the eyes: · Wash out immediately with fresh 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.

SKIN

■ If skin contact occurs: · Immediately remove all contaminated clothing, including footwear · Flush skin and hair with running water (and soap if available).

INHALED

· If fumes or combustion products are inhaled remove from contaminated area. · Lay patient down. Keep warm and rested.

NOTES TO PHYSICIAN

■ Treat symptomatically.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Not available
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	1.126
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA

· Water spray or fog.
· Alcohol stable foam.
· Dry chemical powder.
· Carbon dioxide.

FIRE FIGHTING

- Alert Emergency Responders and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- Combustible.
- Slight fire hazard when exposed to heat or flame.

Combustion products include: carbon dioxide (CO₂), other pyrolysis products typical of burning organic material.

May emit poisonous fumes.

May emit corrosive fumes.

FIRE INCOMPATIBILITY

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

PERSONAL PROTECTION

Glasses:

Chemical goggles.

Gloves:

Respirator:

Type A Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.

MAJOR SPILLS

- Moderate hazard.
- Clear area of personnel and move upwind.
- Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- DO NOT allow clothing wet with material to stay in contact with skin.
- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.

RECOMMENDED STORAGE METHODS

- Metal can or drum
- Packing as recommended by manufacturer.

STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- No smoking, naked lights or ignition sources.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.
- Protect containers against physical damage and check regularly for leaks.
- Observe manufacturer's storing and handling recommendations.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m ³	STEL ppm	STEL mg/m ³	Peak ppm	Peak mg/m ³	TWA F/CC	Notes
Canada - British Columbia Occupational Exposure Limits	crotonic acid (Particles (Insoluble or Poorly Soluble) Not Otherwise Classified (PNOC))		10 (N)						
US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants	crotonic acid (Particulates not otherwise regulated (PNOR)(f)-Respirable fraction)		5						

US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	crotonic acid (Particulates not otherwise regulated Respirable fraction)	-	5	
US - California Permissible Exposure Limits for Chemical Contaminants	crotonic acid (Particulates not otherwise regulated Respirable fraction)	-	5	(n)
US - Oregon Permissible Exposure Limits (Z-1)	crotonic acid (Particulates not otherwise regulated (PNOR) (f) Total Dust)	-	10	Bold print identifies substances for which the Oregon Permissible Exposure Limits (PELs) are different than the federal Limits. PNOR means "particles not otherwise regulated."
US - Michigan Exposure Limits for Air Contaminants	crotonic acid (Particulates not otherwise regulated, Respirable dust)	-	5	
Canada - Prince Edward Island Occupational Exposure Limits	crotonic acid (Particles (Insoluble or Poorly Soluble) [NOS] Inhalable particles)	-	10	See Appendix B current TLV/BEI Book
US - Oregon Permissible Exposure Limits (Z-1)	crotonic acid (Particulates not otherwise regulated (PNOR) (f) Respirable Fraction)	-	5	Bold print identifies substances for which the Oregon Permissible Exposure Limits (PELs) are different than the federal Limits. PNOR means "particles not otherwise regulated."

ENDOELTABLE

The following materials had no OELs on our records

- 3-hydroxybutyric acid: CAS:300-85-6 CAS:625-71-8 CAS:6168-83-8

PERSONAL PROTECTION



RESPIRATOR

Type A Filter of sufficient capacity
Consult your EHS staff for recommendations

EYE

- Safety glasses with side shields.
- Chemical goggles.

HANDS/FEET

■ Wear chemical protective gloves, eg. PVC.

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

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

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).

- When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
- When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
- Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

- Neoprene gloves.

OTHER

- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.
- Eye wash unit.

ENGINEERING CONTROLS

■ General exhaust is adequate under normal operating conditions. Local exhaust ventilation may be required in special circumstances.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Liquid.

Mixes with water.

State	Liquid	Molecular Weight	104.11
Melting Range (°F)	Not available	Viscosity	Not Available
Boiling Range (°F)	244.4- 248 (2 mm)	Solubility in water (g/L)	Miscible
Flash Point (°F)	>230	pH (1% solution)	Not available
Decomposition Temp (°F)	Not available.	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapour Pressure (mmHG)	Not available
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	1.126
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	>1
Volatile Component (%vol)	Not available	Evaporation Rate	Not available

APPEARANCE

■ Family of products which vary in their physical properties as a result of variations in production. Data presented here is for typical family member. Hygroscopic syrup; mixes with water, alcohol, ether. K = 3.86×10^{-5} d-form: White crystalline solid with melting point 43-46. l-form: Hygroscopic monoclinic crystals with melting point 45.5-48.0 deg C. Forms bimolar esterification products up to 35%.

Ecotoxicity of acrylates is a function of n-octanol/ water partition coefficient (log Pow, log Kow). Compounds with a log Pow >5 exhibit simple narcosis, but at lower log Pow the toxicity of acrylates is greater than predicted for simple narcotics. log Kow 0.72

Material	Value
----------	-------

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.

STORAGE INCOMPATIBILITY

■ Avoid reaction with oxidizing agents.

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

Section 11 - TOXICOLOGICAL INFORMATION

3-hydroxybutyric acid

TOXICITY AND IRRITATION

■ unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

■ 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. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.

3-HYDROXYBUTYRIC ACID:

■ No significant acute toxicological data identified in literature search.

CROTONIC ACID:

TOXICITY	IRRITATION
Oral (rat) LD50: 1000 mg/kg	Skin (rabbit): 10 mg/24h (open)
Oral (mouse) LD50: 4800 mg/kg	
Intraperitoneal (mouse) LD50: 25 mg/kg	
Subcutaneous (mouse) LD50: 3590 mg/kg	
Dermal (rabbit) LD50: 600 mg/kg	
Dermal (guinea pig) LD50: 200 mg/kg	

■ The material may be irritating to the eye, with prolonged contact causing inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis.

The material may produce respiratory tract irritation, and result in damage to the lung including reduced lung function.

The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of vesicles, scaling and thickening of the skin.

Based on the available oncogenicity data and without a better understanding of the carcinogenic mechanism the Health and Environmental Review Division (HERD), Office of Toxic Substances (OTS), of the US EPA previously concluded that all chemicals that contain the acrylate or methacrylate moiety ($\text{CH}_2=\text{CHCOO}$ or $\text{CH}_2=\text{C}(\text{CH}_3)\text{COO}$) should be considered to be a carcinogenic hazard unless shown otherwise by adequate testing.

This position has now been revised and acrylates and methacrylates are no longer de facto carcinogens.

CARCINOGEN

VPVB_(VERY~	US - Maine Chemicals of High Concern List	Carcinogen	CA Prop 65; IARC; NTP 11th ROC
-------------	---	------------	--------------------------------

Section 12 - ECOLOGICAL INFORMATION

No data

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
3-hydroxybutyric acid	HIGH		LOW	HIGH
crotonic acid	HIGH		LOW	HIGH

GESAMP/EHS COMPOSITE LIST - GESAMP Hazard Profiles

Name / EHS TRN A1a A1b A1 A2 B1 B2 C1 C2 C3 D1 D2 D3 E1 E2 E3 Cas No / RTECS No _____
_____ [Heavy 226 282 5 2 (2) NR 1 NI 0 0 (1) 1 1 FE 2 Oxo 6 5 Fraction] / CAS:300- 85- 6 /

Legend: EHS=EHS Number (EHS=GESAMP Working Group on the Evaluation of the Hazards of Harmful Substances Carried by Ships)
NRT=Net Register Tonnage, A1a=Bioaccumulation log Pow, A1b=Bioaccumulation BCF, A1=Bioaccumulation, A2=Biodegradation, B1=Acuteaquatic toxicity LC/ECIC50 (mg/l), B2=Chronic aquatic toxicity NOEC (mg/l), C1=Acute mammalian oral toxicity LD50 (mg/kg), C2=Acute mammalian dermal toxicity LD50 (mg/kg), C3=Acute mammalian inhalation toxicity LC50 (mg/kg), D1=Skin irritation & corrosion, D2=Eye irritation & corrosion, D3=Long-term health effects, E1=Tainting, E2=Physical effects on wildlife & benthic habitats, E3=Interference with coastal amenities, For column A2: R=Readily biodegradable, NR=Not readily biodegradable. For column D3: C=Carcinogen, M=Mutagenic, R=Reprotoxic, S=Sensitising, A=Aspiration hazard, T=Target organ systemic toxicity, L=Lung injury, N=Neurotoxic, I=Immunotoxic. For column E1: NT=Not tainting (tested), T=Tainting test positive. For column E2: Fp=Persistent floater, F=Floater, S=Sinking substances. The numerical scales start from 0 (no hazard), while higher numbers reflect increasing hazard. (GESAMP/EHS Composite List of Hazard Profiles - Hazard evaluation of substances transported by ships)

Section 13 - DISPOSAL CONSIDERATIONS

Disposal Instructions

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

‡ 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. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. 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.

DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.

- Recycle wherever possible or consult manufacturer for recycling options.
- Consult Waste Management Authority for disposal.

Section 14 - TRANSPORTATION INFORMATION

NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: DOT, IATA, IMDG

Section 15 - REGULATORY INFORMATION

3-hydroxybutyric acid (CAS: 300-85-6,625-71-8,6168-83-8) is found on the following regulatory lists;

"Canada Domestic Substances List (DSL)", "US Toxic Substances Control Act (TSCA) - Inventory"

Regulations for ingredients

crotonic acid (CAS: 107-93-7,3724-65-0) is found on the following regulatory lists;

"US FDA Indirect Food Additives: Adhesives and Components of Coatings - Substances for Use Only as Components of Adhesives - Adhesives"

Section 16 - OTHER INFORMATION

ND

Substance CAS Suggested codes crotonic acid 107- 93- 7 AUTOID~ crotonic acid 3724- 65- 0 AUTOID~

Ingredients with multiple CAS Nos

Ingredient Name CAS 3-hydroxybutyric acid 300-85-6, 625-71-8, 6168-83-8 crotonic acid 107-93-7, 3724-65-0

Reasonable care has been taken in the preparation of this information, but the author makes no warranty of merchantability or any other warranty, expressed or implied, with respect to this information. The author makes no representations and assumes no liability for any direct, incidental or consequential damages resulting from its use. For additional technical information please call our toxicology department on +800 CHEMCALL.

■ 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. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

This document is copyright. Apart from any fair dealing for the purposes of private study, research, review or criticism, as permitted under the Copyright Act, no part may be reproduced by any process without written permission from CHEMWATCH. TEL (+61 3) 9572 4700.

Issue Date: Feb-3-2009

Print Date:Mar-5-2011