

## MATERIAL SAFETY DATA SHEET

Date Printed: 04/01/2008

Date Updated: 11/01/2007

Version 1.8

## Section 1 - Product and Company Information

Product Name                   HEXANOIC ACID, 99.5+%  
Product Number                153745  
Brand                           ALDRICH

Company                         Sigma-Aldrich  
Address                         3050 Spruce Street  
                                  SAINT LOUIS MO 63103 US

Technical Phone:               800-325-5832  
Fax:                            800-325-5052  
Emergency Phone:               314-776-6555

## Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
CAPROIC ACID	142-62-1	No

Formula                    C6H12O2  
Synonyms                   Butylacetic acid \* n-Caproic acid \* Capronic acid  
                              \* Hexacid 698 \* n-Hexanoic acid \* n-Hexanoic acid \*  
                              Kyselina kapronova (Czech) \* Pentanecarboxylic  
                              acid \* Pentiformic acid \* Pentylformic acid

RTECS Number:               MO5250000

## Section 3 - Hazards Identification

## EMERGENCY OVERVIEW

Corrosive.  
Causes burns.  
Readily absorbed through skin. Stench.

## HMIS RATING

HEALTH: 3  
FLAMMABILITY: 1  
REACTIVITY: 0

## NFPA RATING

HEALTH: 3  
FLAMMABILITY: 1  
REACTIVITY: 0

For additional information on toxicity, please refer to Section 11.

## Section 4 - First Aid Measures

## ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician. Do not induce vomiting.

## INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

#### DERMAL EXPOSURE

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

#### EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

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#### Section 5 - Fire Fighting Measures

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##### FLASH POINT

215.6 °F    102 °C    Method: closed cup

##### EXPLOSION LIMITS

Lower: 2 %    Upper: 10 %

##### AUTOIGNITION TEMP

380 °C

##### FLAMMABILITY

N/A

##### EXTINGUISHING MEDIA

Suitable: Carbon dioxide, dry chemical powder, or appropriate foam.

##### FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.  
Specific Hazard(s): Emits toxic fumes under fire conditions.

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#### Section 6 - Accidental Release Measures

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##### PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area.

##### PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

##### METHODS FOR CLEANING UP

Cover with dry lime or soda ash, pick up, keep in a closed container, and hold for waste disposal. Ventilate area and wash spill site after material pickup is complete.

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#### Section 7 - Handling and Storage

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##### HANDLING

User Exposure: Do not breathe vapor. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

##### STORAGE

Suitable: Keep tightly closed.

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#### Section 8 - Exposure Controls / PPE

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##### ENGINEERING CONTROLS

Safety shower and eye bath. Use only in a chemical fume hood.

## PERSONAL PROTECTIVE EQUIPMENT

**Respiratory:** Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator.  
**Hand:** Compatible chemical-resistant gloves.  
**Eye:** Chemical safety goggles.  
**Other:** Faceshield (8-inch minimum).

## GENERAL HYGIENE MEASURES

Wash contaminated clothing before reuse. Discard contaminated shoes. Wash thoroughly after handling.

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## Section 9 - Physical/Chemical Properties

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Appearance	Physical State: Clear liquid Color: Colorless Odor: Stench.	
Property	Value	At Temperature or Pressure
Molecular Weight	116.16 AMU	
pH	N/A	
BP/BP Range	204.0 - 205.0 °C	
MP/MP Range	- 3.0 °C	
Freezing Point	N/A	
Vapor Pressure	0.18 mmHg	20 °C
Vapor Density	4 g/l	
Saturated Vapor Conc.	N/A	
SG/Density	0.927 g/cm <sup>3</sup>	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	0.003 Pas	20 °C
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	215.6 °F 102 °C	Method: closed cup
Explosion Limits	Lower: 2 % Upper: 10 %	
Flammability	N/A	
Autoignition Temp	380 °C	
Refractive Index	1.416	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

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## Section 10 - Stability and Reactivity

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### STABILITY

**Stable:** Stable.  
**Materials to Avoid:** Bases, Oxidizing agents, Reducing agents, Allyl alcohol.

## HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

## HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

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## Section 11 - Toxicological Information

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### ROUTE OF EXPOSURE

Skin Contact: Causes burns.

Skin Absorption: May be harmful if absorbed through the skin.

Eye Contact: Causes burns.

Inhalation: May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.

Ingestion: May be harmful if swallowed.

### SIGNS AND SYMPTOMS OF EXPOSURE

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin.

Inhalation may result in spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis, and pulmonary edema.

Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting.

### TOXICITY DATA

Oral  
Rat  
2050 UL/KG  
LD50

Oral  
Mouse  
5000 mg/kg  
LD50

Inhalation  
Mouse  
4,100 mg/m<sup>3</sup>  
LC50

Intraperitoneal  
Mouse  
3180 MG/KG  
LD50

Subcutaneous  
Mouse  
3180 MG/KG  
LD50

Intravenous  
Mouse  
1725 MG/KG  
LD50

Remarks: Behavioral: Convulsions or effect on seizure threshold.  
Lungs, Thorax, or Respiration: Respiratory stimulation.

Skin

Rabbit  
630 UL/KG  
LD50

Skin  
Guinea pig  
5 ML/KG  
LD50

#### IRRITATION DATA

Skin  
Rabbit  
10 mg  
24H  
Remarks: Open irritation test

Skin  
Rabbit  
465 mg  
Remarks: Open irritation test

Eyes  
Rabbit  
0.75 mg  
Remarks: Severe irritation effect

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#### Section 12 - Ecological Information

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#### ACUTE ECOTOXICITY TESTS

Test Type: LC50 Fish  
Species: Pimephales promelas (Fathead minnow)  
Time: 96 h  
Value: 88 mg/l

Test Type: LC50 Fish  
Species: Oryzias latipes  
Time: 96 h  
Value: 80 mg/l

Test Type: EC50 Daphnia  
Species: Daphnia magna  
Time: 24 h  
Value: 22 mg/l

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#### Section 13 - Disposal Considerations

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#### APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

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#### Section 14 - Transport Information

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#### DOT

Proper Shipping Name: Caproic acid  
UN#: 2829  
Class: 8  
Packing Group: Packing Group III

Hazard Label: Corrosive

PIH: Not PIH

IATA

Proper Shipping Name: Caproic acid

IATA UN Number: 2829

Hazard Class: 8

Packing Group: III

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Section 15 - Regulatory Information

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EU ADDITIONAL CLASSIFICATION

Symbol of Danger: C

Indication of Danger: Corrosive.

R: 34

Risk Statements: Causes burns.

S: 26-36/37/39-45

Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves, and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Corrosive.

Risk Statements: Causes burns.

Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Take off immediately all contaminated clothing. Wear suitable protective clothing, gloves, and eye/face protection. Do not breathe vapor.

US Statements: Readily absorbed through skin. Stench.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No

TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.

DSL: Yes

NDSL: No

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Section 16 - Other Information

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DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2008 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.