



Pentanoic acid (D₉, 98%)

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Issue date: 4/11/2011 Revision date: 3/5/2024 Supersedes: 8/21/2015 Version: 3.0

SECTION 1: Identification

1.1. Identification

Product form : Substance
Substance name : Pentanoic acid (D₉, 98%)
CAS-No. : 109-52-4
Product code : DLM-572
Formula : C₅H₁₀O₂
Synonyms : Valeric acid; 1-Butanecarboxylic acid

1.2. Recommended use and restrictions on use

No additional information available

1.3. Supplier

Cambridge Isotope Laboratories, Inc.
50 Frontage Rd
01810
ANDOVER, MA, 01810
USA
T 1-800-322-1174
cilsales@isotope.com - www.isotope.com

1.4. Emergency telephone number

Emergency number : 1-703-741-5970
Chemtrec 1-800-424-9300 24 hours

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Acute toxicity (oral) Category 4	H302	Harmful if swallowed
Skin corrosion/irritation Category 1A	H314	Causes severe skin burns and eye damage
Serious eye damage/eye irritation Category 1	H318	Causes serious eye damage
Reproductive toxicity Category 2	H361	(Dermal, Inhalation, oral)
Hazardous to the aquatic environment – Acute Hazard Category 3	H402	Harmful to aquatic life
Hazardous to the aquatic environment – Chronic Hazard Category 3	H412	Harmful to aquatic life with long lasting effects

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US) :



Signal word (GHS US) : Danger
Hazard statements (GHS US) : H302 - Harmful if swallowed
H314 - Causes severe skin burns and eye damage
H318 - Causes serious eye damage
H361 - (Dermal, Inhalation, oral)

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Precautionary statements (GHS US)	: H402 - Harmful to aquatic life H412 - Harmful to aquatic life with long lasting effects P201 - Obtain special instructions before use. P202 - Do not handle until all safety precautions have been read and understood. P260 - Do not breathe dust, fume, gas, mist, spray, vapors. P264 - Wash Both hands thoroughly after handling. P270 - Do not eat, drink or smoke when using this product. P273 - Avoid release to the environment. P280 - Wear protective clothing, protective gloves. P301+P312 - If swallowed: Call a doctor if you feel unwell. P301+P330+P331 - If swallowed: rinse mouth. Do NOT induce vomiting. P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing. P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P308+P313 - If exposed or concerned: Get medical advice/attention. P310 - Immediately call a doctor. P321 - Specific treatment (see Hazard pictograms (CLP) on this label). P330 - Rinse mouth. P363 - Wash contaminated clothing before reuse. P405 - Store locked up. P501 - Dispose of contents/container to Comply with applicable regulations.
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2.3. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	GHS US classification
Pentanoic acid (D ₉ , 98%) (Main constituent)	CAS-No.: 109-52-4	100	Acute Tox. 4 (Oral), H302 Skin Corr. 1A, H314 Eye Dam. 1, H318 Repr. 2, H361 Aquatic Acute 3, H402 Aquatic Chronic 3, H412

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general	: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
First-aid measures after inhalation	: If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.

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First-aid measures after skin contact	: Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.
First-aid measures after eye contact	: Continue rinsing eyes during transport to hospital. Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.
First-aid measures after ingestion	: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2. Most important symptoms and effects (acute and delayed)

Potential Adverse human health effects and symptoms	: This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product. Nausea. Headache. Vomiting. The chemical, physical, and toxicological properties have not been thoroughly investigated.
Symptoms/effects	: Suspected of damaging fertility. Suspected of damaging the unborn child. (in contact with skin, if inhaled, if swallowed).
Symptoms/effects after inhalation	: May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Symptoms/effects after skin contact	: Causes severe skin burns.
Symptoms/effects after eye contact	: Causes severe eye damage.
Symptoms/effects after ingestion	: Harmful if swallowed.

4.3. Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

5.2. Specific hazards arising from the chemical

No additional information available

5.3. Special protective equipment and precautions for fire-fighters

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment. Avoid breathing vapors, mist, or gas. Ensure adequate ventilation. Evacuate personnel to safe area.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Do not discharge the product into the environment.

6.3. Methods and material for containment and cleaning up

For containment : Small quantities of liquid spill: take up in non-combustible absorbent material and shovel into container for disposal. For large spills, confine the spill in a dike and charge it with wet sand or earth for subsequent safe disposal.

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6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Avoid contact with skin and eyes. Avoid inhalation of vapor or mist. Normal measures for preventive fire protection.

Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Store at room temperature away from light and moisture.

Storage conditions : Store at room temperature away from light and moisture.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

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USA - ACGIH - Occupational Exposure Limits

ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
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8.2. Appropriate engineering controls

No additional information available

8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.

Materials for protective clothing:

Wear suitable protective clothing and gloves

Hand protection:

protective gloves

Eye protection:

Chemical goggles or safety glasses

Skin and body protection:

Wear suitable protective clothing, gloves and eye/face protection

Respiratory protection:

When appropriate, use NIOSH/CEN approved respirator.

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Personal protective equipment symbol(s):



SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Clear, Liquid.
Color	: Colorless
Odor	: Stench
Odor threshold	: No data available
pH	: 2.7 at 40 g/l at 20 °C (68 °F)
Melting point	: -20 – -18 °C (-4 - 0 °F) - lit
Freezing point	: No data available
Boiling point	: 110 – 111 °C (230 - 232 °F) at 13 hPa (10 mmHg) - lit. 185 °C (365 °F) - lit
Flash point	: 96 °C (205 °F) - closed cup
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: 0.2 hPa (0.15 mmHg) at 20 °C (68 °F)
Relative vapor density at 20°C	: 3.53 - (Air = 1.0)
Relative density	: No data available
Density	: 0.939 g/ml at 25 °C (77 °F)
Molecular mass	: 111.19 g/mol (Unlabeled)
Solubility	: Water: 40 g/l
Partition coefficient n-octanol/water (Log Pow)	: 1.39
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: 1.6 – 7.6 % (V)
Explosive properties	: No data available
Oxidizing properties	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

No additional information available

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10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

formed under fire conditions: Carbon oxides.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral) : Harmful if swallowed.
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Not classified

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ATE US (oral)	500 mg/kg body weight
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Skin corrosion/irritation : Causes severe skin burns.
pH: 2.7 at 40 g/l at 20 °C (68 °F)
Serious eye damage/irritation : Causes serious eye damage.
pH: 2.7 at 40 g/l at 20 °C (68 °F)
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified

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National Toxicology Program (NTP) Status	No component of this product present at levels greater than or equal to 0.1 % is identified as a known or anticipated carcinogen by NTP.
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Reproductive toxicity : (Dermal, Inhalation, oral).
STOT-single exposure : Not classified
STOT-repeated exposure : Not classified
Aspiration hazard : Not classified
Viscosity, kinematic : No data available
Potential Adverse human health effects and symptoms : This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product. Nausea. Headache. Vomiting. The chemical, physical, and toxicological properties have not been thoroughly investigated.
Symptoms/effects : Suspected of damaging fertility. Suspected of damaging the unborn child. (in contact with skin, if inhaled, if swallowed).
Symptoms/effects after inhalation : May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Symptoms/effects after skin contact : Causes severe skin burns.
Symptoms/effects after eye contact : Causes severe eye damage.
Symptoms/effects after ingestion : Harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - water : Harmful to aquatic life with long lasting effects.

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EC50 - Crustacea [1]	45 mg/l Daphnia magna (Water flea) - 48 h
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12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

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Partition coefficient n-octanol/water (Log Pow)	1.39
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12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Other adverse effects : Environmental precautions. Avoid release to the environment. Disposal must be done according to official regulations.

SECTION 13: Disposal considerations

13.1. Disposal methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.

Product/Packaging disposal recommendations : Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Ecology - waste materials : Dispose of as unused product.

SECTION 14: Transport information

In accordance with DOT / TDG / IMDG / IATA

14.1. UN number

DOT NA No	: UN3265
UN-No. (TDG)	: UN3265
UN-No. (IMDG)	: 3265
UN-No. (IATA)	: 3265

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Corrosive liquid, acidic, organic, n.o.s.
Proper Shipping Name (TDG)	: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.
Proper Shipping Name (IMDG)	: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.
Proper Shipping Name (IATA)	: Corrosive liquid, acidic, organic, n.o.s.

14.3. Transport hazard class(es)

DOT

Transport hazard class(es) (DOT)	: 8
Hazard labels (DOT)	: 8



TDG

Transport hazard class(es) (TDG)	: 8
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Hazard labels (TDG) : 8



IMDG

Transport hazard class(es) (IMDG) : 8

Hazard labels (IMDG) : 8



IATA

Transport hazard class(es) (IATA) : 8

Hazard labels (IATA) : 8



14.4. Packing group

Packing group (DOT) : III

Packing group (TDG) : III

Packing group (IMDG) : III

Packing group (IATA) : III

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

DOT

UN-No.(DOT) : UN3265

DOT Special Provisions (49 CFR 172.102) : 386 - Notwithstanding the provisions of §177.834(l) of this subchapter, cargo heaters may be used when weather conditions are such that the freezing of a wetted explosive material is likely. Shipments must be made by private, leased or contract carrier vehicles under exclusive use of the offeror. Cargo heaters must be reverse refrigeration (heat pump) units. Shipments made in accordance with this Special provision are excepted from the requirements of §173.60(b)(4) of this subchapter.

IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672).

T7 - 4 178.274(d)(2) Normal..... 178.275(d)(3)

TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = $97 / 1 + a (tr - tf)$ Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.

TP28 - A portable tank having a minimum test pressure of 2.65 bar (265 kPa) may be used provided the calculated test pressure is 2.65 bar or less based on the MAWP of the hazardous material, as defined in 178.275 of this subchapter, where the test pressure is 1.5 times the MAWP.

DOT Packaging Exceptions (49 CFR 173.xxx) : 154

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DOT Packaging Non Bulk (49 CFR 173.xxx)	: 203
DOT Packaging Bulk (49 CFR 173.xxx)	: 241
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 60 L
DOT Vessel Stowage Location	: A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
DOT Vessel Stowage Other	: 40 - Stow "clear of living quarters",53 - Stow "separated from" alkaline compounds,58 - Stow "separated from" cyanides

TDG

UN-No. (TDG)	: UN3265
TDG Special Provisions	: 16 - (1) The technical name of at least one of the most dangerous substances that predominantly contributes to the hazard or hazards posed by the dangerous goods must be shown, in parentheses, on the shipping document following the shipping name in accordance with clause 3.5(1)(c)(ii)(A) of Part 3 (Documentation). The technical name must also be shown, in parentheses, on a small means of containment or on a tag following the shipping name in accordance with subsections 4.11(2) and (3) of Part 4 (Dangerous Goods Safety Marks). (2) Despite subsection (1), the technical name for the following dangerous goods is not required to be shown on a shipping document or on a small means of containment when Canadian law for domestic transport or an international convention for international transport prohibits the disclosure of the technical name: (a) UN1544, ALKALOID SALTS, SOLID, N.O.S. or ALKALOIDS, SOLID, N.O.S; (b) UN1851, MEDICINE, LIQUID, TOXIC, N.O.S; (c) UN3140, ALKALOID SALTS, LIQUID, N.O.S. or ALKALOIDS, LIQUID, N.O.S; (d) UN3248, MEDICINE, LIQUID, FLAMMABLE, TOXIC, N.O.S; or (e) UN3249, MEDICINE, SOLID, TOXIC, N.O.S. (3) Despite subsection (1), the technical name for the following dangerous goods is not required to be shown on a small means of containment: (a) UN2814, INFECTIOUS SUBSTANCE, AFFECTING HUMANS; or (b) UN2900, INFECTIOUS SUBSTANCE, AFFECTING ANIMALS.
Explosive Limit and Limited Quantity Index	: 5 L
Excepted quantities (TDG)	: E1
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index	: 5 L
Emergency Response Guide (ERG) Number	: 153

IMDG

Special provision (IMDG)	: 223, 274
Limited quantities (IMDG)	: 5 L
Excepted quantities (IMDG)	: E1
Packing instructions (IMDG)	: P001, LP01
IBC packing instructions (IMDG)	: IBC03
Tank instructions (IMDG)	: T7
Tank special provisions (IMDG)	: TP1, TP28
EmS-No. (Fire)	: F-A - FIRE SCHEDULE Alfa - GENERAL FIRE SCHEDULE
EmS-No. (Spillage)	: S-B - SPILLAGE SCHEDULE Bravo - CORROSIVE SUBSTANCES
Stowage category (IMDG)	: A
Stowage and handling (IMDG)	: SW2
Segregation (IMDG)	: SGG1, SG36, SG49
Flash point (IMDG)	: '
Properties and observations (IMDG)	: Causes burns to skin, eyes and mucous membranes.
MFAG-No	: 153

IATA

PCA Excepted quantities (IATA)	: E1
PCA Limited quantities (IATA)	: Y841
PCA limited quantity max net quantity (IATA)	: 1L

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PCA packing instructions (IATA)	: 852
PCA max net quantity (IATA)	: 5L
CAO packing instructions (IATA)	: 856
CAO max net quantity (IATA)	: 60L
Special provision (IATA)	: A3, A803
ERG code (IATA)	: 8L

14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

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SARA Section 302 Threshold Planning Quantity (TPQ)	SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.
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SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard
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Commercial status of components according to the United States Environmental Protection Agency's Toxic Substances Control Act (TSCA):

Name	CAS-No.	Listing	Commercial status	Flags
Pentanoic acid (D ₉ , 98%)	109-52-4	Not present	-	

15.2. International regulations

CANADA

Pentanoic acid (D₉, 98%) (109-52-4)

Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

Pentanoic acid (D₉, 98%) (109-52-4)

Listed on INSQ (Mexican National Inventory of Chemical Substances)

15.3. US State regulations

Pentanoic acid (D₉, 98%) (109-52-4)

State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List
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SECTION 16: Other information

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Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

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Full text of H-phrases	
H302	Harmful if swallowed
H314	Causes severe skin burns and eye damage
H318	Causes serious eye damage
H361	Suspected of damaging fertility or the unborn child
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Safety Data Sheet (SDS), USA

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