

SAFETY DATA SHEET

Version 6.2
Revision Date 04/29/2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : AB-PINACA 5-Pentanoic acid metabolite

Product Number : S-085

Brand : Cerilliant

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - single exposure (Category 1), H370

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)
H225 : Highly flammable liquid and vapor.

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H301 + H311 + H331 H370	Toxic if swallowed, in contact with skin or if inhaled. Causes damage to organs.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P307 + P311	IF exposed: Call a POISON CENTER or doctor/ physician.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Molecular weight : 32.04 g/mol

Component		Classification	Concentration
Methanol			
CAS-No.	67-56-1	Flam. Liq. 2; Acute Tox. 3;	>= 90 - <= 100 %
EC-No.	200-659-6	STOT SE 1; H225, H301,	
Index-No.	603-001-00-X	H331, H311, H370	
Registration number	01-2119433307-44-XXXX	Concentration limits:	
		>= 10 %: STOT SE 1, H370; 3 - < 10 %: STOT SE 2, H371;	

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

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, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

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

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Use explosion-proof equipment. **Advice on protection against fire and explosion**
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage stability

Recommended storage temperature
-20 °C

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Methanol	67-56-1	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		
		STEL	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Danger of cutaneous absorption		
		TWA	200 ppm 260 mg/m ³	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		

		ST	250 ppm 325 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200 ppm 260 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	250 ppm 325 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		TWA	200 ppm 260 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		C	1,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		PEL	200 ppm 260 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	250 ppm 325 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Methanol	67-56-1	Methanol	15 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (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. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

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

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: colorless
b) Odor	pungent
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -98.0 °C (-144.4 °F)
f) Initial boiling point and boiling range	64.0 - 65.0 °C 147.2 - 149.0 °F at 1013 hPa
g) Flash point	9.7 °C (49.5 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 36 %(V) Lower explosion limit: 6 %(V)
k) Vapor pressure	130.3 hPa at 20.0 °C (68.0 °F) 546.6 hPa at 50.0 °C(122.0 °F) 169.27 hPa at 25.0 °C(77.0 °F)
l) Vapor density	1.11
m) Relative density	No data available
n) Water solubility	completely miscible
o) Partition coefficient: n-octanol/water	log Pow: -0.77
p) Autoignition temperature	455.0 °C (851.0 °F) at 1,013 hPa
q) Decomposition temperature	No data available

- r) Viscosity No data available
s) Explosive properties Not explosive
t) Oxidizing properties The substance or mixture is not classified as oxidizing.

9.2 Other safety information

Minimum ignition energy	0.14 mJ
Conductivity	< 1 µS/cm
Relative vapor density	1.11

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.

Vapors may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks.
Heat, flames and sparks.

10.5 Incompatible materials

Acid chlorides, Acid anhydrides, Oxidizing agents, Alkali metals, Reducing agents, Acids

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Not available

Methyl alcohol may be fatal or cause blindness if swallowed.

Effects due to ingestion may include:, Headache, Dizziness, Drowsiness, metabolic acidosis, Coma, Seizures.

Symptoms may be delayed., Damage of the:, Liver, Kidney

Stomach - Irregularities - Based on Human Evidence

Components**Methanol****Acute toxicity**

Acute toxicity estimate Oral - 100.1 mg/kg

(Expert judgment)

Symptoms: Nausea, Vomiting

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l

(Expert judgment)

Symptoms: Irritation symptoms in the respiratory tract.

Acute toxicity estimate Dermal - 300.1 mg/kg
(Expert judgment)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks:

(ECHA)

Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Remarks:

(ECHA)

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Based on available data the classification criteria are not met.

Ames test

Salmonella typhimurium

Result: negative

In vitro mammalian cell gene mutation test

Chinese hamster lung cells

Result: negative

OECD Test Guideline 474

Mouse - male and female - Bone marrow

Result: negative

Carcinogenicity

Did not show carcinogenic effects in animal experiments.

Reproductive toxicity

Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

Causes damage to organs. - Eyes, Central nervous system

Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Acute oral toxicity - Nausea, Vomiting

Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

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12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

Components

Methanol

Toxicity to fish	flow-through test LC50 - <i>Lepomis macrochirus</i> (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - ca. 22,000.0 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 1230 Class: 3 Packing group: II
Proper shipping name: MethanolSOLUTION

Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

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UN number: 1230 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D
Proper shipping name: METHANOLSOLUTION

IATA

UN number: 1230 Class: 3 (6.1) Packing group: II
Proper shipping name: MethanolSOLUTION

SECTION 15: Regulatory information

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

SECTION 16: Other information

Further information

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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 Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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