

## SAFETY DATA SHEET

Version 5.4  
Revision Date 09/23/2016  
Print Date 08/10/2017

**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : a-Pyrrolidinovalerophenone-D8 hydrochloride solution

Product Number : P-101  
Brand : Cerilliant  
Index-No. : 603-001-00-X

**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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

**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 vapour.  
H301 + H311 + H331 : Toxic if swallowed, in contact with skin or if inhaled  
H370 : 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/ vapours/ 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	IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P307 + P311	IF exposed: Call a POISON CENTER or doctor/ physician.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P361	Remove/Take off immediately all contaminated clothing.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.2 Mixtures

Molecular weight : 275.84 g/mol

#### Hazardous components

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

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this 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

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### 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

No data available

#### 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.

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### 6. ACCIDENTAL RELEASE MEASURES

#### 6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours 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.

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### 7. HANDLING AND STORAGE

#### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.

#### 7.2 Conditions for safe storage, including any incompatibilities

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.

Recommended storage temperature -20 °C

#### 7.3 Specific end use(s)

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

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### 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

#### 8.1 Control parameters

##### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Methanol	67-56-1	TWA	200.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Headache Nausea Dizziness		

		Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		STEL	250.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Headache Nausea Dizziness Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		TWA	200.000000 ppm 260.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		ST	250.000000 ppm 325.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200.000000 ppm 260.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Headache Nausea Dizziness Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		STEL	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Headache Nausea Dizziness Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		TWA	200 ppm 260 mg/m3	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
		The value in mg/m3 is approximate.		

		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	15.0000 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			
		Methanol	15 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Colour: colourless
b) Odour	pungent
c) Odour 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 1,013 hPa (760 mmHg)
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) Vapour pressure	130.3 hPa (97.7 mmHg) at 20.0 °C (68.0 °F) 546.6 hPa (410.0 mmHg) at 50.0 °C (122.0 °F) 169.27 hPa (126.96 mmHg) at 25.0 °C (77.0 °F)
l) Vapour density	1.11
m) Relative density	0.79 g/cm <sup>3</sup> at 20 °C (68 °F)
n) Water solubility	completely miscible
o) Partition coefficient: n-octanol/water	log Pow: -0.77
p) Auto-ignition temperature	455.0 °C (851.0 °F) at 1,013 hPa (760 mmHg)
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 vapour density	1.11

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## 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

Vapours may form explosive mixture with air. Vapours may form explosive mixture with air.

#### 10.4 Conditions to avoid

Heat, flames and sparks.

Heat, flames and sparks. Extremes of temperature and direct sunlight.

#### 10.5 Incompatible materials

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

#### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

##### 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 sensitisation

No data available

##### Germ cell mutagenicity

No data available

##### Carcinogenicity

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

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: 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.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

##### Reproductive toxicity

No data available

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

##### Additional Information

RTECS: 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  
Stomach - Irregularities - Based on Human Evidence  
Stomach - Irregularities - Based on Human Evidence ( $\alpha$ -Pyrrolidinovalerophenone-d8 HCl)

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

No data available

### 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

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## 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.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 1230      Class: 3      Packing group: II

Proper shipping name: Methanol, solution

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

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

Proper shipping name: METHANOL, SOLUTION

### IATA

UN number: 1230      Class: 3 (6.1)      Packing group: II

Proper shipping name: Methanol, solution

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## 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



Methanol	CAS-No. 67-56-1	Revision Date 2007-07-01
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#### **Pennsylvania Right To Know Components**

Methanol	CAS-No. 67-56-1	Revision Date 2007-07-01
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#### **New Jersey Right To Know Components**

Methanol	CAS-No. 67-56-1	Revision Date 2007-07-01
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#### **California Prop. 65 Components**

WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.	CAS-No. 67-56-1	Revision Date 2012-03-16
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Methanol

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## **16. OTHER INFORMATION**

### **Full text of H-Statements referred to under sections 2 and 3.**

Acute Tox.	Acute toxicity
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H370	Causes damage to organs.
STOT SE	Specific target organ toxicity - single exposure

### **HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	0

### **NFPA Rating**

Health hazard:	2
Fire Hazard:	3
Reactivity Hazard:	0

### **Further information**

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### **Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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