

## 1: Identification of substance / mixture

### 1. Product Identifier

Substance

Product Name **4-(2,2,2-trifluoroacetyl)benzotrile**  
Product Code NCS K1322251  
CAS Number 23516-85-0  
Other Names  
IUPAC  
MFCD Number MFCD01319971  
EC/EINECS  
REACH Number

### 2. Relevant identified uses of the substance or mixture and uses advised against

Research and Development

### 3. Details of the supplier of the safety data sheet

Rieke Metals, LLC  
1001 Kingbird Road,  
Lincoln  
Nebraska  
68521  
US



Telephone: 402 434 2775  
Fax: 402 434 2777  
Email: sales@riekemetals.com

### 4. Emergency telephone number

800-535-5053 / International 1-352-323-3500 -

## 2. Hazards Identification

### 1. Classification of the substance or mixture

H303	Acute Tox. 5	
H315	Skin Irrit. 2	
H319	Eye Irrit. 2	
H335	STOT SE 3a	

### 2. Label elements

Signal Word **Warning**



### Hazard Statements

H303	Maybe harmful if swallowed
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

### Precautionary Phrases

P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P264	Wash skin thoroughly after handling.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position 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.
P312	Call a POISON CENTER or doctor/physician if you feel unwell.

P501	Dispose of contents/container to licensed professional waste disposal service to dispose of this material
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### 3. Other Hazards

Additional precautionary phrases are located throughout the safety data sheet

## 3. Composition / Information on Ingredients

### 1. Substances

4-(2,2,2-trifluoroacetyl)benzotrile

Assay:100% CAS Number :23516-85-0

### 2. Mixtures

Not Relevant

## 4. First Aid Measures

### 1. Description of first aid measures

*Skin Contact* P302 + P352: IF ON SKIN: Wash with plenty of soap and water.  
Remove all contaminated clothes and footwear immediately unless stuck to skin. Wash off with soap and plenty of water. Consult a physician

*Eye Contact* P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
Rinse opened eye for several minutes under running water.  
Consult a physician.

*Ingestion* Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water.  
Consult a physician.

*Inhalation* P304 + P340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

### 2. Most important symptoms and effects

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly tested.

### 3. Indication of any immediate medical attention

P312: Call a POISON CENTER or doctor/physician if you feel unwell.

## 5. Firefighting measures

### 1. Extinguishing Media

*Suitable* Use water spray, alcohol-resistant foam, dry chemical, CO2, or appropriate foam.

*Unsuitable* No recommendations.

### 2. Special Hazards arising from the substance or mixture

In combustion toxic fumes may form.  
In combustion emits toxic fumes of hydrogen bromides  
In combustion emits toxic fumes of carbon dioxide / carbon monoxide.

### 3. Advice for Fire Fighters

Wear self contained breathing apparatus for firefighting if necessary.  
Wear protective clothing to prevent contact with skin and eyes.

## 6. Accidental Release Measures

### 1. Personal Precautions

Use personal protective equipment. 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.

### 2. Environmental Precautions

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

### 3. Methods & Materials

Contain spillage then pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.  
Do not flush with water.

### 4. Preventing the occurrence of secondary hazards.

No Data Available.

## 7. Handling and Storage

### 1. Personal Precautions

<i>Safe Handling</i>	Avoid direct contact with the substance. Avoid inhalation of vapors or mist. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust and vapor is formed. P264: Wash skin thoroughly after handling.
<i>Protection against explosions and fires</i>	Keep away from sources of ignition-No smoking.

### 2. Conditions for safe storage, including any incompatibilities

<i>Managing Storage Risks</i>	Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept in an upright to prevent leakage. Avoid extremes of temperatures.
<i>Storage Controls</i>	No special requirements
<i>Maintaining Integrity</i>	No special requirements
<i>Other advice</i>	No further information available.

### 3. Specific End Uses

The end use(s) have not been fully determined. The substance is supplied for Research and Development purposes by professionals only.

## 8. Exposure Controls/Personal Protection

### 1. Control Parameters

No Data Available

### 2. Exposure Controls

<i>General protective and hygiene measures</i>	P280: Wear protective gloves/protective clothing/eye protection/face protection. The standard precautionary measures should be adhered to when handling Avoid contact with skin and eyes
<i>Engineering measures</i>	Ensure there is exhaust ventilation of the area. Use only in a chemicals fume hood.
<i>Eye / Face Protection</i>	Tightly fitting safety goggles. Safety Glasses with side-shields.
<i>Hand protection</i>	Handle with protective 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.
<i>Respiratory protection</i>	P260: Do not breathe dust/fume/gas/mist/vapours/spray. P261: Avoid breathing dust/fume/gas/mist/vapours/spray.
<i>Skin protection</i>	Protective clothing, antistatic. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
<i>Other personal protection advice</i>	No Data Available.

## 9. Physical and Chemical Properties

### 1. Physical and Chemical Properties

Appearance	White Solid
Odour	No Data Available
Odour threshold	No Data Available
PH	No Data Available
Melting point / Freezing point	51.0 - 52.0 °C

Initial boiling point and boiling range	No Data Available
Flash point	No Data Available
Evaporation rate	No Data Available
Flammability(solid, gas)	No Data Available
Upper/lower flammability or explosive limits	No Data Available
Vapour pressure	No Data Available
Vapour density	No Data Available
Relative density	No Data Available
Solubility(ies):	No Data Available
Partition coefficient: n-octanol/water	No Data Available
Auto-ignition temperature	No Data Available
Decomposition temperature	No Data Available
Viscosity	No Data Available
Explosive properties	No Data Available
Oxidising properties	No Data Available

## 2. Other Information

199.13 g/mol  
C9H4F3NO

## 10. Stability and Reactivity

### 1. Reactivity

Hazardous Reactions No information available

### 2. Stability

Stable under recommended storage conditions.

### 3. Possibility of Hazardous Reactions

No hazardous reactions known.

### 4. Conditions to Avoid

Heat, Flames and sparks. Extremes of temperature and direct sunlight. Exposure to moisture.

### 5. Incompatible Materials

Oxidizing agents, Strong oxidizing agents, Strong reducing agents.

### 6. Hazardous Decomposition Products

Hazardous decomposition products formed under fire conditions.  
Carbon oxides, Carbon monoxides, Hydrogen Bromides.  
Other decomposition products - no data available

## 11. Toxicology information

### 1. Information

<i>Acute Toxicity</i>	No data available
<i>Skin corrosion/irritation</i>	No data available
<i>Serious eye Damage/irritation</i>	No data available
<i>Respiratory or skin sensitisation</i>	No data available
<i>Germ Cell mutagenicity</i>	No data available
<i>Carcinogenicity</i>	No data available
<i>Reproductive toxicity</i>	No data available
<i>STOT-single exposure</i>	No data available
<i>STOT-repeated exposure</i>	No data available
<i>Aspiration hazard</i>	No data available

### 2. Additional

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.  
No additional information available

## 12. Ecological Information

### 1. Toxicity

No data available

### 2. Persistence and degradability

No data available

### 3. Bio-Accumulative Potential

No data available

### 4. Mobility and Soil

No data available

### 5. Results of PBT & vPvB assessment

No data available

### 6. Other adverse effects

No data available

## 13. Disposal Considerations

### 1. Waste Treatment Methods

*Disposal Operations*

*Disposal of Packaging* Disposal must be made according to official regulations.

## 14. Transport Information

### Air (ICAO)

1. **UN Number:**
2. **Shipping Name:** Non Hazardous
3. **Transport hazard class(es):** : Sub Class :
  
4. **Packing group:**
5. **Environmental hazards:**
6. **Special Precautions for user:**
7. **Transport in bulk:**

### Road (ADR)

1. **UN Number:**
2. **Shipping Name:** None Hazardous
3. **Transport hazard class(es):** : Sub Class :
  
4. **Packing group:**
5. **Environmental hazards:**
6. **Special Precautions for user:**
7. **Transport in bulk:**

### Sea (IMDG)

1. **UN Number:**
2. **Shipping Name:** Non Hazardous
3. **Transport hazard class(es):** : Sub Class :

- 4. **Packing group:**
- 5. **Environmental hazards:**
- 6. **Special Precautions for user:**
- 7. **Transport in bulk:**

## 15. Safety, health, environmental and national regulations

### 1. Safety, health, environmental and national regulations:

OSHA Hazards  
Irritant

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

SARA 313 Components  
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards  
Acute Health Hazard

### 2. Safety Assessment

No Chemical Safety Assessment

## 16. Other Information

### 1. Other Information:

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

### 2. Associated risk phrases according to European directive 67/548/EEC

### 3. Disclaimer

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 or fitness for a particular use. Rieke Metals, LLC shall not be held liable for any damage resulting from handling or from contact with the above product.

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