

## SAFETY DATA SHEET

Version 6.6  
Revision Date 03/05/2021  
Print Date 07/31/2021

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Bromo-4'-cyanoacetophenone

Product Number : 539392  
Brand : Aldrich  
CAS-No. : 20099-89-2

**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)**

Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 4), H332  
Acute toxicity, Dermal (Category 4), H312  
Skin corrosion (Category 1B), H314  
Serious eye damage (Category 1), H318

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) H302 + H312 + H332 H314	Harmful if swallowed, in contact with skin or if inhaled. Causes severe skin burns and eye damage.
Precautionary statement(s) P260 P264 P270 P271 P280	Do not breathe dusts or mists. Wash skin thoroughly after handling. Do not eat, drink or smoke when using this product. Use only outdoors or in a well-ventilated area. Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331 P303 + P361 + P353	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P363	Wash contaminated clothing before reuse.
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

Lachrymator.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula : C<sub>9</sub>H<sub>6</sub>BrNO  
Molecular weight : 224.05 g/mol  
CAS-No. : 20099-89-2

Component	Classification	Concentration
<b>2-Bromo-4'-cyanoacetophenone</b>	Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; H302, H332, H312, H314, H318	<= 100 %

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**

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

**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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**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

Nitrogen oxides (NO<sub>x</sub>)

Hydrogen bromide gas

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**6.3 Methods and materials for containment and cleaning up**

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

**6.4 Reference to other sections**

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### Advice on safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. **Advice on safe handling**

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

#### Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.

#### Hygiene measures

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

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.

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

### 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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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

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

#### 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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min  
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact  
Material: Nitrile rubber  
Minimum layer thickness: 0.11 mm  
Break through time: 480 min  
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### **Body Protection**

Complete suit protecting against chemicals, 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 particle respirator type N100 (US) or type P3 (EN 143) 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**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

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|---|---|
| a) Appearance                                   | Form: solid   |
| b) Odor   | No data available                                     |
| c) Odor Threshold                               | No data available                                     |
| d) pH   | No data available                                     |
| e) Melting point/freezing point                 | Melting point/range: 92 - 96 °C (198 - 205 °F) - lit. |
| f) Initial boiling point and boiling range      | No data available                                     |
| g) Flash point                                  | ( )No data available                                  |
| h) Evaporation rate                             | No data available                                     |
| i) Flammability (solid, gas)                    | No data available                                     |
| j) Upper/lower flammability or explosive limits | No data available                                     |

- |  |                   |
|--|-------------------|
| k) Vapor pressure                            | No data available |
| l) Vapor density                             | No data available |
| m) Relative density                          | No data available |
| n) Water solubility                          | No data available |
| o) Partition coefficient:<br>n-octanol/water | No data available |
| p) Autoignition<br>temperature               | No data available |
| q) Decomposition<br>temperature              | No data available |
| r) Viscosity                                 | No data available |
| s) Explosive properties                      | No data available |
| t) Oxidizing properties                      | No data available |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Avoid moisture.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

LD50 Oral - 500.1 mg/kg

LC50 Inhalation - 4 h - 1.5 mg/l

(Acute toxicity estimate)

LD50 Dermal - 1,100 mg/kg

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

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

Cough, Shortness of breath, Headache, Nausea, Vomiting

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**SECTION 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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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. 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.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

UN number: 2928 Class: 6.1 (8) Packing group: II  
Proper shipping name: Toxic solids, corrosive, organic, n.o.s. (2-Bromo-4'-cyanoacetophenone)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 2928 Class: 6.1 (8) Packing group: II EMS-No: F-A, S-B  
Proper shipping name: TOXIC SOLID, CORROSIVE, ORGANIC, N.O.S. (2-Bromo-4'-cyanoacetophenone)

### IATA

UN number: 2928 Class: 6.1 (8) Packing group: II  
Proper shipping name: Toxic solid, corrosive, organic, n.o.s. (2-Bromo-4'-cyanoacetophenone)

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## SECTION 15: Regulatory information

### SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

### SARA 313 Components

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

### Massachusetts Right To Know Components

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

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

### Pennsylvania Right To Know Components



2-Bromo-4'-cyanoacetophenone

CAS-No.  
20099-89-2

Revision Date

**New Jersey Right To Know Components**

2-Bromo-4'-cyanoacetophenone

CAS-No.  
20099-89-2

Revision Date

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**SECTION 16: Other information**

**Further information**

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