

## Safety Data Sheet (United States)

Isocaffeine

**1. Identification**

Product name: Isocaffeine  
Catalog#: 0051BA  
IUPAC name: 1,3,9-trimethylpurine-2,6-dione  
Product use restrictions: Only for research and development use by, or directly under the supervision of, a technically qualified individual.  
Company: AK Scientific, Inc.  
30023 Ahern Ave.  
Union City, CA 94587  
Telephone: (510) 429-8835  
Fax: (510) 429-8836  
Website: www.aksci.com  
Emergency contact number: 1-800-633-8253 United States & Canada  
1-801-629-0667 International

**2. Hazard Identification:****GHS Classification (United States)**

Skin irritation (Category 2)

Eye irritation (Category 2A)

Specific target organ toxicity - single exposure (Category 3), Respiratory system

**Pictogram(s)****Signal word:**

Warning

**Hazard statement(s)**

H302

Harmful if swallowed.

**Precautionary statement(s):**

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P301+P312 IF SWALLOWED: Call a poison center or doctor if you feel unwell.

P330 Rinse mouth.

P501 Dispose of contents/container to an approved waste disposal plant.

**Hazards not otherwise classified (HNOC) or not covered by GHS:**

None

**3. Composition/Information on Ingredients**

Synonyms: Isocaffeine; 519-32-4; 1,3,9-Trimethylxanthine; 1,3,9-trimethylpurine-2,6-dione; 1,3,9-trimethyl-3,9-dihydro-1H-purine-2,6-dione

CAS#: 519-32-4

Purity: 95%

EC: 208-267-7

**4. First Aid Measures****General Information:** Immediately remove any clothing contaminated by the product. Move out of dangerous area. Consult a physician and show this safety data sheet.**Inhalation:** Move person to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Obtain medical aid.

**Skin contact:** Immediately flush skin with running water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Obtain medical aid immediately.

**Eye contact:** Immediately flush open eyes with running water for at least 15 minutes. Obtain medical aid immediately.

**Ingestion:** Do NOT induce vomiting without medical advice. Rinse mouth with water. Never administer anything by mouth to an unconscious person. Obtain medical aid immediately.

**Most important symptoms and effects, both acute and delayed:** No further information available. Please see sections 2 and 11.

**Indication of any immediate medical attention and special treatment needed:** No further information available.

## 5. Fire Fighting Measures

**Suitable extinguishing media:** Use water spray, dry chemical, carbon dioxide, or chemical foam.

**Specific hazards arising from the chemical:** Carbon oxides, Nitrogen oxides.

**Advice for firefighters:** As in any fire, wear a NIOSH-approved or equivalent, pressure-demand, self-contained breathing apparatus and full protective gear. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion.

## 6. Accidental Release Measures

**Personal precautions, protective equipment and emergency procedures:** Wear protective equipment and keep unprotected personnel away. Ensure adequate ventilation. Remove all sources of ignition. Prevent further leak or spill if safe to do so. For personal protective equipment, please refer to section 8.

**Environmental precautions:** Do not let product enter drains, other waterways, or soil.

**Methods and materials for containment and cleaning up:** Prevent further leak or spill if safe to do so. Vacuum, sweep up, or absorb with inert material and place into a suitable disposal container. Consult local regulations for disposal. See section 13 for further disposal information.

## 7. Handling and Storage

**Precautions for safe handling:** Avoid contact with skin, eyes, and personal clothing. Wash hands thoroughly after handling. Avoid breathing fumes. Use only with adequate ventilation. Wear suitable protective clothing, gloves, and eye/face protection. Keep away from sources of ignition. Minimize dust generation and accumulation. Keep container tightly closed. Open and handle container with care. Do not eat, drink, or smoke while handling.

**Conditions for safe storage, including any incompatibilities:** Store in a tightly-closed container when not in use. Store in a cool, dry, well-ventilated area away from incompatible substances. Keep away from sources of ignition. Store long-term in a cool, dry place.

## 8. Exposure Controls/Personal Protection

### Exposure limits:

OSHA PEL: Not available.

NIOSH REL: Not available.

ACGIH TLV: Not available.

**Appropriate engineering controls:** Avoid contact with skin, eyes, and clothing. Wash hands before breaks and immediately after handling the product. Facilities storing or utilizing this material should be equipped with an eyewash fountain. Use adequate general and local exhaust ventilation to keep airborne concentrations low.

**Personal protection**

Eyes:	Not Available.
Hands:	Not Available.
Skin and body:	Not Available.
Respiratory:	Not Available.

**9. Physical and Chemical Properties**

Physical State:	Not available.
Molecular Formula:	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>
Molecular Weight:	194.19
Odor:	Not available.
pH:	Not available.
Boiling Point Range:	Not available.
Freezing/Melting Point:	Not available.
Flash Point:	Not available.
Evaporation Rate:	Not available.
Flammability(solid,gas):	Please see section 2.
Explosive limits:	Not available.
Vapor Pressure:	Not available.
Vapor Density:	Not available.
Solubility:	Not available.
Relative Density:	Not available.
Refractive Index:	Not available.
Volatility:	Not available.
Auto-ignition Temperature:	Not available.
Decomposition Temperature:	Not available.
Partition Coefficient:	Not available.

**10. Stability and Reactivity**

Reactivity:	Not available.
Chemical stability:	Stable under recommended temperatures and pressures.
Possibility of hazardous reactions:	Not available.
Conditions to avoid:	Dust generation.
Incompatible materials:	Strong oxidizing agents.
Hazardous decomposition products:	Carbon oxides, Nitrogen oxides.

**11. Toxicological Information**

RTECS#	Not available.
Acute toxicity:	Not available.
Routes of exposure:	Inhalation,eye contact,skin contact,ingestion.
Symptoms related to the physical,chemical and toxicological characteristics:	Skin contact may result in inflammation characterized by itching, scaling, reddening, blistering, pain or dryness. Eye contact may result in redness, pain or severe eye damage. Inhalation may cause irritation of the lungs and respiratory system. Overexposure may result in serious illness or death.

**Carcinogenicity**

IARC:	Not classified.
NTP:	Not listed.
OSHA:	Not Available..
Acute toxic effects:	Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

**12. Ecological Information**

Ecotoxicity:	Not available.
Persistence and degradability:	Not available.
Bioaccumulative potential:	Not available.
Mobility in soil:	Not available.
Other adverse effects:	Not available.

**13. Disposal Considerations**

Disposal of waste:	Not listed
Disposal of packaging:	Not listed

**14. Transportation Information****DOT (United States)**

UN number:	Not hazardous material.
Proper shipping name:	Not available.
Transport hazard class:	Not available.
Packing group:	Not available.

**IATA**

UN Number:	Not dangerous good.
Proper shipping name:	Not available.
Transport hazard class:	Not available.
Packing group:	Not available.

**15. Regulatory Information****TSCA (United States)**

Not Available.

California Proposition 65:	Not Available..	
NFPA Rating:	Health:	Not available.
	Flammability:	Not available.
	Instability:	Not available.

**16. Additional Information**

Revision Date: 03/07/2022

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