

Date : 07.03.2024.

## SAFETY DATA SHEET

### 1. PRODUCT AND COMPANY INFORMATION

Product Name : Isocaffeine-d<sub>3</sub>, 98% (CP)

Product No. : SL-4149

Product Use : For laboratory research use only, not for drug, household or other uses.

Manufacture & Supplier : SynInnova Laboratories Inc,  
4-105A NINT Innovation Center,  
11421 Saskatchewan Drive,  
Edmonton, AB, Canada T6G 2M9.  
Tel : 780 485 2962, Fax : 780 485 2963  
e-mail : sales@syninnova.com, www.syninnova.com

### 2. HAZARDS IDENTIFICATION

Hazardous statement(s) : H303 May be harmful if swallowed  
H313 May be harmful in contact with skin  
H320 Causes eye irritation  
H333 May be harmful if inhaled

Precautionary statement(s) : P260 : Do not breathe dust / fume / gas / mist / vapours / spray.  
P280 : Wear protective gloves / protective clothing / eye protection / face protection.  
P301 + P310 : IF SWALLOWED: Immediately call a POISON CENTER or doctor / physician.  
P303 + 361 + 353 : IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water / shower.  
P304 + 312 : IF INHALED: Call a POISON CENTER or doctor/physician if you feel unwell.  
P305 + P351 + P338 : IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do  continue rinsing.

Potential Health Effects : Inhalation : May be harmful if inhaled. May cause respiratory tract irritation.  
Skin : May be harmful if absorbed through skin. May cause skin irritation.  
Eyes : May cause eye irritation.  
Ingestion : May be harmful if swallowed.

### 3. COMPOSITION / INFORMATION ON INGREDIENTS

Ingredient Name : Isocaffeine-d<sub>3</sub>

Synonym : 1,3,9-Trimethyl-1H-purine-2,6(3H,9H)-dione-d<sub>3</sub>;  
9-Methyltheophylline-d<sub>3</sub>; Caffeine-d<sub>3</sub> EP impurity C; NSC 28332-d<sub>3</sub>

Molecular formula : C<sub>8</sub>H<sub>7</sub>D<sub>3</sub>N<sub>4</sub>O<sub>2</sub>

Molecular weight : 197.21

Chemical concentration : <=100%

#### **4. FIRST AID MEASURES**

Skin contact : Immediately wash skin with copious amounts of water for at least 15 minutes while removing contaminated clothing and shoes. If irritation persists, seek medical attention.

Eye contact : Immediately wash skin with copious amounts of water for at least 15 minutes. Assure adequate flushing of the eyes by separating the eyelids with fingers. If irritation persists, seek medical attention.

Inhalation : Remove to fresh air. In severe cases or if symptoms persist, seek medical attention.

Ingestion : Wash out mouth with copious amounts of water for at least 15 minutes. Seek medical attention.

#### **5. FIRE FIGHTING MEASURES**

In the event of a fire involving this material, alone or in combination with other materials, use dry powder or carbon dioxide extinguishers. Protective clothing and self-contained breathing apparatus should be worn.

#### **6. ACCIDENTAL RELEASE MEASURES**

Personal precautions : Wear suitable personal protective equipment which performs satisfactorily and meets local/state/national standards.

Respiratory precaution : Wear approved mask/respirator

Hand precaution : Wear suitable gloves/gauntlets

Skin protection : Wear suitable protective clothing

Eye protection : Wear suitable eye protection

Methods for cleaning up : Mix with sand or similar inert absorbent material, sweep up and keep in a tightly closed container for disposal. See section 12.

Environmental precautions : Do not allow material to enter drains or watercourses.

#### **7. HANDLING AND STORAGE**

Handling : This product should be handled only by, or under the close supervision of, those properly qualified in the handling and use of potentially hazardous chemicals, who should take into account the fire, health and chemical hazard data given on this sheet.

Storage : Keep container tightly closed under nitrogen or argon and refrigerate for long-term shelf life.

#### **8. EXPOSURE CONTROLS / PERSONAL PROTECTION**

Engineering Controls : Use only in a chemical fume hood.

Personal protective equipment : Wear laboratory clothing, chemical-resistant gloves, safety goggles and appropriate respirator mask.

General hygiene measures : Wash thoroughly after handling. Wash contaminated clothing before reuse.

## **9. PHYSICAL AND CHEMICAL PROPERTIES**

Appearance : Off-white solid  
Boiling point : No data available  
Melting point : Not available  
Flash point : No data available  
Density : No data available

## **10. STABILITY AND REACTIVITY**

Conditions to avoid : Heat, flames and sparks.  
Materials to avoid : Strong-oxidizing agents.  
Possible hazardous : Carbon dioxide, Carbon monoxide, nitrogen oxides (NOx), and other  
combustion products decomposition products.

## **11. TOXICOLOGICAL INFORMATION**

No data available

## **12. ECOLOGICAL INFORMATION**

No data available

## **13. DISPOSAL CONSIDERATION**

Arrange disposal as special waste, by licensed disposal company, in consultation with local waste disposal authority, in accordance with national and regional regulations.

## **14. TRANSPORTATION INFORMATION**

Non-hazardous for air and ground transportation.

## **15. REGULATORY INFORMATION**

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the SDS contains all the information required by the Controlled Products Regulations.

## **16. OTHER INFORMATION**

This SDS is correct to the best of our knowledge at the date of publication but we cannot accept liability for any loss, injury or damage, which may result from its use.