

## 1 Identification

### Product identifier

**Product name:** 3-Isobutyl-1-methylxanthine

**Stock number:** J64598

**CAS Number:**

28822-58-4

**EC number:**

249-259-3

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

**Identified use:** SU24 Scientific research and development

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

#### Manufacturer/Supplier:

Alfa Aesar

Thermo Fisher Scientific Chemicals, Inc.

30 Bond Street

Ward Hill, MA 01835-8099

Tel: 800-343-0660

Fax: 800-322-4757

Email: tech@alfa.com

www.alfa.com

**Information Department:** Health, Safety and Environmental Department

**Emergency telephone number:**

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

## 2 Hazard(s) identification

**Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)**



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

**Hazards not otherwise classified** No information known.

### Label elements

**GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

### Hazard pictograms



GHS07

**Signal word** Warning

### Hazard statements

H302 Harmful if swallowed.

### Precautionary statements

P264 Wash thoroughly after handling.

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

P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor/.../if you feel unwell.

P330 Rinse mouth.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

**WHMIS classification** Not controlled

### Classification system

**HMIS ratings (scale 0-4)**

(Hazardous Materials Identification System)

**HEALTH** **2** Health (acute effects) = 2

**FIRE** **1** Flammability = 1

**REACTIVITY** **1** Physical Hazard = 1

### Other hazards

### Results of PBT and vPvB assessment

**PBT:** Not applicable.

**vPvB:** Not applicable.

## 3 Composition/information on ingredients

**Chemical characterization:** Substances

**CAS# Description:**

28822-58-4 3-Isobutyl-1-methylxanthine

**Identification number(s):**

**EC number:** 249-259-3

## 4 First-aid measures

### Description of first aid measures

#### After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

#### After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

**After eye contact** Rinse opened eye for several minutes under running water. Then consult a doctor.

**After swallowing** Seek medical treatment.

### Information for doctor

**Most important symptoms and effects, both acute and delayed** No further relevant information available.

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

## 5 Fire-fighting measures

### Extinguishing media

**Suitable extinguishing agents** Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

**Product name: 3-Isobutyl-1-methylxanthine**

(Contd. of page 1)

**Special hazards arising from the substance or mixture**

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Nitrogen oxides (NOx)

**Advice for firefighters**

**Protective equipment:**

Wear self-contained respirator.

Wear fully protective impervious suit.

**6 Accidental release measures**

**Personal precautions, protective equipment and emergency procedures**

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

**Environmental precautions:** Do not allow material to be released to the environment without proper governmental permits.

**Methods and material for containment and cleaning up:** Dispose of contaminated material as waste according to section 13.

**Prevention of secondary hazards:** No special measures required.

**Reference to other sections**

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

**7 Handling and storage**

**Handling**

**Precautions for safe handling**

Keep container tightly sealed.

Ensure good ventilation at the workplace.

**Information about protection against explosions and fires:** No information known.

**Conditions for safe storage, including any incompatibilities**

**Storage**

**Requirements to be met by storerooms and receptacles:** Store in freezer (-20 °C).

**Information about storage in one common storage facility:**

Protect from heat.

Store away from oxidizing agents.

**Further information about storage conditions:** Keep container tightly sealed.

**Specific end use(s)** No further relevant information available.

**8 Exposure controls/personal protection**

**Additional information about design of technical systems:**

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

**Control parameters**

**Components with limit values that require monitoring at the workplace:**

The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.

**Additional information:** No data

**Exposure controls**

**Personal protective equipment**

**General protective and hygienic measures**

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Maintain an ergonomically appropriate working environment.

**Breathing equipment:** Use suitable respirator when high concentrations are present.

**Recommended filter device for short term use:**

Use a respirator with type P100 (USA) or P3 (EN 143) cartridges as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards.

**Protection of hands:**

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

**Material of gloves** Nitrile rubber, NBR

**Penetration time of glove material (in minutes)** Not determined

**Eye protection:** Safety glasses

**Body protection:** Protective work clothing.

**9 Physical and chemical properties**

**Information on basic physical and chemical properties**

**General Information**

**Appearance:**

**Form:** Solid

**Color:** White

**Odor:** Not determined

**Odor threshold:** Not determined.

**pH-value:** Not applicable.

**Change in condition**

**Melting point/Melting range:** 200-201 °C (392-394 °F)

**Boiling point/Boiling range:** Not determined

**Sublimation temperature / start:** Not determined

**Flammability (solid, gaseous)** Not determined.

**Ignition temperature:** Not determined

**Decomposition temperature:** Not determined

**Auto igniting:** Not determined.

**Danger of explosion:** Not determined.

**Explosion limits:**

**Lower:** Not determined

**Upper:** Not determined

**Vapor pressure:** Not applicable.

**Density:** Not determined

(Contd. on page 3)  
USA

Product name: **3-Isobutyl-1-methylxanthine**

(Contd. of page 2)

Relative density	Not determined.
Vapor density	Not applicable.
Evaporation rate	Not applicable.
Solubility in / Miscibility with Water:	Not determined
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not applicable.
kinematic:	Not applicable.
Other information	No further relevant information available.

10 Stability and reactivity

**Reactivity** No information known.  
**Chemical stability** Stable under recommended storage conditions.  
**Thermal decomposition / conditions to be avoided:** Decomposition will not occur if used and stored according to specifications.  
**Possibility of hazardous reactions** Reacts with strong oxidizing agents  
**Conditions to avoid** No further relevant information available.  
**Incompatible materials:**  
Oxidizing agents  
Heat  
**Hazardous decomposition products:**  
Carbon monoxide and carbon dioxide  
Nitrogen oxides

11 Toxicological information

**Information on toxicological effects**  
**Acute toxicity:**  
Harmful if swallowed.  
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for this substance.  
**LD/LC50 values that are relevant for classification:** No data  
**Skin irritation or corrosion:** May cause irritation  
**Eye irritation or corrosion:** May cause irritation  
**Sensitization:** No sensitizing effects known.  
**Germ cell mutagenicity:** The Registry of Toxic Effects of Chemical Substances (RTECS) contains mutation data for this substance.  
**Carcinogenicity:** No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.  
**Reproductive toxicity:** No effects known.  
**Specific target organ system toxicity - repeated exposure:** No effects known.  
**Specific target organ system toxicity - single exposure:** No effects known.  
**Aspiration hazard:** No effects known.  
**Subacute to chronic toxicity:** No effects known.  
**Additional toxicological information:** To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

**Toxicity**  
**Aquatic toxicity:** No further relevant information available.  
**Persistence and degradability** No further relevant information available.  
**Bioaccumulative potential** No further relevant information available.  
**Mobility in soil** No further relevant information available.  
**Additional ecological information:**  
**General notes:**  
Do not allow material to be released to the environment without proper governmental permits.  
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.  
Avoid transfer into the environment.  
**Results of PBT and vPvB assessment**  
**PBT:** Not applicable.  
**vPvB:** Not applicable.  
**Other adverse effects** No further relevant information available.

13 Disposal considerations

**Waste treatment methods**  
**Recommendation** Consult state, local or national regulations to ensure proper disposal.  
**Uncleaned packagings:**  
**Recommendation:** Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, ADN, IMDG, IATA	Not applicable
UN proper shipping name DOT, ADN, IMDG, IATA	Not applicable
Transport hazard class(es) DOT, ADR, ADN, IMDG, IATA Class	Not applicable
Packing group DOT, IMDG, IATA	Not applicable
Environmental hazards:	Not applicable.
Special precautions for user	Not applicable.
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	-

**Product name: 3-Isobutyl-1-methylxanthine**

(Contd. of page 3)

**15 Regulatory information**

**Safety, health and environmental regulations/legislation specific for the substance or mixture**  
**GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)  
**Hazard pictograms**



GHS07

**Signal word** Warning

**Hazard statements**

H302 Harmful if swallowed.

**Precautionary statements**

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P330 Rinse mouth.

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**National regulations**

This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.

This product is not listed on the Canadian Domestic Substances List (DSL) or the Canadian Non-Domestic Substances List (NDSL).

**SARA Section 313 (specific toxic chemical listings)** Substance is not listed.

**California Proposition 65**

**Prop 65 - Chemicals known to cause cancer** Substance is not listed.

**Prop 65 - Developmental toxicity** Substance is not listed.

**Prop 65 - Developmental toxicity, female** Substance is not listed.

**Prop 65 - Developmental toxicity, male** Substance is not listed.

**Information about limitation of use:** For use only by technically qualified individuals.

**Other regulations, limitations and prohibitive regulations**

**Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006.** Substance is not listed.

**The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.**

Substance is not listed.

**Annex XIV of the REACH Regulations (requiring Authorisation for use)** Substance is not listed.

**Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

**16 Other information**

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

**Department issuing SDS:** Global Marketing Department

**Date of preparation / last revision** 11/24/2015 / -

**Abbreviations and acronyms:**

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

DOT: US Department of Transportation

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

vPvB: very Persistent and very Bioaccumulative

ACGIH: American Conference of Governmental Industrial Hygienists (USA)

OSHA: Occupational Safety and Health Administration (USA)

NTP: National Toxicology Program (USA)

IARC: International Agency for Research on Cancer

EPA: Environmental Protection Agency (USA)