

Revision Date 02-Jul-2012

Revision Number 4

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

Product Identifier

Product Description:

3-Isobutyl-1-methylxanthine

Cat No.

228420000; 228420010; 228420050

Synonyms

1-Methyl-3-isobutylxanthine; IBMX; MIX

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

Recommended Use

Laboratory chemicals

Uses advised against

No Information available

Details of the supplier of the safety data sheet

Company

Acros Organics BVBA
Janssen Pharmaceuticaaan 3a
2440 Geel, Belgium

E-mail address

begel.sdsdesk@thermofisher.com

Emergency Telephone Number

For information in the US, call: 001-800-ACROS-01

For information in Europe, call: +32 14 57 52 11

Emergency Number, Europe: +32 14 57 52 99

Emergency Number, US: 001-201-796-7100

CHEMTREC Phone Number, US: 001-800-424-9300

CHEMTREC Phone Number, Europe: 001-703-527-3887

SECTION 2. HAZARDS IDENTIFICATION

Classification of the substance or mixture

REGULATION (EC) No 1272/2008

Acute oral toxicity

Category 4

Classification according to EU Directives 67/548/EEC or 1999/45/EC

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

Symbol(s)

Xn - Harmful

R-phrases(s)

R22 - Harmful if swallowed

Label Elements

3-Isobutyl-1-methylxanthine
Revision Date 02-Jul-2012
SECTION 2. HAZARDS IDENTIFICATION

Signal Word
Warning
Hazard Statements

H302 - Harmful if swallowed

Precautionary Statements - EU (§28, 1272/2008)

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

Other Hazards

No information available.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	EC-No.	Weight %	CAS-No	67/548/EEC Classification	CLP Classification - Regulation (EC) No 1272/2008	REACH No.
3,7-Dihydro-3-isobutyl-1-methyl-1H-purine-2,6-dione 28822-58-4	EEC No. 249-259-3	>95	28822-58-4	Xn;R22	Acute Tox. 4 (H302)	-

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16
SECTION 4. FIRST AID MEASURES
Description of first aid measures
Eye Contact

Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Obtain medical attention. Take off contaminated clothing and shoes immediately.

Ingestion

Never give anything by mouth to an unconscious person. Drink plenty of water. Call a physician immediately. If possible drink milk afterwards.

Inhalation

Remove from exposure, lie down. Move to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Immediate medical attention is required.

3-Isobutyl-1-methylxanthine

Revision Date 02-Jul-2012

Notes to Physician

Treat symptomatically

SECTION 5. FIRE-FIGHTING MEASURES**Extinguishing media****Suitable Extinguishing Media**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Extinguishing media which must not be used for safety reasons

No information available.

Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors

Advice for fire-fighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal precautions, protective equipment and emergency procedures**

Ensure adequate ventilation

Environmental precautions

Prevent further leakage or spillage if safe to do so

Methods and material for containment and cleaning up

Sweep up or vacuum up spillage and collect in suitable container for disposal.

SECTION 7. HANDLING AND STORAGE**Precautions for Safe Handling**

Avoid contact with skin and eyes. Avoid contact with clothing. Remove and wash contaminated clothing before re-use. Avoid breathing vapors or mists. Do not ingest. Wash thoroughly after handling.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in freezer.

Specific End Uses

3-Isobutyl-1-methylxanthine

Revision Date 02-Jul-2012

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control parameters

Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies.

Derived No Effect Level (DNEL)

No information available.

Predicted No Effect Concentration (PNEC)

No information available.

Exposure controls

Engineering Measures

Ventilation systems

Personal protective equipment

Eye Protection

Goggles

Hand Protection

Protective gloves

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure

Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice

Environmental exposure controls

No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Physical State

Powder, Solid

Appearance

Beige

pH

No information available.

Boiling Point/Range

No information available.

Melting Point/Range

200 - 203°C / 392 - 397.4°F

Flash Point

No information available.

Autoignition Temperature

No information available.

Water Solubility

almost insoluble

Molecular Formula

C₁₀ H₁₄ N₄ O₂

Molecular Weight

222.25

SECTION 10. STABILITY AND REACTIVITY

Reactivity

Chemical Stability

Stable under normal conditions.

3-Isobutyl-1-methylxanthine

Revision Date 02-Jul-2012

Possibility of Hazardous Reactions**Hazardous Polymerization
Hazardous Reactions .**

Hazardous polymerization does not occur.
No information available.

Conditions to Avoid

Heat, flames and sparks

Incompatible Materials

Oxidizing agents.

Hazardous Decomposition Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x).

SECTION 11. TOXICOLOGICAL INFORMATION**Information on Toxicological Effects****Acute Toxicity****Component Information****Chronic Toxicity****Carcinogenicity**

There are no known carcinogenic chemicals in this product

Sensitization

No information available.

Mutagenic Effects

No information available

Reproductive Effects

No information available.

Developmental Effects

No information available.

Target Organs

No information available.

Other Adverse Effects

The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information

Endocrine Disruptor Information

None known

SECTION 12. ECOLOGICAL INFORMATION**Toxicity****Ecotoxicity effects**

Do not empty into drains

3-Isobutyl-1-methylxanthine

Revision Date 02-Jul-2012

SECTION 12. ECOLOGICAL INFORMATION

Persistence and degradability

No information available

Bioaccumulative potential

No information available.

Component	log Pow
3,7-Dihydro-3-isobutyl-1-methyl-1H-purine-2,6-dione	1.582

Mobility in soil

No information available.

Results of PBT and vPvB assessment

Other adverse effects

No information available

SECTION 13. DISPOSAL CONSIDERATIONS

Waste treatment methods

Waste from Residues / Unused Products

Dispose of in accordance with local regulations

Contaminated Packaging

Empty containers should be taken to local recyclers for disposal

SECTION 14. TRANSPORT INFORMATION

IMDG/IMO

Not regulated

ADR

Not regulated

IATA

Not regulated

SECTION 15. REGULATORY INFORMATION

Safety, health and environmental regulations/legislation specific for the substance or mixture

International Inventories

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	CHINA	AICS	KECL
3,7-Dihydro-3-isobutyl-1-methyl-1H-purine-2,6-dione	249-259-3	-		-	-	-	-	-	X	-	-

3-Isobutyl-1-methylxanthine**Revision Date 02-Jul-2012****Legend****TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List**PICCS** - Philippines Inventory of Chemicals and Chemical Substances**ENCS** - Japan Existing and New Chemical Substances**CHINA** - China Inventory of Existing Chemical Substances**AICS** - Inventory of Chemical Substances**KECL** - Existing and Evaluated Chemical Substances**Chemical Safety Assessment****SECTION 16. OTHER INFORMATION****Full text of R-phrases referred to under sections 2 and 3**

No information available.

Revision Date 02-Jul-2012**Revision Summary****Reason for revision** (M)SDS sections updated, 7.**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006****Disclaimer**

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

End of Safety Data Sheet