

Safety Data Sheet (SDS) According to the REACH Regulation (EC) No. 1907/2006

Issuing Date: 2014-07-17

Revision Date: 2017-08-31

Version: 2

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product No 13630
Product name IBMX
Reach registration number This substance/mixture contains only ingredients which have been registered, or are exempt from registration, according to Regulation (EC) No. 1907/2006.

Contains

Chemical Name	Index No.	CAS No
1-methyl-3-(2-methylpropyl)-7H-purine-2,6-dione (90 - 100%)	Not Listed	28822-58-4

Formula	C ₁₀ H ₁₄ N ₄ O ₂
Molecular Weight	222.24 g/mol

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

Identified uses For research use only

1.3. Details of the supplier of the safety data sheet

Importer (Applicable in EU only)	Manufacturer
Cell Signaling Technology Europe B.V. Schuttersveld 2 2316 ZA Leiden The Netherlands TEL: +31 (0)71 7200 200 FAX: +31 (0)71 891 0098	Cell Signaling Technology, Inc. 3 Trask Lane Danvers, MA 01923 United States TEL: +1 978 867 2300 FAX: +1 978 867 2400

Website	www.cellsignal.com
E-mail Address	info@cellsignal.eu

1.4. Emergency telephone number

CHEMTREC 24 hours a day, 7 days a week, 365 days a year
 +1 703 527 3887 (INTERNATIONAL) +1 800 424 9300 (NORTH AMERICA)

Europe 112

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No. 1272/2008

Acute oral toxicity	Category 4 - (H302)
Reproductive toxicity	Category 2 - (H361d)

For the full text of the H-phrases & EUH-phrases mentioned in this Section, see Section 16

2.2. Label elements



Signal word

Warning

Hazard statement(s)

H302 - Harmful if swallowed

H361d - Suspected of damaging the unborn child

Precautionary statement(s)

P201 - Obtain special instructions before use

P264 - Wash face, hands and any exposed skin thoroughly after handling

P281 - Use personal protective equipment as required

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

P330 - Rinse mouth

P308 + P313 - IF exposed or concerned: Get medical advice/attention

2.3. Other hazards

None under normal use conditions.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms

IBMX; IMX; Isobutylmethylxanthine; 3-Isobutyl-1-methylxanthine; Methylisobutylxanthine; Xanthine, 1-methyl-3-(2-methylpropyl)

Formula

C₁₀H₁₄N₄O₂

Chemical nature

Monoconstituent substance.

Chemical Name	CAS No	Weight %	EC No	Classification (1272/2008)	REACH Registration Number
1-methyl-3-(2-methylpropyl)-7H-purine-2,6-dione	28822-58-4	100	249-259-3	Acute Tox. 4 (H302) Repr. 2 (H361)	no data available

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

SECTION 4: First aid measures

4.1. Description of first aid measures

General advice

If symptoms persist, call a physician. Show this safety data sheet to the doctor in attendance. Do not breathe dust/fume/gas/mist/vapors/spray.

Inhalation

Move to fresh air. Consult a physician. If not breathing, give artificial respiration.

Skin contact

Consult a physician if necessary. Wash off immediately with soap and plenty of water removing all contaminated clothes and shoes.

Eye contact

Rinse thoroughly with plenty of water, also under the eyelids. Keep eye wide open while

Ingestion rinsing.
Rinse mouth. Drink plenty of water. If symptoms persist, call a physician. Do NOT induce vomiting. Never give anything by mouth to an unconscious person.

Protection of first-aiders Use personal protective equipment.

4.2. Most important symptoms and effects, both acute and delayed

4.3. Indication of any immediate medical attention and special treatment needed

Notes to physician Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

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

Unsuitable Extinguishing Media No information available.

5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors.

5.3. Advice for firefighters

Wear self-contained breathing apparatus and protective suit. Use personal protective equipment.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel Evacuate personnel to safe areas. Ensure adequate ventilation.

For emergency responders Use personal protection recommended in Section 8.

6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system.

6.3. Methods and material for containment and cleaning up

Methods for containment Prevent further leakage or spillage if safe to do so.

Methods for cleaning up Use personal protective equipment. Cover powder spill with plastic sheet or tarp to minimize spreading and keep powder dry. Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation. Clean contaminated surface thoroughly.

6.4. Reference to other sections

See Sections 8 & 13 for additional information.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Avoid contact with skin, eyes and clothing. Wear personal protective equipment. Prevent the formation of vapors, mists and aerosols. Do not eat, drink or smoke when using this product. Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Keep out of the reach of children.

7.3. Specific end use(s)

Use as a laboratory reagent.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters**8.2. Exposure controls****Appropriate engineering controls**

Showers, eyewash stations, and ventilation systems.

Individual protection measures, such as personal protective equipment

Eye/face protection	Tightly fitting safety goggles.
Skin protection	
Hand protection	Impervious gloves.
Other	Wear suitable protective clothing.
Respiratory protection	In case of inadequate ventilation wear respiratory protection.

Environmental Exposure Controls

Do not allow material to contaminate ground water system.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	Solid
Appearance	Crystalline Powder
Color	No information available
Odor	No information available
Odor Threshold	No information available

<u>Property</u>	<u>Values</u>	<u>Remarks • Method</u>
pH		No information available
Melting point/freezing point	205 °C	
Initial boiling point and boiling range		No information available
Flash point		No information available.
Evaporation rate		No information available
Flammability (solid, gas)		No information available
Upper flammability limit		No information available
Lower flammability limit		No information available
Vapor pressure		No information available
Vapor density		No information available
Relative density		No information available
Solubility		No information available
Partition coefficient: n-octanol/water		No information available
Autoignition temperature		No information available
Decomposition temperature		No information available.
Viscosity		No information available
Explosive properties		No information available
Oxidizing properties		No information available

9.2. Other information

Softening point	No information available
Molecular Weight	222.24 g/mol
Solubility in other solvents	Soluble in ethanol (EtOH) @ 5 mg/mL, Soluble in dimethyl formamide (DMF) @ 5 mg/mL
VOC content	No information available

Density No information available.

SECTION 10: Stability and reactivity

10.1. Reactivity

No information available.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous polymerization Hazardous polymerization does not occur.
Hazardous reactions None under normal processing.

10.4. Conditions to avoid

None known based on information supplied.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Thermal decomposition can lead to release of irritating gases and vapors: Nitrogen oxides (NO_x), Carbon oxides (CO_x).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

This material should only be handled by, or under the close supervision of, those properly qualified in the handling and use of potentially hazardous chemicals. It should be borne in mind that the toxicological and physiological properties of this compound is not well defined.

ATEmix (oral) 500 mg/kg

Information on likely routes of exposure

Inhalation There is no data available for this product.
Eye contact There is no data available for this product.
Skin contact There is no data available for this product.
Ingestion May be harmful if swallowed.

Symptoms No information available.
Skin corrosion/irritation No information available.
Serious eye damage/eye irritation No information available.
Sensitization No information available.
Mutagenic effects No information available.
Carcinogenic effects No information available.
Reproductive toxicity IBMX, a phosphodiesterase inhibitor also known to be an adenosine receptor antagonist, was the most potent developmental toxicant of the materials evaluated using the Frog Embryo Teratogenesis Assay Xenopus (FETAX).
Teratogenicity Possible risk of harm to the unborn child. IBMX (0.5-5 umol) was applied topically to the extraembryonic membrane of 4-day chickembryo (Hamburger-Hamilton developmental stage 24). Cardiovascular malformations were demonstrated in 53% of chick embryos treated with 2.5 umol IBMX where survival rate was 89%. Malformation rate was dose-dependent. Cardiovascular anomalies demonstrated were ventricular septal defect, dextroposition of the aorta, double outletright ventricle, truncus arteriosus communis and

STOT - single exposure	aortic arch anomalies.
STOT - repeated exposure	No information available.
Aspiration Hazard	No information available.
Other information	Intraperitoneal LD50 = 44 mg/kg (Mouse).

SECTION 12: Ecological information

12.1. Toxicity

No information available.

12.2. Persistence and degradability

No information available.

12.3. Bioaccumulative potential

Bioaccumulation	Not likely to bioaccumulate.
Bioconcentration factor (BCF)	No information available.

Chemical Name	Octanol-Water Partition Coefficient
1-methyl-3-(2-methylpropyl)-7H-purine-2,6-dione	1.15

12.4. Mobility in soil

No information available.

12.5. Results of PBT and vPvB assessment

No information available.

12.6. Other adverse effects

No information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste from residues / unused products	Dispose of in accordance with local regulations.
Contaminated packaging	Empty containers should be taken to an approved waste handling site for recycling or disposal.
Other information	According to the European Waste Catalogue, Waste Codes are not product specific, but application specific. Waste codes should be assigned by the user based on the application for which the product was used.

SECTION 14: Transport information

IMDG/IMO

14.1 UN number	Not regulated
14.2 UN proper shipping name	Not regulated
14.3 Transport hazard class(es)	Not regulated
14.4 Packing group	Not regulated
14.5 Environmental hazards	None
14.6 Special precautions for user	None
14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	Not regulated

ADR/RID

14.1 UN number	Not regulated
14.2 UN proper shipping name	Not regulated
14.3 Transport hazard class(es)	Not regulated
14.4 Packing group	Not regulated
14.5 Environmental hazards	None
14.6 Special precautions for user	None

IATA

14.1 UN number	Not regulated
14.2 UN proper shipping name	Not regulated
14.3 Transport hazard class(es)	Not regulated
14.4 Packing group	Not regulated
14.5 Environmental hazards	None
14.6 Special precautions for user	None

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture**Candidate List of Substances of Very High Concern for Authorization Information**

This product does not contain Substances of Very High Concern (SVHC).

SEVESO Directive Information

This product does not contain substances identified in the SEVESO Directive.

International inventories

TSCA 8(b)	-
DSL/NDSL	-
EINECS/ELINCS	Complies
ENCS	-
IECSC	Complies
KECL	-
PICCS	-
AICS	-

International inventories legend

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
 DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List
 EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances
 ENCS - Japan Existing and New Chemical Substances
 IECSC - China Inventory of Existing Chemical Substances
 KECL - Korean Existing and Evaluated Chemical Substances
 PICCS - Philippines Inventory of Chemicals and Chemical Substances
 AICS - Australian Inventory of Chemical Substances

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out

SECTION 16: Other information

Full text of H-Statements referred to under Sections 2 and 3

H302 - Harmful if swallowed
 H361d - Suspected of damaging the unborn child

Classification procedure: Expert judgment and weight of evidence determination. Bridging principle "Interpolation within one toxicity category".

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Disclaimer

The information provided in 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 guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered 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 materials or in any process, unless specified in the text.