

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

Issuing Date: 2014-07-15

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 13055
Product name PX-866
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
[(3aR,6E,9S,9aR,10R,11aS)-6-[[bis(prop-2-enyl)amino]methylidene]-5-hydroxy-9-(methoxymethyl)-9a,11a-dimethyl-1,4,7-trioxo-2,3,3a,9,10,11-hexahydroindeno[4,5-h]isochromen-10-yl] acetate (90 - 100%)	Not Listed	502632-66-8

Formula $C_{29}H_{35}NO_8$
Molecular Weight 525.59

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)
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Acute dermal toxicity	Category 4 - (H312)
Acute inhalation toxicity	Category 4 - (H332)
Skin corrosion/irritation	Category 2 - (H315)
Serious eye damage/eye irritation	Category 2 - (H319)

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
 H312 - Harmful in contact with skin
 H332 - Harmful if inhaled
 H315 - Causes skin irritation
 H319 - Causes serious eye irritation

Precautionary statement(s)

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
 P264 - Wash face, hands and any exposed skin thoroughly after handling
 P280 - Wear protective gloves/protective clothing/eye protection/face protection
 P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
 P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
 P312 - Call a POISON CENTER or doctor if you feel unwell

2.3. Other hazards

None under normal use conditions.

SECTION 3: Composition/information on ingredients

Synonyms

Sonolisib; UNII-987796874T; DJM166; DJM-2-166;
 (4E)-4-(((Bis(prop-2-en-1-yl)amino)methylidene)-6-hydroxy-1alpha-(methoxymethyl)-3,7,17-trioxo-2-oxaandrost-5,8-dien-11alpha-yl) acetate

Formula

C₂₉H₃₅NO₈

Chemical nature

Derivative of Wortmannin.

Chemical Name	CAS No	Weight %	EC No	Classification (1272/2008)	REACH Registration Number
[(3aR,6E,9S,9aR,10R,11aS)-6-[[bis(prop-2-enyl)amino]methylidene]-5-hydroxy-9-(methoxymethyl)-9a,11a-dimethyl-1,4,7-trioxo-2,3,3a,9,10,11-hexahydroindeno[4,5-h]isochromen-10-yl] acetate	502632-66-8	100	-	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332) Skin Irrit. 2 (315) Eye Irrit. 2 (H319)	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	Use first aid treatment according to the nature of the injury. When symptoms persist or in all cases of doubt seek medical advice.
Inhalation	Move to fresh air.
Skin contact	Wash off immediately with soap and plenty of water removing all contaminated clothes and shoes.
Eye contact	Rinse thoroughly with plenty of water for at least 15 minutes, lifting lower and upper eyelids. Consult a physician.
Ingestion	Clean mouth with water and afterwards drink plenty of water.

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

Diarrhea, Nausea, Vomiting, tiredness, In animal studies, the major side effects included leukocytosis (raised white blood cell count), gastrointestinal irritation, and hyperglycemia with decreased glucose tolerance.

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

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.

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	Safety glasses with side-shields.
Skin protection	
Hand protection	Impervious gloves.
Other	Wear suitable protective clothing.
Respiratory protection	In case of inadequate ventilation wear respiratory protection.

Environmental Exposure Controls

No information available.

SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state	Solid
Appearance	Crystalline Powder
Color	Yellow
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	98-110 °C	No information available
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	Practically insoluble	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	525.59
Solubility in other solvents	Soluble in ethanol (EtOH) @ 200 mg/mL, Soluble in dimethyl sulfoxide (DMSO) @ 200 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

Incompatible with strong acids and bases.

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
ATEmix (dermal)	1100 mg/kg
ATEmix (inhalation-dust/mist)	1.5 mg/l

Information on likely routes of exposure

Inhalation	May be harmful if inhaled.
Eye contact	May cause temporary eye irritation.
Skin contact	May be harmful in contact with skin. May cause irritation.
Ingestion	May be harmful if swallowed.

Symptoms	Diarrhea. Nausea. Vomiting. tiredness. In animal studies, the major side effects included leukocytosis (raised white blood cell count), gastrointestinal irritation, and hyperglycemia with decreased glucose tolerance.
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Skin corrosion/irritation	Irritating to skin.
Serious eye damage/eye irritation	Irritating to eyes.
Sensitization	No information available.
Mutagenic effects	No information available.
Carcinogenic effects	No information available.
Reproductive toxicity	No information available.
STOT - single exposure	No information available.
STOT - repeated exposure	No information available.
Aspiration Hazard	No information available.
Other information	No information available.

SECTION 12: Ecological information

12.1. Toxicity

No information available.

12.2. Persistence and degradability

No information available.

12.3. Bioaccumulative potential

Bioaccumulation	No information available.
Bioconcentration factor (BCF)	No information available.

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	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	Not regulated

IBC Code**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	-
ENCS	-
IECSC	-
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
H312 - Harmful in contact with skin
H332 - Harmful if inhaled
H319 - Causes serious eye irritation
H315 - Causes skin irritation

Classification procedure: Expert judgment and weight of evidence determination. By analogy.

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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.