

Product Name: Ketoenamine
Issued: Feb-06-2013

SAFETY DATA SHEET

Section 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product Identifier

Product Name: Ketoenamine
Chemical Name: 2-Amino-5-S-dibenzylamino-4-oxo-1,6-diphenylhex-2-ene
Synonyms: Ketoenamina; Ritonavir Intermediate
Drug Code Number: 22192

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

Recommended use: Process Intermediate
Scientific research and development

1.3 Details of the supplier of the safety data sheet

Supplier: AbbVie Inc.
1 North Waukegan Road
North Chicago, IL 60064
USA
1-800-255-5162
+1-847-937-7433
Customer Service Telephone: 1-800-255-5162 (US and Canada only)
+1-847-937-7433
E-mail Address: AbbVie.SDS@abbvie.com

1.4 Emergency telephone number

Emergency Telephone: CHEMTREC: 1(800) 424-9300 (in USA and Canada)
or +1-703-527-3887 (international)

Section 2. Hazards identification

2.1 Classification of the substance or mixture

Regulation (EC) No 1272/2008

Serious eye damage/eye irritation Category 2

Chronic aquatic toxicity Chronic toxicity 4

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

2.2 Label elements

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Section 2. Hazards identification



Signal Word: Warning

Hazard Statements: H319 - Causes serious eye irritation
H413 - May cause long lasting harmful effects to aquatic life

P264 - Wash face, hands and any exposed skin thoroughly after handling
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes.
Remove contact lenses, if present and easy to do. Continue rinsing
P337 + P313 - If eye irritation persists: Get medical advice/attention

2.3 Other hazards

Not determined

Section 3. Composition/information on ingredients

Chemical Name	Percent	EINECS/ELINCS Number	EEC Classification	EU - GHS Substance Classification	REACH No.
Ketoenamine 156732-13-7	100	NA	Xi, R36; R53	Eye Irrit. 2 (H319) Aquatic Chronic 4 (H413)	01-00000-16960-68-0003

Not Hazardous* - Based on available data, not classified as hazardous according to the criteria of the Globally Harmonized System.

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

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

Section 4. First aid measures

4.1 Description of first aid measures

Eye Contact: Remove from source of exposure. Flush with copious amounts of water. If irritation persists or signs of toxicity occur, seek medical attention. Provide symptomatic/supportive care as necessary.

Skin Contact: Remove from source of exposure. Flush with copious amounts of water. If irritation persists or signs of toxicity occur, seek medical attention. Provide symptomatic/supportive care as necessary.

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Inhalation: Remove from source of exposure. If signs of toxicity occur, seek medical attention. Provide symptomatic/supportive care as necessary.

Ingestion: Remove from source of exposure. If signs of toxicity occur, seek medical attention. Provide symptomatic/supportive care as necessary.

Protection of First-aiders: Use personal protective equipment

4.2 Most important symptoms and effects, both acute and delayed

Signs and Symptoms: None known from occupational exposure.

Medical Conditions Aggravated by Exposure: None known from occupational exposure.

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 agent suitable for type of surrounding fire

Unsuitable Extinguishing Media: Not determined

5.2 Special hazards arising from the substance or mixture

Special Exposure Hazards: Not determined

5.3 Advice for firefighters

Protective Equipment and Precautions for Firefighters: As in any fire, wear self-contained breathing apparatus and full protective gear

Section 6. Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal Precautions: For personal protection see section 8

6.2. Environmental precautions

Environmental Precautions: Contain material and prevent release to waterways or soil.

6.3. Methods and material for containment and cleaning up

Methods for Cleaning Up: Recover product and place in an appropriate container for disposal.

6.4. Reference to other sections

Refer to Sections 8, 12, and 13 for further information.

Section 7. Handling and storage

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Section 7. Handling and storage

7.1. Precautions for safe handling

Avoid contact with skin, eyes and clothing. Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Store according to label instructions

7.3. Specific end use(s)

Recommended use: Process Intermediate
Scientific research and development

Section 8. Exposure controls/personal protection

8.1. Control parameters

Exposure limits:

Chemical Name	Employee Exposure Limit	Skin Notation
Ketoenamine 156732-13-7	Not Applicable	None

8.2. Exposure controls

Engineering Controls: Local exhaust ventilation as necessary to maintain exposures to within applicable limits.

Respiratory Protection: An approved respirator (i.e. NIOSH, EN, etc.) should be worn when exposures are expected to exceed the applicable limits.

Eyes: Wear eye protection appropriate to handling activities.

Gloves: Impervious gloves.

Other PPE Data: Wear appropriate body coverings if contact may occur.

Environmental Exposure Controls: Not determined

Section 9. Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance: White to light yellow Solid
Odor: Not determined.
Odor Threshold: Not determined
pH: Not determined.
Boiling Pt. @ 760 mm Hg (°C): > 300 with decomposition.
Melting/Freezing Point (°C): 98-103
Flash Point (°C): Not determined.
Evaporation Rate at 20°C: Not determined.
Flammability (Solid): Not determined.

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Lower Explosive Limit:	Not determined.
Upper Explosive Limit:	Not determined.
Vapor Pressure (mm Hg):	0.000009at 25 deg. C
Vapor Density (Air = 1):	Not determined.
Density, g / mL:	1.104
Specific Gravity:	Not determined.
Solubility(ies):	Soluble in: methylene chloride, ethyl acetate. Insoluble in: water, alcohol.
Partition coefficient: n-octanol/water	Not determined.
Log Po/w	6.3
Autoignition Temp. (°C):	> 400
Decomposition temperature (°C):	Not determined.
Viscosity (centipoise):	Not determined.
Explosion Severity:	Not determined.
Oxidizer Properties:	Not determined.

9.2. Other information

Min. Ignition Energy-Cloud (mJ):	2
Min. Explosive Conc. (g/m³):	25

Section 10. Stability and reactivity

10.1. Reactivity

Not determined

10.2. Chemical stability

Stable under normal conditions

10.3. Possibility of hazardous reactions

Hazardous reactions: Not determined.

10.4. Conditions to avoid

Not determined.

10.5 Incompatible materials

Not determined

10.6 Hazardous decomposition products

Carbon oxides, Nitrogen oxides (NOx)

Section 11. Toxicological information

11.1. Information on toxicological effects

Routes of Exposure:	
Oral:	Not determined.
Dermal:	Not determined.

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Inhalation: Not determined.

Acute Toxicity - Oral: Data for component (s) given below.

Chemical Name	Acute Test	Value	Units	Species
Ketoenamine 156732-13-7	LD50 >	2000	mg/kg	Rats

Acute Toxicity - Dermal: Data for component (s) given below.

Chemical Name	Acute Test	Value	Units	Species
Ketoenamine 156732-13-7	LD50 >	2000	mg/kg	Rats

Acute Toxicity - Inhalation: Not determined.

Corrosivity: Not determined.

Dermal Irritation: Not an irritant.

Eye Irritation: Not an eye irritant in rabbits.

Sensitization: Negative in the maximization assay in guinea pigs at challenge concentrations.

Toxicokinetics/Metabolism: Not determined.

Target Organ Effects: Data for component (s) given below.

Chemical Name	Target Organs:	Species	Dosage	Units	Route	Duration
Ketoenamine 156732-13-7	None	Rats	15-500	mg/kg/day	Oral Gavage	1 Month

Reproductive Effects: Not determined.

Carcinogenicity: Not determined.

Mutagenicity: Data for component (s) given below.

Chemical Name	Micronucleus Assay	Ames Test:	Mouse Lymphoma Assay	Chromosomal Abbr. Assay
Ketoenamine 156732-13-7	No Data.	Negative	No Data.	Negative

Aspiration hazard: Not determined

Notes:

1. ALD: Approximate lethal dosage
2. LC50: Concentration in air that produces 50% mortality
3. LD50: Oral or dermal dosage that produces 50% mortality

Section 12. Ecological information

12.1. Toxicity

No aquatic toxicity detected at the limit of solubility

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12.2. Persistence and degradability

Not readily biodegradable

Persistence: Not determined.

12.3. Bioaccumulative potential

Not determined

12.4. Mobility in soil

Not determined.

12.5. Results of PBT or vPvB assessment

Chemical safety report is not required for this substance/product.

12.6. Other adverse effects

Do not allow undiluted material or large quantities to reach groundwater, bodies of water or sewer system.

Notes:

1. EC50: Concentration in water that produces 50% mortality in *Daphnia* sp.
2. LC50: Concentration in water that produces 50% mortality in fish.
3. EbC50/ErC50: Concentration in water that produces 50% inhibition of growth and in algae.

Section 13. Disposal considerations

13.1 Waste treatment methods

Waste Disposal Methods: Disposal should be made in accordance with country, federal, state and local regulations.

Section 14. Transport information

ADR, DOT, ICAO/IATA, IMDG/IMO

Status: Not regulated

- 14.1. UN Number:** Not applicable
14.2. Proper shipping name: Not applicable
14.3. Hazard class: Not applicable
14.4. Packing group: Not applicable
14.5. Environmental hazard: Not applicable
14.6. Special Provisions: Not applicable
14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code: Not applicable

Section 15. Regulatory Information

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

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International Inventories

Chemical Name	EINECS/ ELINCS	TSCA	DSL	NDSL	PICCS
Ketoenamine 156732-13-7	-	-	-	Not listed.	-

Chemical Name	ENCS	ISHL	IECSC	AICS	KECL	New Zealand
Ketoenamine 156732-13-7	-	-	-	-	-	

Legend

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

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

ISHL - Japan Industrial Safety and Health Law

IECSC - China Inventory of Existing Chemical Substances

AICS - Australian Inventory of Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

Carcinogenicity Rating:

Chemical Name	Percent	NTP:	IARC:	ACGIH:
Ketoenamine	100	Not Listed	Not Listed	Not Listed

SARA 313 Information

Chemical Name	Percent	SARA 313 Chemical:	CERCLA RQ/SARA EHS RQ (lbs):	SARA EHS TPQ (lbs):
Ketoenamine	100	No	Not Applicable	Not applicable

Immediate Health: Yes

Delayed Health: No

Fire: No

Sudden Pressure: No

Reactivity: No

RCRA Status: Not determined.

Proposition 65 Status: Does not contain chemicals known to the state of California to cause cancer or reproductive harm.

WHMIS Hazard Class: Not determined.

NFPA Rating:

Health: 1

Fire: 1

Reactivity: 0

Notes:

1. SARA = Superfund Amendments and the Reauthorization Act.
2. CERCLA = Comprehensive Environmental Response, Compensation and Liability Act.
3. FIFRA = Federal Insecticide, Fungicide and Rodenticide Act.
4. TSCA = Toxic Substances Control Act.
5. EC = European Community.
6. WHMIS = Canadian Workplace Hazardous Materials Information System.
7. UN GHS = United Nations Globally Harmonized System for Hazard Identification.

15.2. Chemical safety assessment

Product Name: Ketoenamine
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Chemical safety assessment has not been conducted on the substance/product.

Section 16. Other information

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

H319 - Causes serious eye irritation, H413 - May cause long lasting harmful effects to aquatic life

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Disclaimer:

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