

SAFETY DATA SHEETS

According to the UN GHS revision 10

Version: 1.1
Creation Date: July 15, 2024
Revision Date: January 11, 2025

SECTION 1: Identification

1.1 GHS Product identifier

Product name Isavuconazole Impurity 60

1.2 Other means of identification

Product number C4X-123660
Other names 2-BUTENAL; Topanel; CH₃CH=CHCHO

1.3 Recommended use of the chemical and restrictions on use

Identified uses For laboratory and Industrial use only.
Uses advised against no data available

1.4 Supplier's details

Company CATO Research Chemicals Inc.
Address 3/F,Building B,No.179 BASIGO, Guangpu Rd East,Huangpu Dist,Guangzhou
Telephone +86-20-81960175

1.5 Emergency phone number

Emergency phone number +86-20-81960175
Service hours 'Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Flammable liquids, Category 2
Acute toxicity - Category 3, Oral
Acute toxicity - Category 3, Dermal
Skin irritation, Category 2
Serious eye damage, Category 1
Acute toxicity - Category 2, Inhalation
Specific target organ toxicity – single exposure, Category 3
Germ cell mutagenicity, Category 2
Specific target organ toxicity – repeated exposure, Category 2
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H301 Toxic if swallowed
H311 Toxic in contact with skin
H315 Causes skin irritation
H318 Causes serious eye damage
H330 Fatal if inhaled
H335 May cause respiratory irritation
H341 Suspected of causing genetic defects
H373 May cause damage to organs through prolonged or repeated exposure
H400 Very toxic to aquatic life

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] wear respiratory protection.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P203 Obtain, read and follow all safety instructions before use.
P273 Avoid release to the environment.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P320 Specific treatment is urgent (see ... on this label).
P319 Get medical help if you feel unwell.
P318 IF exposed or concerned, get medical advice.
P391 Collect spillage.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Isavuconazole Impurity 60	(E)-crotonaldehyde	123-73-9	204-647-1	≈ 99%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention. Half-upright position. Artificial respiration may be needed.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Give one or two glasses of water to drink. Refer for medical attention.

4.2 Most important symptoms/effects, acute and delayed

Although slightly less toxic, crotonaldehyde is similar chemically and toxicologically to acrolein, which is rated as extremely toxic. Toxic concentrations for human inhalation have been reported at 12 mg/m³/10 minutes. Irritant dose to human eye is 45 ppm. As with acrolein, vapor exposures cause severe and painful eye irritation, damage to cornea, lacrimation (tearing), irritation of nasal membranes, pulmonary edema (filling of lungs with fluid) and gastrointestinal distress when ingested. (EPA, 1998)

This compound is an extreme eye, respiratory, and skin irritant and can cause corneal damage. A 15 minute exposure at 4.1 ppm is highly irritating to the nose and upper respiratory tract and causes tearing. Brief exposure at 45 ppm proved very disagreeable with prominent eye irritation. (EPA, 1998)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Prehospital Management. Victims exposed only to crotonaldehyde vapor do not pose contamination risks to rescuers. Victims whose clothing or skin is contaminated with liquid crotonaldehyde can secondarily contaminate response personnel by direct contact or by off-gassing vapor. Crotonaldehyde is a direct irritant to mucous membranes, skin, eyes, and the respiratory system. Acute inhalation exposure may lead to respiratory distress and noncardiogenic pulmonary edema. There is no antidote for crotonaldehyde. Treatment consists of respiratory and cardiovascular support.

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Evacuation: If fire becomes uncontrollable or container is exposed to direct flame-consider evacuation of one-third (1/3) mile radius. Crotonaldehyde, stabilized

5.2 Specific hazards arising from the chemical

Vapors form explosive mixtures in air or in sewers. Hazardous peroxides and acids emitted when heated to decomposition. Avoid nitric acid. Unstable, avoid oxygen, heat, elevated pressures. Hazardous polymerization may occur. Avoid contact with alkaline materials such as caustic ammonia or amines, or at elevated temperatures. (EPA, 1998)

Flammable/combustible material; may be ignited by heat, sparks or flames. Vapor may travel to a source of ignition and flash back. Container may explode in heat of fire. Vapor explosion and poison hazard indoors, outdoors or in sewers. Runoff to sewer may create fire or explosion hazard. Readily converted by oxygen to hazardous peroxides and acids and is incompatible with caustics, ammonia, organic amines, mineral acids, and strong oxidizers. Readily resinifies to dimer when pure and slowly oxidizes to crotonic acid. Altered by light and air. Hazardous polymerization may occur. Polymerization may take place at high temperatures. (EPA, 1998)

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

6.2 Environmental precautions

Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Ventilation. Remove all ignition sources. Do NOT absorb in saw-dust or other combustible absorbents. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

6.3 Methods and materials for containment and cleaning up

Environmental considerations land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner./ Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete. Absorb bulk liquid with fly ash or cement powder. Apply appropriate foam to diminish vapor and fire hazard. Add sodium bisulfite (NaHSO₃). Crotonaldehyde, stabilized

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Fireproof. Separated from food and feedstuffs. See Chemical Dangers. Cool. Keep in the dark. Well closed. Store only if stabilized. Store in cool place with containers tightly sealed & away from sources of ignition or heat.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

Component	(E)-crotonaldehyde			
CAS No.	123-73-9			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m ³	ppm	mg/m ³
Austria	0,34	1	1,36	4

Component	(E)-crotonaldehyde			
CAS No.	123-73-9			
Denmark	2	6	4	12
Finland	0,1	0,29	0,3 (1)	0,87 (1)
France	2	6		
Ireland	2	6	6 (1)	18 (1)
Spain			0,3	0,87
Switzerland	0,34	1		
USA - NIOSH	2	6		
USA - OSHA	2	6		
	Remarks			
Austria	TRK value (based on technical feasibility)			
Finland	(1) 15 minutes average value			
Ireland	(1) 15 minutes reference period			
Spain	skin			

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	(e)-crotonaldehyde is a water-white to straw-colored liquid with a pungent, suffocating odor. Used as a chemical intermediate in a variety of industrial processes (surfactants, textiles, paper, fuels, insecticides, leather tanning, etc.). Used in chemical warfare. (EPA, 1998)
Colour	Water-white, mobile liquid
Odour	Pungent, suffocating odor
Melting point/freezing point	-74°C
Boiling point or initial boiling point and boiling range	101-103°C
Flammability	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit	IN AIR % BY VOL-- LOWER 2.1, UPPER 15.5
Flash point	13°C
Auto-ignition temperature	450° F (USCG, 1999)
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	less than 0.1 mg/mL at 65.3° F (NTP, 1992)
Partition coefficient n-octanol/water	log Kow = 0.60 (est)
Vapour pressure	32 mm Hg (20 °C)
Density and/or relative density	0.858
Relative vapour density	2.41 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity



10.1 Reactivity

The substance can presumably form explosive peroxides. The substance may polymerize. This generates fire or explosion hazard. The substance is a strong reducing agent. It reacts violently with oxidants and many other substances. This generates fire and explosion hazard. Attacks plastics and many other substances.

10.2 Chemical stability

May deteriorate in normal storage & cause hazard.

10.3 Possibility of hazardous reactions

Fire hazard ... when exposed to heat or flame; can react with oxidizing materials. The vapour is heavier than air and may travel along the ground; distant ignition possible. (E)-CROTONALDEHYDE is an aldehyde. It can react violently with strong oxidizing reagents, e.g., reaction with conc. nitric acid leads to instantaneous ignition [Andrussow, L., Chim. Ind. (Paris), 1961, 86, p. 542]. In contact with strong acids or bases it will undergo an exothermic condensation reaction. Reaction with 1,3-butadiene is particularly violent [Greenlee, K. W., Chem. Eng. News, 1948, 26, p. 1985]. Crotonaldehyde may rapidly polymerize with ethyl acetoacetate (Soriano, D.S. et al. 1988. Journal of Chemical Education 65:637.).

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

The Diels-Adler reaction between ... /1,3-butadiene & crotonaldehyde/ under pressure is a logical approach to the prepn of a number of cyclic aldehydes, alcohols, & hydrocarbons. A destructive explosion, including a secondary gas explosion, occurred in carrying out this reaction.

10.6 Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 206 mg/kg
- Inhalation: LC50 Rat inhalation 200 mg/cu m/ 2hr
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

CLASSIFICATION: C; possible human carcinogen. BASIS FOR CLASSIFICATION: Based on no human data and an increased incidence of hepatocellular carcinomas and hepatic neoplastic nodules (combined) in male F344 rats. The possible carcinogenicity of crotonaldehyde is supported by genotoxic activity and the expected reactivity of croton oil and aldehyde. Crotonaldehyde is also a suspected metabolite of N-nitrosopyrrolidine, a probable human carcinogen. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: Limited.

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50; Species: Lepomis macrochirus (Bluegill sunfish); Conditions: static bioassay in fresh water at 23 deg C with mild aeration applied after 24 hr; Concentration: 3.5 ppm for 96 hr (85% aqueous)
- Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea); Conditions: freshwater, static;

- Concentration: 3900 ug/L for 24 hr; Effect: behavior equilibrium
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

Crotonaldehyde (isomer not reported) was observed to have a 5-day BODT of 37% using the AFNOR T.90 test protocol(1). (E)-Crotonaldehyde has been found to be degradable via anaerobic (methane fermentation) biotechnology(2,3).

12.3 Bioaccumulative potential

An estimated BCF value of 0.74 was calculated for (E)-crotonaldehyde(SRC), using an experimental water solubility of 150,000 mg/L at 20 deg C(1), and a recommended regression-derived equation(2). According to a recommended classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms will not be an important fate process(SRC).

12.4 Mobility in soil

The Koc of (E)-crotonaldehyde is estimated to be approximately 6.2(SRC), using an experimental water solubility of 150,000 mg/L at 20 deg C(1) and a regression-derived equation(2,SRC). According to a recommended classification scheme(3), this estimated Koc value suggests that (E)-crotonaldehyde has very high mobility in soil(SRC).

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.2 UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.3 Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
(E)-crotonaldehyde	(E)-crotonaldehyde	123-73-9	204-647-1
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.

New Zealand Inventory of Chemicals (NZIoC)	Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Listed.
Vietnam National Chemical Inventory	Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Listed.
Korea Existing Chemicals List (KECL)	Listed.

SECTION 16: Other information

Information on revision

Creation Date July 15, 2024
Revision Date January 11, 2025

Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Any questions regarding this SDS, Please send your inquiry to info@cato-chem.com

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