

SAFETY DATA SHEETS

According to the UN GHS revision 10

Version: 1.1
Creation Date: July 15, 2024
Revision Date: January 09, 2025

SECTION 1: Identification

1.1 GHS Product identifier

Product name Pregabalin Impurity 79

1.2 Other means of identification

Product number C4X-131279

Other names ethyl 2-cyanoacetate; Ethyl Cyanoacetate; Acetic acid, cyano-, ethyl ester

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

Acute toxicity - Category 4, Oral

Acute toxicity - Category 4, Dermal

Acute toxicity - Category 4, Inhalation

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H302 Harmful if swallowed

H312 Harmful in contact with skin

H332 Harmful if inhaled

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P317 Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

Storage

none

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
Pregabalin Impurity 79	Ethyl cyanoacetate	105-56-6	203-309-0	≈ 99%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

4.2 Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 151 [Substances - Toxic (Non-combustible)]: Highly toxic, may be fatal if inhaled, swallowed or absorbed through skin. Avoid any skin contact. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Esters and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Carbon dioxide, dry chemical

5.2 Specific hazards arising from the chemical

Excerpt from ERG Guide 151 [Substances - Toxic (Non-combustible)]: Non-combustible, substance itself does not burn but may decompose upon heating to produce corrosive and/or toxic fumes. Containers may explode when heated. Runoff may pollute waterways. (ERG, 2016)

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

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

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	Ethyl cyanoacetate is a colorless liquid. Denser than water. Contact may irritate skin, eyes and mucous membranes. May be toxic by ingestion. Used to make other chemicals.
Colour	Colorless liquid
Odour	Slight, pleasant odor
Melting point/freezing point	270°C(dec.)(lit.)
Boiling point or initial boiling point and boiling range	288°C(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	110°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Very soluble in ethyl ether, ethanol
Partition coefficient n-octanol/water	no data available
Vapour pressure	1 mm Hg (67.8 °C)
Density and/or relative density	1.063
Relative vapour density	3.9 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Slightly soluble in water.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

Combustible when exposed to heat or flame. ETHYL CYANOACETATE is both a nitrile and an ester. Esters react with acids to liberate heat along with alcohols and acids. Strong oxidizing acids may cause a vigorous reaction that is sufficiently exothermic to ignite the reaction products. Heat is also generated by the interaction of esters with caustic solutions. Flammable hydrogen is generated by mixing

esters with alkali metals and hydrides. Nitriles may polymerize in the presence of metals and some metal compounds. They are incompatible with acids; mixing nitriles with strong oxidizing acids can lead to extremely violent reactions. Nitriles are generally incompatible with other oxidizing agents such as peroxides and epoxides. The combination of bases and nitriles can produce hydrogen cyanide. Nitriles are hydrolyzed in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids). These reactions generate heat. Peroxides convert nitriles to amides. Nitriles can react vigorously with reducing agents. Acetonitrile and propionitrile are soluble in water, but nitriles higher than propionitrile have low aqueous solubility. They are also insoluble in aqueous acids.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Will react with water or steam to produce toxic and flammable vapors.

10.6 Hazardous decomposition products

When heated to decomposition or on contact with acid or acid fumes, it emits highly toxic fumes of /cyanides/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: LC50 Rat inhalation >7380 mg/cu m 1hr
- 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

no data available

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: no data available
- Toxicity to daphnia and other aquatic invertebrates: no data available
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC: Ethyl cyanoacetate, present at 30 mg/L, reached 68% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 100 mg/L in the Japanese MITI test(1,2).

12.3 Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for ethyl cyanoacetate(SRC), using an estimated log Kow of 0.02(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of ethyl cyanoacetate can be estimated to be 4(SRC). According to a classification scheme(2), this estimated Koc value suggests that ethyl cyanoacetate is expected to have very high mobility in soil.

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: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

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
Ethyl cyanoacetate	Ethyl cyanoacetate	105-56-6	203-309-0
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			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

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January 09, 2025

Abbreviations and acronyms



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- 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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