

## Chemical Safety Data Sheet MSDS / SDS

## Cyano (3-phenoxybenzyl)-2-(4-chlorophenyl)-3-methylbutyrate SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: Cyano (3-phenoxybenzyl)-2-(4-chlorophenyl)-3-methylbutyrate

CAS: 51630-58-1

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

Relevant identified uses: For R&amp;D use only. Not for medicinal, household or other use.

Uses advised against: none

**Company Identification**

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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**SECTION 2: Hazards identification****Classification of the substance or mixture**Acute toxicity - Category 3, Oral  
Skin irritation, Category 2

Eye irritation, Category 2  
Specific target organ toxicity - single exposure, Category 3

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

### Hazard statement(s)

H301 Toxic if swallowed  
H315 Causes skin irritation  
H319 Causes serious eye irritation  
H335 May cause respiratory irritation  
H410 Very toxic to aquatic life with long lasting effects

### 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+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/...  
P332+P317 If skin irritation occurs: Get medical help.  
P362+P364 Take off contaminated clothing and wash it before reuse.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P319 Get medical help if you feel unwell.

### Storage

P405 Store locked up.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

#### **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.

#### **Other hazards which do not result in classification**

no data available

### **SECTION 3: Composition/information on ingredients**

#### **Substance**

Chemical name:	Cyano (3-phenoxybenzyl)-2-(4-chlorophenyl)-3-methylbutyrate
Common names and synonyms:	Cyano (3-phenoxybenzyl)-2-(4-chlorophenyl)-3-methylbutyrate
CAS number:	51630-58-1
EC number:	257-326-3
Concentration:	100%

### **SECTION 4: First aid measures**

#### **Description of necessary first-aid measures**

##### **If inhaled**

Fresh air, rest. Refer for medical attention.

##### **Following skin contact**

Remove contaminated clothes. Rinse and then wash skin with water and soap.

##### **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. Refer for medical attention .

#### **Most important symptoms/effects, acute and delayed**

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]: TOXIC; inhalation, ingestion or skin contact with material may cause severe injury or death. Contact with molten substance may cause severe burns to skin and eyes. 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)

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

In an antidotal study, phenobarbital, pentobarbital, and diphenylhydantoin were found to be effective in relieving the acute signs of intoxication in the rat. Intraperitoneal injection of phenobarbital (50 mg/kg) prevented tremor, diphenylhydantoin (100 mg/kg) by the same route reduced the toxic reaction, and pentobarbital (35 mg/kg intraperitoneally) removed the tremor reaction completely within 30 min. The combination of diphenylhydantoin with either of the barbiturates was effective in reducing the onset and severity of tremors whereas various other agents d-tubocurarine, atropine, meprobamate, diazepam, biperiden, and trimethadione) were ineffective .

### **SECTION 5: Firefighting measures**

#### **Suitable extinguishing media**

Liquid formulations containing organic solvents may be flammable. Water foam carbon dioxide powder

#### **Specific hazards arising from the chemical**

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]: Non-combustible, substance itself does not burn but may decompose upon heating to produce corrosive and/or toxic fumes. Some are oxidizers and may ignite combustibles (wood, paper, oil, clothing, etc.). Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. For electric vehicles or equipment, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. (ERG, 2016)

#### **Special protective actions for fire-fighters**

Use water, foam, carbon dioxide, powder.

### **SECTION 6: Accidental release measures**

### Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

### Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

### Methods and materials for containment and cleaning up

Personal protection: filter respirator for organic gases and vapors. 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 and remove to safe place.

## SECTION 7: Handling and storage

### Precautions for safe handling

NO open flames. 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.

### Conditions for safe storage, including any incompatibilities

Store in an area without drain or sewer access. Keep in a well-ventilated room. Separated from strong oxidants, strong bases and food and feedstuffs. Store in an area without drain or sewer access. Keep in a well-ventilated room. Separated from strong oxidants, strong bases, food and feedstuffs

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

Component	Cyano (3-phenoxybenzyl)-2-(4-chlorophenyl)-3-methylbutyrate	
CAS No.	51630-58-1	
	Limit value - Eight hours	Limit value - Short term

	ppm	mg/m <sup>3</sup>	ppm	mg/m <sup>3</sup>
People's Republic of China	?	0,05	?	?
	Remarks			

### Biological limit values

no data available

### 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.

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

#### Eye/face protection

Wear safety goggles or eye protection in combination with breathing protection.

#### Skin protection

Protective gloves. Protective clothing.

#### Respiratory protection

Use ventilation, local exhaust or breathing protection.

#### Thermal hazards

no data available

## SECTION 9: Physical and chemical properties and safety characteristics

**Physical state:** Fenvalerate is a clear viscous yellow liquid with a mild odor. Used as broad spectrum insecticide.

**Colour:** Clear yellow viscous liquid

**Odour:** Mild odor

**Melting point/freezing point:** 39.5 - 53.7 °C

Boiling point or initial boiling point and boiling range:	300°C
Flammability:	Combustible. Liquid formulations containing organic solvents may be flammable. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	279.7°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Solubility at 20 deg c (g/L): acetone >450; chloroform >450; methanol >450; hexane 77
Partition coefficient n-octanol/water:	log Kow = 6.20
Vapour pressure:	1.5X10 <sup>-9</sup> mm Hg at 25 deg C
Density and/or relative density:	1.21 g/cm <sup>3</sup>
Relative vapour density:	no data available
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Decomposes on heating between 150 and 300°C. This produces toxic fumes including hydrogen cyanide (see ICSC 0492) and hydrogen chloride (see ICSC 0163). Reacts with strong bases and strong oxidants.

### **Chemical stability**

More stable in acidic solution than in alkaline solution.

### **Possibility of hazardous reactions**

Pyrethrins/ ... burn with difficulty. /Pyrethrins/A pyrethroid. This compound is an ester and nitrile. 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).

### **Conditions to avoid**

no data available

### **Incompatible materials**

Incompatible with alkaline materials.

### **Hazardous decomposition products**

When heated to decomposition it emits toxic fumes of /hydrogen chloride, nitrogen oxides and hydrogen cyanide/.

## **SECTION 11: Toxicological information**

### **Acute toxicity**

Oral: LD50 Rat oral 451 mg/kg

Inhalation: LC50 Rat inhalation > 101 g/cu m/4 hr

Dermal: LD50 Rat percutaneous > 5000 mg/kg



**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**

Cancer Classification: Group E Evidence of Non-carcinogenicity for Humans

**Reproductive toxicity**

no data available

**STOT-single exposure**

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the nervous system.

**STOT-repeated exposure**

Repeated or prolonged contact may cause skin sensitization.

**Aspiration hazard**

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

**SECTION 12: Ecological information****Toxicity**

Toxicity to fish: LC50 *Pimephales promelas* (fathead minnow) 0.42 mg/L/96 hr (confidence limit 0.39-0.46 mg/L), flow-through bioassay with measured concentrations, 24.5 deg C, dissolved oxygen 7.3 mg/L, hardness 44.8 mg/L calcium carbonate, alkalinity 40.9 mg/L calcium carbonate, and pH 7.8.

Toxicity to daphnia and other aquatic invertebrates: LC50; Species: *Daphnia magna* (Water flea, age <24 hr); Conditions: freshwater, static, 20 deg C, pH 6.5; Concentration: 4.3 ug/L for 48 hr />95% purity

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

### **Persistence and degradability**

AEROBIC: In a laboratory study using sediment and seawater collected from a salt marsh near Escambia County, FL, fenvalerate was observed to have a half-life of about 34 days(1); when the media was sterilized, fenvalerate showed no appreciable degradation after 28 days of incubation(1), thus suggesting that degradation was occurring through biotic means(SRC). In degradation tests using an activated sludge inoculum, the aerobic degradation rate of fenvalerate was 50-72% faster than in sterile controls(2); addition of a glucose medium to cometabolize the non-sterile flasks resulted in a 6-fold increase in the degradation rate(2). The aerobic (semi-open system, activated sludge inocula) biodegradation rate of fenvalerate was determined in tests using both inoculated and non-inoculated (control) experiments(3); the biodegradation half-life was determined to be 13 days(3). In seawater and seawater-sediment microcosm studies, the half-life of fenvalerate was determined to be 14-17 days in non-sterile systems and 33-41 days in sterile systems suggesting a presence of microbial activity(4). Through the application of an aquatic ecosystem model, fenvalerate added at concentrations of 5 and 25 ug/L, exhibited aquatic biodegradation half-lives of 3.5-4.3 days using moderately polluted river water (pH 7.7, dissolved oxygen 1.5 mg O<sub>2</sub>/L, 126 mg CaCO<sub>3</sub>/L; sand, carp, maintained at 15-19 deg C)(5).

### **Bioaccumulative potential**

A BCF of 1,100 was measured for one isomer of fenvalerate (S,S-isomer) in carp in a 24 hr renewal exposure following 7 days of exposure(1). In a 28 day laboratory study, a steady-state BCF of 570 was measured in sheepshead minnow (*Cyprinodon variegatus*)(1). Log BCF values of 2.61 and 2.96, corresponding to BCFs of 407 and 912, respectively, in rainbow trout were reported(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high to very high(SRC), provided the compound is not metabolized by the organism(SRC). In a 28 day laboratory study, a steady-state BCF of 4,700 was measured in eastern oysters (*Crassostrea virginica*)(1). In a 30 day aquatic ecosystem study, fenvalerate BCFs of 100 for fish, 491 for snails and 412 for algae were measured(1); relatively low residues in the organisms were attributed to metabolism, especially by the fish(1). The presence of dissolved organic matter (concentration of 6.7 mg/L) may enhance bioconcentration in *Oncorhynchus mykiss* (rainbow trout) by up to a factor of 300(4).

### **Mobility in soil**

The US Dept of Agriculture's Pesticide Properties Database reports a fenvalerate Koc of 5,300(1). Based upon measured isotherms and organic carbon content(2), the Koc values for fenvalerate in the silty-clay and clay sediments are log 4.04-4.22(2),

corresponding to Koc values of 10,964 to 16,595(SRC). Freundlich sorption isotherms on corundum, quartz, kaolinite, and montmorillonite were 0.71, 0.6, 0.07, and 0.09, respectively(3). According to a classification scheme(4), this estimated Koc value suggests that fenvalerate is expected to be immobile in soil.

#### **Other adverse effects**

no data available

### **SECTION 13: Disposal considerations**

#### **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**

#### **UN Number**

ADR/RID: UN2811 (For reference only, please check.)

IMDG: UN2811 (For reference only, please check.)

IATA: UN2811 (For reference only, please check.)

#### **UN Proper Shipping Name**

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

IATA: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

#### **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.)

**Packing group, if applicable**

ADR/RID: I (For reference only, please check.)  
IMDG: I (For reference only, please check.)  
IATA: I (For reference only, please check.)

**Environmental hazards**

ADR/RID: No  
IMDG: No  
IATA: No

**Special precautions for user**

no data available

**Transport in bulk according to IMO instruments**

no data available

**SECTION 15: Regulatory information**

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

**European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

**EC Inventory**

Listed.

**United States Toxic Substances Control Act (TSCA) Inventory**

Not Listed.

**China Catalog of Hazardous chemicals 2015**

Not Listed.

#### **New Zealand Inventory of Chemicals (NZIoC)**

Listed.

#### **(PICCS)**

Listed.

#### **Vietnam National Chemical Inventory**

Listed.

#### **IECSC)**

Listed.

#### **Korea Existing Chemicals List (KECL)**

Listed.

### **SECTION 16: Other information**

#### **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](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/>

### **Other Information**

Carrier solvents used in commercial formulations may change physical and toxicological properties. If the substance is formulated with solvents also consult the ICSCs of these materials. Do NOT take working clothes home. See ICSC 1516.

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any