

Chemical Safety Data Sheet MSDS / SDS

IR-1061

Revision Date:2026-05-31 Revision Number:1

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

Product identifier

Product name : IR-1061
CBnumber : CB4499231
CAS : 155614-01-0
Synonyms : 4-[2-[2-chloro-3-[(2,6-diphenyl-4h-thiopyran-4-ylidene)ethylidene]-1-cyclohexen-1-yl]ethenyl]-2,6-diphenylthiopyrylium tetrafluoroborate

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Warning

Precautionary statements

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P302+P352 IF ON SKIN: wash with plenty of soap and water.

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

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

P264 Wash skin thoroughly after handling.

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

Hazard statements

H335 May cause respiratory irritation

H319 Causes serious eye irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: IR-1061
Synonyms	: 4-[2-[2-chloro-3-[(2,6-diphenyl-4h-thiopyran-4-ylidene)ethylidene]-1-cyclohexen-1-yl]ethenyl]-2,6-diphenylthiopyrylium tetrafluoroborate
CAS	: 155614-01-0
MF	: C44H34ClS2.BF4
MW	: 749.141

SECTION 4: First aid measures

General advice

Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of HF. After decontamination with water, further damage can occur due to penetration/absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or Milk of Magnesia to conscious victims. Conditions such as hypocalcemia, hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure. Show this safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

First treatment with calcium gluconate paste. In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting

Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products

Carbon oxides Sulphur oxides Hydrogen chloride gas Hydrogen fluoride Borane/boron oxides

Specific extinguishing methods

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7: Handling and storage

Handling

Avoidance of contact

Strong oxidizing agents

Storage**Further information on storage conditions**

Tightly closed. Dry.

Storage class

11, Combustible Solids

Recommended storage temperature

-20 °C

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

No data available

Personal protective equipment**Respiratory protection**

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type

Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Safety glasses

Skin and body protection

protective clothing

Hand protection**Material**

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Full contact

Manufacturer

KCL 741 L

Material

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Splash contact

Manufacturer

KCL 741 L

Remarks

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D- 36124 Eichenzell, Internet: www.kcl.de).

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

solid

Color

Brown to black

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

222 °C

Method: dec.

Boiling point/boiling range

No data available

Flash point

No data available

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

No data available

Density

No data available

Water solubility

No data available

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

No data available

Oxidizing properties

No data available

Molecular weight

749.13 g/mol

Particle characteristics Particle size

No data available

Physical state

Solid

SECTION 10: Stability and reactivity

Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

No data available

Conditions to avoid

no information available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information**Ecotoxicity****Components:****IR-1061:****Toxicity to fish**

Remarks: No data available

Persistence and degradability**Components:****IR-1061:****Biodegradability**

Remarks: No data available

Bioaccumulative potential

Components:

IR-1061:

Bioaccumulation

Remarks: No data available

Mobility in soil

Components:

IR-1061:

Stability in soil

Remarks: No data available

Other adverse effects

Components:

IR-1061:

Additional ecological information

No data available

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Packing instruction (cargo aircraft) : Not applicable

Packing instruction (passenger aircraft) : Not applicable

IMDG-Code

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

EmS Code : Not applicable

Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National Regulations

JT/T 617

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Environmentally hazardous : no

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

Catalogue of Hazardous Chemicals : This product is not listed in the catalogue of hazardous chemicals, but it meets the definition of hazardous chemicals and its principles of determination.

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

Not listed

Hazardous Chemicals for Priority Management

Not listed under SAWS

Regulations on Labour Protection in Workplaces where Toxic Substances are Used

Catalogue of Highly Toxic Chemicals

Not listed

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

B1A222215924 B1A222241375

SECTION 16: Other information

Full text of other abbreviations

AllC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonised System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Cancer

IATA - International Air Transport Association

IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC₅₀ - Half maximal inhibitory concentration

ICAO - International Civil Aviation Organization

IECSC - Inventory of Existing Chemical Substances in China

IMDG - International Maritime Dangerous Goods

IMO - International Maritime Organisation

ISHL - Industrial Safety and Health Law (Japan)

ISO - International Organisation for Standardisation
KECI - Korea Existing Chemicals Inventory
LC50 - Lethal Concentration to 50 % of a test population
LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)
MARPOL - International Convention for the Prevention of Pollution from Ships
MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods
n.o.s. - Not Otherwise Specified
Nch - Chilean Norm
NO(A)EC - No Observed (Adverse) Effect Concentration
NO(A)EL - No Observed (Adverse) Effect Level
NOELR - No Observable Effect Loading Rate
NOM - Official Mexican Norm
NTP - National Toxicology Program
NZIoC - New Zealand Inventory of Chemicals
OECD - Organisation for Economic Co-operation and Development
OPPTS - Office of Chemical Safety and Pollution Prevention
PBT - Persistent, Bioaccumulative and Toxic substance
PICCS - Philippines Inventory of Chemicals and Chemical Substances
(Q)SAR - (Quantitative) Structure Activity Relationship
REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals
SADT - Self-Accelerating Decomposition Temperature
SDS - Safety Data Sheet
TCSI - Taiwan Chemical Substance Inventory
TDG - Transportation of Dangerous Goods
TECI - Thailand Existing Chemicals Inventory
TSCA - Toxic Substances Control Act (United States)
UN - United Nations
UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods
vPvB - Very Persistent and Very Bioaccumulative
WHMIS - Workplace Hazardous Materials Information System

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.