

Chemical Safety Data Sheet MSDS / SDS

Isophthalic acid 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: Isophthalic acid
CAS: 121-91-5

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.in
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SECTION 2: Hazards identification**Classification of the substance or mixture**

Not classified.

GHS label elements, including precautionary statements

Signal word No signal word

Hazard statement(s)

none

Precautionary statement(s)**Prevention**

none

Response

none

Storage

none

Disposal

none

Other hazards which do not result in classification

no data available

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

Chemical name: Isophthalic acid

Common names and
synonyms: Isophthalic acid

CAS number: 121-91-5

EC number: 204-506-4

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

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.

Most important symptoms/effects, acute and delayed

May cause slight to moderate irritation of eyes, skin, and mucous membranes on prolonged contact. Ingestion may cause gastrointestinal irritation. (USCG, 1999)

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 if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the 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. Poisons A and B

SECTION 5: Firefighting measures

Suitable extinguishing media

Fire Extinguishing Agents: Water, dry powder, foam, carbon dioxide (USCG, 1999)

Specific hazards arising from the chemical

Behavior in Fire: Dust forms explosive mixture in air. (USCG, 1999)

Special protective actions for fire-fighters

Use water spray, foam, powder, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust. 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 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

Control parameters

Occupational Exposure limit values

MAK: (inhalable fraction): 5 mg/m³; peak limitation category: I(2); pregnancy risk group: C

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 spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state: Solid. Crystalline powder.

Colour: White, when purified to the grade required for use as a polyester feedstock.

Odour: no data available

Melting point/freezing point:	$\geq 345 - \leq 348$ °C. Atm. press.: > 1 atm. Remarks:Melting point determined by the closed tube method [Ref. Doc. Table 24]. Sublimation occurs under normal atmospheric pressure; heat of sublimation at 25 degrees C is given as 106.7 kJ/mol. Sublimation temperature not stated.
Boiling point or initial boiling point and boiling range:	348 °C. Atm. press.: > 760 mm Hg. Remarks:The melting point of IPA under sealed tube conditions was 345 to 348 degrees C.
Flammability:	Combustible.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	107°C(lit.)
Auto-ignition temperature:	>650 °C
Decomposition temperature:	no data available
pH:	3.5. Remarks:PH measured.;3.43. Remarks:PH measured.;3.33. Remarks:PH measured.
Kinematic viscosity:	0.00025186 Pa-s at 619.15K (346 deg C)
Solubility:	Soluble in 8000 parts cold water, 460 parts boiling water; freely soluble in alcohol; practically insoluble in petroleum ether
Partition coefficient n-octanol/water:	$\log P_{ow} = 1.76$. Remarks:Temp and pH not relevant as theoretical result.
Vapour pressure:	Ca. 0 mm Hg. Temperature:Ca. 25 °C. Remarks:The vapour pressure at 25 degrees C is extrapolated beyond the range of the data used to construct the equation relating VP to temperature. Nevertheless, the estimate is very low compared to standard atmospheric pressure.
Density and/or relative density:	1.53 g/cm ³ . Temperature:25 °C.
Relative vapour density:	no data available

Particle characteristics:

no data available

SECTION 10: Stability and reactivity

Reactivity

Dust forms explosive mixture in air (USCG, 1999).

Chemical stability

Sublimes without decomp

Possibility of hazardous reactions

Dust explosion possible if in powder or granular form, mixed with air. ISOPHTHALIC ACID is a carboxylic acid. Carboxylic acids donate hydrogen ions if a base is present to accept them. They react in this way with all bases, both organic (for example, the amines) and inorganic. Their reactions with bases, called "neutralizations", are accompanied by the evolution of substantial amounts of heat. Neutralization between an acid and a base produces water plus a salt. Carboxylic acids with six or fewer carbon atoms are freely or moderately soluble in water; those with more than six carbons are slightly soluble in water. Soluble carboxylic acid dissociate to an extent in water to yield hydrogen ions. The pH of solutions of carboxylic acids is therefore less than 7.0. Many insoluble carboxylic acids react rapidly with aqueous solutions containing a chemical base and dissolve as the neutralization generates a soluble salt. Carboxylic acids in aqueous solution and liquid or molten carboxylic acids can react with active metals to form gaseous hydrogen and a metal salt. Such reactions occur in principle for solid carboxylic acids as well, but are slow if the solid acid remains dry. Even "insoluble" carboxylic acids may absorb enough water from the air and dissolve sufficiently in it to corrode or dissolve iron, steel, and aluminum parts and containers. Carboxylic acids, like other acids, react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slower for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H₂S and SO₃), dithionites (SO₂), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information**Acute toxicity**

Oral: LD50 Rat oral 12200 mg/kg bw

Inhalation: no data available

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

May cause mechanical irritation to the eyes.

STOT-repeated exposure

no data available

Aspiration hazard

Evaporation at 20°C is negligible; a nuisance-causing concentration of airborne particles can, however, be reached quickly.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Leuciscus idus melanotus* - > 907 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - > 952 mg/L - 48 h.

Toxicity to algae: NOEC - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 1 000 mg/L - 96 h.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - 617.1 mg/L - 3 h. Remarks: Respiration rate.

Persistence and degradability

AEROBIC: Isophthalic acid, present at 100 mg/L, reached 78 of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test indicating ready biodegradability(1). Under aerobic conditions and following OECD guideline 301B, approximately 9%, 46%, 64%, and 77% of isophthalic acid contained in sludge was degraded after 2, 5, 7, and 12 days, respectively(2). Isophthalic acid is degraded by aerobic microorganisms isolated from soil and marine sediment(3,4); cultures isolated from marine cultures also degraded isophthalic acid under anaerobic conditions(4). After an acclimation to an activated sludge inoculum over a 24 day period, 84% of isophthalate was consumed in a respiratory test(5). Isophthalic acid completely degraded in 8 days in a biodegradation test that used a soil inoculum(6). In another screening test, 95% of COD was removed in 5 days using an acclimated activated sludge inoculum(7). In anaerobic biodegradation tests using granular and digested sewage sludge inoculum, isophthalic acid (as isophthalate) could be completely mineralized with a lag phase for 50% degradation ranging from 74 to 156 days(8). Using bacteria from river water as inocula (Songhua River, China) and a sealed-bottled method, isophthalic acid was found to be readily biodegradable with first-order rate constant of 1.43/day(9).

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for isophthalic acid(SRC), using a log Kow of 1.66(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.

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of isophthalic acid can be estimated to be 79(SRC). According to a classification scheme(2), this estimated Koc value suggests that isophthalic acid is expected to have high mobility in soil(SRC). Isophthalic acid is a dibasic (2 displaceable hydrogen atoms) acid whose pKa1 is 3.70 and pKa2 is 4.60 at 25 deg C(3) indicating that isophthalic acid will be largely dissociated in the environment in the anion form and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4).

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: 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.)

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.)

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.)

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.)

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

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

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

Sublimes without decomposition.

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