

# Isophthalonitrile



[Identification](#) | [Characterisation](#) | [Formula](#) | [Physical and chemical properties](#) | [Toxicology / Ecotoxicology](#) | [Occupational health and first aid](#) | [Safe handling](#) | [Regulations](#) | [Links](#) | [Literature register](#)

## IDENTIFICATION

### Isophthalonitrile

1,3-Dicyanobenzene  
Benzenedicarbonitrile

**ZVG No:** 530294  
**CAS No:** 626-17-5  
**EC No:** 210-933-7

## CHARACTERISATION

### SUBSTANCE GROUP CODE

146100 Nitriles

### STATE OF AGGREGATION

The substance is solid.

### PROPERTIES

crystalline powder  
white  
bitter almond-like odour

### CHEMICAL CHARACTERISATION

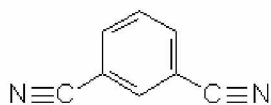
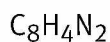
Combustible substance, poorly flammable.  
Very slightly soluble in water.  
Acute or chronic health hazards result from the substance.  
(see: chapter REGULATIONS).

### DUST EXPLOSIVENESS

There is a risk of a dust explosion if the following conditions are met:

- The substance is given in very finely distributed form (powder, dust).
- The substance is whirled up in sufficient quantity in the air.
- An ignition source is present (flame, spark, electrostatic discharge, etc.)

Quelle: 06806

**FORMULA**

**Molar mass:** 128,13 g/mol

**PHYSICAL AND CHEMICAL PROPERTIES**

Melting point | Boiling point | Density | Flash point | Ignition temperature | Explosion data | Solubility | Partition coefficient

**MELTING POINT**

Melting point: 162 ... 163 °C

Reference: 01211

**BOILING POINT**

Boiling Point: 288 °C

Reference: 01211

**DENSITY**

DENSITY

Value: 1,3 g/cm<sup>3</sup>

Temperature: 20 °C

Reference: 01211

**FLASH POINT**

Flash point: > 150 °C

Reference: 01251

**IGNITION TEMPERATURE**

Ignition temperature: > 360 °C

Reference: 01251

**EXPLOSION DATA**

Lower explosion limit:  
40 g/m<sup>3</sup>

Reference: 01251

**SOLUBILITY IN WATER**

Concentration: 0,7 g/l

Temperature: 20 °C

Reference: 01211

**PARTITION COEFFICIENT (octanol/water)**

log Kow: 0,8

Recommended value of LOG KOW Databank.

Reference: 02070

## TOXICOLOGY / ECOTOXICOLOGY

### TOXICOLOGICAL DATA

#### LD50 oral rat

Value: 860 mg/kg

National Technical Information Service. Vol. OTS0533488,

#### LD50 dermal

Species: Rabbit

Value: > 2000 mg/kg

National Technical Information Service. Vol. OTS0533488,

Reference: 02071

## OCCUPATIONAL HEALTH AND FIRST AID

Toxic effects |  
First Aid

### TOXIC EFFECTS

#### Annotation

At present time the occupational health information for this substance is only available in german. Please consult our database in german.

### FIRST AID

#### Annotation

At present time the first aid information for this substance is only available in German. Please consult our database in German.

## SAFE HANDLING

Handling | Storage | Fire and explosion protection | Organisational measures | Personal protection | Disposal considerations | Accidental release measures | Fire fighting measures

### TECHNICAL MEASURES - HANDLING

#### Workplace

Provision of good ventilation in the working area.

Washing facility at the workplace required.

#### Equipment

If release of the substance cannot be prevented, then it should be suctioned off at the point of exit.

Consider emission limit values, a purification of waste gases if necessary.

Label containers and pipelines clearly.

#### Advice on safer handling

Take care to maintain clean working place.

Do not leave container open.

Sufficient ventilation must be guaranteed for refilling, transfer, or open use.

Avoid spillage.

Fill only into labelled container.

Avoid rising dust.

### **Cleaning and maintenance**

Use protective equipment while cleaning if necessary.

Avoid dust formation. Dust formation that cannot be avoided must be collected regularly.

Use tested explosion-proof industrial vacuum cleaners of class M.

Do not raise dust while cleaning.

Use of a blower for cleaning is not permitted.

Only conduct maintenance and other work on or in the vessel or closed spaces after obtaining written permission.

## **TECHNICAL MEASURES - STORAGE**

### **Storage**

Do not use any food containers - risk of mistake.

Containers have to be labelled clearly and permanently.

Store in the original container as much as possible.

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage at room temperature.

### **Conditions of collocated storage**

Storage class 10 - 13 (Other liquids and solids)

Only substances of the same storage class should be stored together.

Collocated storage with the following substances is prohibited:

- Pharmaceuticals, foods, and animal feeds including additives.
- Infectious, radioactive und explosive substances.
- Strongly oxidizing substances of storage class 5.1A.

Under certain conditions the collocated storage with the following sub-stances is permitted (For more details see [TRGS 510](#)):

- Gases.
- Flammable liquids of storage class 3.
- Other explosive substances of storage class 4.1A.
- Pyrophoric substances.
- Substances liberating flammable gases in contact with water.
- Oxidizing substances of storage class 5.1B.
- Ammonium nitrate and preparations containing ammonium nitrate.
- Organic peroxides and self reactive substances.
- Combustible and non combustible acutely toxic substances of storage classes 6.1A and 6.1B.

The substance should not be stored with substances with which hazardous chemical reactions are possible.

## **TECHNICAL MEASURES - FIRE AND EXPLOSION PROTECTION**

### **Technical, constructive measures**

Substance is combustible.

Fire fighting equipment must be available.

If there is a risk of a dust explosion due to the dust-like distribution and the quantities used, measures according to [TRGS 722](#) (prevention of formation), [723](#) (prevention of ignition) and [TRGS 724](#) (constructive explosion protection) may become necessary.

### **Precaution on handling**

Areas in which the substance can arise as a dust in such quantities that a dust explosion could occur are to be considered as at a risk of explosion.

Keep away from sources of ignition (e.g. open flames, heat sources and sparks).

## ORGANISATIONAL MEASURES

Instruction on the hazards and the protective measures using instruction manual ([TRGS 555](#)) are required with signature if just more than one minor hazard was detected.

Instruction must be provided before employment and then at a minimum of once per annum thereafter.

Observe the restrictions on juvenile employment as defined in the "Jugendarbeitsschutzgesetz".

## PERSONAL PROTECTION

### Body protection

Wear an apron or a lab coat.

### Respiratory protection

In an emergency (e.g.: unintentional release of the substance) respiratory protection must be worn. Consider the maximum period for wear.

Respiratory protection: Particle filter P1, colour code white.

### Eye protection

Sufficient eye protection should be worn.

Wear glasses with side protection.

### Hand protection

The use of resistant protective gloves is recommended.

Skin protection cremes do not protect as effectively against the substance as protective gloves. Therefore suitable protective gloves should be preferred as far as possible.

Currently there is no information available regarding suitable glove materials.

Experience says that polychloroprene, nitrile rubber, butyl rubber, fluoro-caoutchouc, and polyvinyl chloride are suitable as glove materials for protection against un-dissolved solids.

### Occupational hygiene

Foods, beverages and other articles of consumption must not be consumed at the work areas. Suitable areas are to be designated for these purposes.

Avoid contact with clothing. Contaminated clothes must be exchanged and cleaned carefully.

The skin must be washed with soap and water before breaks and at the end of work.

Apply fatty skin-care products after washing.

## DISPOSAL CONSIDERATIONS

Hazardous waste according to Waste Catalogue Ordinance (AVV).

If there is no way of recycling it must be disposed of in compliance with the respective national and local regulations.

Collection of small amounts of substance:

Collect in container for solid organic residues.

Collection vessels must be clearly labelled with a systematic description of their contents. Store the vessels in a well-ventilated location. Entrust them to the appropriate authorities for disposal.

## ACCIDENTAL RELEASE MEASURES

Wear personal protective equipment (see chapter Personal Protection).

Pick up without creating dust.

Afterwards ventilate area and wash spill site.

Endangerment of water:

Low hazard to waters. Inform the responsible authorities when very large quantities get into water, drainage, sewer, or the ground.

## FIRE FIGHTING MEASURES

### Classes of fires

B liquid or melting substances

### Suitable extinguishing media

Water (spray - not splash)  
Dry extinguishing powder  
Alcohol resistant foam  
Carbon dioxide

### Instructions

Seek immediate cover in case of sudden release and raising of large quantities of dust.  
Cool surrounding containers with water spray.  
If possible, take container out of dangerous zone.  
Shut off sources of ignition.

### Special protective equipment

In the case of a fire hazardous substances can be released.  
Nitrous gases (nitric oxides)  
Hydrogen cyanide vapours  
Carbon monoxide and carbon dioxide  
Wear self-contained breathing apparatus and special tightly sealed suit.

## REGULATIONS

[GHS Classification/ Labelling](#) | [Workplace labelling](#) | [Water hazard class](#) | [Air quality control](#) | [Transport Regulations](#) | [Technical rules](#) | [Regulations of accident insurers](#)

## EUROPEAN GHS CLASSIFICATION AND LABELLING

### Classification

Acute toxicity, Category 4, oral; H302



**Signal Word** "Warning"

### Hazard Statement - H-phrases

H302: Harmful if swallowed.

### Precautionary Statement - P-phrases

P301+P312+P330: IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.  
Rinse mouth.

Manufacturer's specification by Sigma-Aldrich

Reference: 01221

State: 2017

Checked: 2017

## GHS-CLASSIFICATION OF MIXTURES

The classification of mixtures containing this substance results from Annex 1 of Regulation (EC) 1272/2008.

Reference: 99999

## WORKPLACE LABELLING ACCORDING TO GERMAN ASR A1.3

### Precept label



Use safety goggles

## GERMAN WATER HAZARD CLASS

Substance No: 5334

WGK 1 - low hazard to waters

Classification according to the announcement of the list of substances hazardous to water in the Federal Register of 10.08.2017, last update 17.08.2021

## TECHNICAL INSTRUCTIONS ON AIR QUALITY CONTROL (TA LUF)

Chapter 5.2.5 Organic Substances, dust

To be treated as overall dust. The emissions of dust in the exhaust gas are not allowed to exceed the following values:

Mass flow: 0,20 kg/hr

or

Mass conc.: 20 mg/m<sup>3</sup>

The mass per unit volume of 0,15 g/m<sup>3</sup> in exhaust gas is not allowed to be exceeded also on observance or lower deviation of a mass flow of 0,20 kg/h.

## TRANSPORT REGULATIONS

Not subject to transport regulations.

Reference: 01221

## TECHNICAL RULES FOR HAZARDOUS SUBSTANCES

### TRGS 201

Einstufung und Kennzeichnung bei Tätigkeiten mit Gefahrstoffen; Ausgabe Februar 2017, zuletzt geändert und ergänzt April 2018

### TRGS 400

Gefährdungsbeurteilung für Tätigkeiten mit Gefahrstoffen; Ausgabe Juli 2017

### TRGS 555

Betriebsanweisung und Information der Beschäftigten; Ausgabe Februar 2017

### TRGS 600

Substitution; Ausgabe Juli 2020

### TRGS 500

Schutzmaßnahmen; Ausgabe September 2019

[TRGS 509](#)

Lagern von flüssigen und festen Gefahrstoffen in ortsfesten Behältern sowie Füll- und Entleerstellen für ortsbewegliche Behälter; Ausgabe September 2014, zuletzt berichtigt, geändert und ergänzt Oktober 2020

[TRGS 510](#)

Lagerung von Gefahrstoffen in ortsbeweglichen Behältern; Ausgabe Januar Dezember 2020

[TRGS 800](#)

Brandschutzmaßnahmen; Ausgabe Dezember 2010

[TRGS 720](#)

Gefährliche explosionsfähige Gemische - Allgemeines; Ausgabe Juli 2020, zuletzt berichtigt März 2021

[TRGS 721](#)

Gefährliche explosionsfähige Gemische - Beurteilung der Explosionsgefährdung; Ausgabe Oktober 2020, zuletzt berichtigt Dezember 2020

[TRGS 722](#)

Vermeidung oder Einschränkung gefährlicher explosionsfähiger Atmosphäre, Ausgabe Februar 2021

[TRGS 723](#)

Gefährliche explosionsfähige Gemische - Vermeidung der Entzündung gefährlicher explosionsfähiger Gemische; Ausgabe Juli 2019, zuletzt geändert Oktober 2020

[TRGS 724](#)

Gefährliche explosionsfähige Gemische - Maßnahmen des konstruktiven Explosionsschutzes, welche die Auswirkung einer Explosion auf ein unbedenkliches Maß beschränken, Ausgabe Juli 2019

**REGULATIONS OF GERMAN ACCIDENT INSURERS**

DGUV Regel 112-190

Benutzung von Atemschutzgeräten, Ausgabe Dezember 2011

<http://publikationen.dguv.de/dguv/pdf/10002/r-190.pdf>

(in German only)

DGUV Regel 112-195

Benutzung von Schutzhandschuhen, Aktualisierte Nachdruckfassung Oktober 2007

<http://publikationen.dguv.de/dguv/pdf/10002/bgr195.pdf>

(in German only)

**LINKS**

[International Limit Values](#)

**REFERENCES**



Quelle: 00001

IFA: Erfassungs- und Pflegehandbuch der GESTIS-Stoffdatenbank (nicht öffentlich)  
Data acquisition and maintenance manual of the GESTIS substance database (non-public)

Quelle: 00454

Hazardous Substances Data Bank (HSDB)

Quelle: 01211

GHS-Sicherheitsdatenblatt, Merck  
GHS Material Safety Data Sheet, Merck

Quelle: 01221

GHS-Sicherheitsdatenblatt, Sigma-Aldrich  
GHS Material Safety Data Sheet, Sigma-Aldrich

Quelle: 01251

GHS-Sicherheitsdatenblatt, Alfa Aesar (eine Marke von Thermo Fisher Scientific)  
GHS Material Safety Data Sheet, Alfa Aesar (A Thermo Fisher <sup>ZE</sup> )

Quelle: 02070

LOG KOW Databank, compiled by <sup>ZE</sup> Sangster Research Laboratories, Montreal, Canada, distributed by Technical Database Services (TDS), New York

Quelle: 02071

Toxicological Data, compiled by the National Institute of Health (NIH), USA, selected and distributed by Technical Database Services (TDS), New York, 2009

Quelle: 05300

[TRGS 510](#) "Lagerung von Gefahrstoffen in ortsbeweglichen Behältern" Ausgabe Dezember 2020

Quelle: 06806

GESTIS-STAU-EX-Datenbank des IFA [www.dguv.de/ifa/gestis-staub-ex](http://www.dguv.de/ifa/gestis-staub-ex)

Quelle: 07580

Bekanntmachung der Liste der wassergefährdenden Stoffe im Bundesanzeiger vom 10.08.2017, zuletzt geändert 17.08.2021

Quelle: 99999

Angabe des Bearbeiters  
Indication of the editor

[Identification](#) | [Characterisation](#) | [Formula](#) | [Physical and chemical properties](#) |  
[Toxicology / Ecotoxicology](#) | [Occupational health and first aid](#) | [Safe handling](#) | [Regulations](#) | [Links](#) |  
[Literature register](#)

**This material data sheet was carefully compiled. However no liability can be assumed for the data content, whatever the legal cause may be.**