

ALFAAA11954

4-Isopropylbenzotrile

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明:
Product Description: 4-异丙基苯甲腈
4-Isopropylbenzotrile

Cat No. : A11954
CAS No 13816-33-6
Molecular Formula C10 H11 N

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

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Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
No information available

Odor
No information available

Emergency Overview
May be harmful if swallowed. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

Classification of the substance or mixture

| | |
|----------------------------------------------------|------------|
| Acute Oral Toxicity | Category 5 |
| Skin Corrosion/Irritation | Category 2 |
| Serious Eye Damage/Eye Irritation | Category 2 |
| Specific target organ toxicity - (single exposure) | Category 3 |

Label Elements



Signal Word

Warning

4-Isopropylbenzotrile

Hazard Statements

H303 - May be harmful if swallowed
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

Precautionary Statements**Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P264 - Wash face, hands and any exposed skin thoroughly after handling
P270 - Do not eat, drink or smoke when using this product
P271 - Use only outdoors or in a well-ventilated area
P280 - Wear protective gloves/protective clothing/eye protection/face protection

Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P312 - Call a POISON CENTER or doctor if you feel unwell
P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

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

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

None identified.

Health Hazards

May be harmful if swallowed. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its volatility. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

| Component | CAS No | Weight % |
|--------------------------------|------------|----------|
| Benzotrile, 4-(1-methylethyl)- | 13816-33-6 | <=100 |

SECTION 4. FIRST AID MEASURES**General Advice**

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

Ingestion

Clean mouth with water and drink afterwards plenty of water.

Most important symptoms and effects

None reasonably foreseeable.

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.

Storage

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

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of

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exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls**Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments |
|----------------|-----------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers recommendations | - | EN 374 | (minimum requirement) |
| Neoprene | | | | |
| Natural rubber | | | | |
| PVC | | | | |

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection Long sleeved clothing

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Valve filtering: EN405; or, Half mask: EN140; plus filter, EN 141
When RPE is used a face piece Fit Test should be conducted

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**Appearance**

Physical State Liquid

Odor No information available

Odor Threshold No data available

pH No information available

4-Isopropylbenzotrile

| | | |
|------------------------------------------------|-----------------------------|------------------------------------------|
| Melting Point/Range | No data available | |
| Softening Point | No data available | |
| Boiling Point/Range | 88 - 90 °C / 190.4 - 194 °F | |
| Flash Point | 94 °C / 201.2 °F | Method - No information available |
| Evaporation Rate | No data available | |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Vapor Pressure | No data available | |
| Vapor Density | No data available | (Air = 1.0) |
| Specific Gravity / Density | No data available | |
| Bulk Density | Not applicable | Liquid |
| Water Solubility | No information available | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Component | log Pow | |
| Benzotrile, 4-(1-methylethyl)- | 2.6 | |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| Viscosity | No data available | |
| Explosive Properties | No information available | |
| Oxidizing Properties | No information available | |
| Molecular Formula | C10 H11 N | |
| Molecular Weight | 145.21 | |

SECTION 10. STABILITY AND REACTIVITY

| | |
|---------------------------------|---------------------------------|
| Stability | Stable under normal conditions. |
| Hazardous Reactions | None under normal processing. |
| Hazardous Polymerization | No information available. |
| Conditions to Avoid | None known. |
| Materials to avoid | No information available. |

Hazardous Decomposition Products None under normal use conditions.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

| Component | LD50 Oral | LD50 Dermal | LC50 Inhalation |
|--------------------------------|---------------------------|------------------------------|-----------------|
| Benzotrile, 4-(1-methylethyl)- | LD50 = 3900 mg/kg (Rat) | LD50 > 5000 mg/kg (Rabbit) | |

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

SAFETY DATA SHEET

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(f) carcinogenicity; No data available
There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3
Results / Target organs Respiratory system

(i) STOT-repeated exposure; No data available
Target Organs No information available.

(j) aspiration hazard; No data available

Symptoms / effects,both acute and delayed No information available

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects .

Persistence and Degradability No information available
Persistence Persistence is unlikely, based on information available.

Bioaccumulative Potential Bioaccumulation is unlikely

| Component | log Pow | Bioconcentration factor (BCF) |
|--------------------------------|---------|-------------------------------|
| Benzotrile, 4-(1-methylethyl)- | 2.6 | No data available |

Mobility in soil The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Will likely be mobile in the environment due to its volatility Disperses rapidly in air

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport Not Regulated

4-Isopropylbenzotrile

IMDG/IMO Not regulated**IATA** Not regulated**Special Precautions for User** No special precautions required**SECTION 15. REGULATORY INFORMATION****International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

| Component | The Inventory of Hazardous Chemicals (2015 Edition) | List of dangerous goods GB 12268 - 2012 | TCSI | IECSC | EINECS | TSCA | DSL | PICCS | ENCS | ISHL | AICS | KECL |
|--------------------------------|-----------------------------------------------------|-----------------------------------------|------|-------|-----------|------|-----|-------|------|------|------|------|
| Benzotrile, 4-(1-methylethyl)- | - | - | X | X | 237-492-3 | X | X | X | - | | X | - |

National Regulations**SECTION 16. OTHER INFORMATION**

Prepared By Health, Safety and Environmental Department
Revision Date 01-May-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend**CAS** - Chemical Abstracts Service**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances**PICCS** - Philippines Inventory of Chemicals and Chemical Substances**IECSC** - Chinese Inventory of Existing Chemical Substances**KECL** - Korean Existing and Evaluated Chemical Substances**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List**ENCS** - Japanese Existing and New Chemical Substances**AICS** - Australian Inventory of Chemical Substances**NZIoC** - New Zealand Inventory of Chemicals**WEL** - Workplace Exposure Limit**ACGIH** - American Conference of Governmental Industrial Hygienists**DNEL** - Derived No Effect Level**RPE** - Respiratory Protective Equipment**LC50** - Lethal Concentration 50%**NOEC** - No Observed Effect Concentration**TWA** - Time Weighted Average**IARC** - International Agency for Research on Cancer**PNEC** - Predicted No Effect Concentration**LD50** - Lethal Dose 50%**EC50** - Effective Concentration 50%**POW** - Partition coefficient Octanol:Water

4-Isopropylbenzotrile

PBT - Persistent, Bioaccumulative, Toxic

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet