

**SAFETY DATA SHEET**

Revision Date 25-Mar-2024

Revision Number 4

**1. Identification**

**Product Name** 4-Isopropylbenzoic acid

**Cat No. :** B20704

**CAS No** 536-66-3  
**Synonyms** Cuminic acid

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

**Details of the supplier of the safety data sheet****Company**

Thermo Fisher Scientific Chemicals, Inc.  
30 Bond Street  
Ward Hill, MA 01835-8099  
Tel: 800-343-0660  
Fax: 800-322-4757

**Emergency Telephone Number**

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
**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

**2. Hazard(s) identification****Classification**

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

|                                                  |            |
|--------------------------------------------------|------------|
| Skin Corrosion/Irritation                        | Category 2 |
| Serious Eye Damage/Eye Irritation                | Category 2 |
| Specific target organ toxicity (single exposure) | Category 3 |
| Target Organs - Respiratory system.              |            |

**Label Elements****Signal Word**

Warning

**Hazard Statements**

Causes skin irritation  
Causes serious eye irritation

May cause respiratory irritation

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling  
Wear protective gloves/protective clothing/eye protection/face protection  
Avoid breathing dust/fume/gas/mist/vapors/spray  
Use only outdoors or in a well-ventilated area

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
Call a POISON CENTER or doctor/physician if you feel unwell

**Skin**

IF ON SKIN: Wash with plenty of soap and water  
If skin irritation occurs: Get medical advice/attention  
Take off contaminated clothing and wash before reuse

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
If eye irritation persists: Get medical advice/attention

**Storage**

Store in a well-ventilated place. Keep container tightly closed  
Store locked up

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

None identified

### 3. Composition/Information on Ingredients

| Component                        | CAS No   | Weight % |
|----------------------------------|----------|----------|
| Benzoic acid, 4-(1-methylethyl)- | 536-66-3 | <=100    |

### 4. First-aid measures

|                                            |                                                                                                                   |
|--------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <b>General Advice</b>                      | If symptoms persist, call a physician.                                                                            |
| <b>Eye Contact</b>                         | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.   |
| <b>Skin Contact</b>                        | Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician. |
| <b>Inhalation</b>                          | Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.      |
| <b>Ingestion</b>                           | Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.             |
| <b>Most important symptoms and effects</b> | None reasonably foreseeable.                                                                                      |

## Notes to Physician

Treat symptomatically

## 5. Fire-fighting measures

**Suitable Extinguishing Media** Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam.

**Unsuitable Extinguishing Media** No information available

**Flash Point** No information available

**Method -** No information available

**Autoignition Temperature** No information available

**Explosion Limits**

**Upper** No data available

**Lower** No data available

**Sensitivity to Mechanical Impact** No information available

**Sensitivity to Static Discharge** No information available

**Specific Hazards Arising from the Chemical**

Keep product and empty container away from heat and sources of ignition.

**Hazardous Combustion Products**

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

**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.

**NFPA**

**Health**  
2

**Flammability**  
0

**Instability**  
0

**Physical hazards**  
N/A

## 6. Accidental release measures

**Personal Precautions** Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

**Environmental Precautions** Should not be released into the environment.

**Methods for Containment and Clean Up** Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

## 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. Avoid dust formation.

**Storage.** Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents.

## 8. Exposure controls / personal protection

**Exposure Guidelines** This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

**Engineering Measures** Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

**Personal Protective Equipment**

|                                 |                                                                                                                                                                                                                                                   |
|---------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Eye/face Protection</b>      | Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.                                                                       |
| <b>Skin and body protection</b> | Wear appropriate protective gloves and clothing to prevent skin exposure.                                                                                                                                                                         |
| <b>Respiratory Protection</b>   | Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. |
| <b>Recommended Filter type:</b> | Particulates filter conforming to EN 143.                                                                                                                                                                                                         |
| <b>Hygiene Measures</b>         | Handle in accordance with good industrial hygiene and safety practice.                                                                                                                                                                            |

## 9. Physical and chemical properties

|                                               |                               |
|-----------------------------------------------|-------------------------------|
| <b>Physical State</b>                         | Powder Solid                  |
| <b>Appearance</b>                             | White                         |
| <b>Odor</b>                                   | Odorless                      |
| <b>Odor Threshold</b>                         | No information available      |
| <b>pH</b>                                     | Not applicable                |
| <b>Melting Point/Range</b>                    | 116 - 120 °C / 240.8 - 248 °F |
| <b>Boiling Point/Range</b>                    | No information available      |
| <b>Flash Point</b>                            | No information available      |
| <b>Evaporation Rate</b>                       | Not applicable                |
| <b>Flammability (solid,gas)</b>               | No information available      |
| <b>Flammability or explosive limits</b>       |                               |
| Upper                                         | No data available             |
| Lower                                         | No data available             |
| <b>Vapor Pressure</b>                         | No information available      |
| <b>Vapor Density</b>                          | Not applicable                |
| <b>Specific Gravity</b>                       | No information available      |
| <b>Solubility</b>                             | No information available      |
| <b>Partition coefficient; n-octanol/water</b> | No data available             |
| <b>Autoignition Temperature</b>               | No information available      |
| <b>Decomposition Temperature</b>              | No information available      |
| <b>Viscosity</b>                              | Not applicable                |
| <b>Molecular Formula</b>                      | C10 H12 O2                    |
| <b>Molecular Weight</b>                       | 164.2                         |

## 10. Stability and reactivity

|                                         |                                                         |
|-----------------------------------------|---------------------------------------------------------|
| <b>Reactive Hazard</b>                  | None known, based on information available              |
| <b>Stability</b>                        | Stable under normal conditions.                         |
| <b>Conditions to Avoid</b>              | Incompatible products.                                  |
| <b>Incompatible Materials</b>           | Strong oxidizing agents                                 |
| <b>Hazardous Decomposition Products</b> | Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ) |
| <b>Hazardous Polymerization</b>         | No information available.                               |
| <b>Hazardous Reactions</b>              | None under normal processing.                           |

## 11. Toxicological information

### Acute Toxicity

### Product Information

**Component Information****Toxicologically Synergistic Products**

No information available

**Delayed and immediate effects as well as chronic effects from short and long-term exposure****Irritation**

No information available

**Sensitization**

No information available

**Carcinogenicity**

The table below indicates whether each agency has listed any ingredient as a carcinogen.

| Component                        | CAS No   | IARC       | NTP        | ACGIH      | OSHA       | Mexico     |
|----------------------------------|----------|------------|------------|------------|------------|------------|
| Benzoic acid, 4-(1-methylethyl)- | 536-66-3 | Not listed | Not listed | Not listed | Not listed | Not listed |

**Mutagenic Effects**

No information available

**Reproductive Effects**

No information available.

**Developmental Effects**

No information available.

**Teratogenicity**

No information available.

**STOT - single exposure**

Respiratory system

**STOT - repeated exposure**

None known

**Aspiration hazard**

No information available

**Symptoms / effects, both acute and delayed**

No information available

**Endocrine Disruptor Information**

No information available

**Other Adverse Effects**

The toxicological properties have not been fully investigated.

## 12. Ecological information

**Ecotoxicity**

Do not empty into drains.

**Persistence and Degradability**

Soluble in water Persistence is unlikely based on information available.

**Bioaccumulation/ Accumulation**

No information available.

**Mobility**

Will likely be mobile in the environment due to its water solubility.

## 13. Disposal considerations

**Waste Disposal Methods**

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## 14. Transport information

**DOT**

Not regulated

**TDG**

Not regulated

**IATA**

Not regulated

**IMDG/IMO**

Not regulated

## 15. Regulatory information

**United States of America Inventory**

| Component                        | CAS No   | TSCA | TSCA Inventory notification - Active-Inactive | TSCA - EPA Regulatory Flags |
|----------------------------------|----------|------|-----------------------------------------------|-----------------------------|
| Benzoic acid, 4-(1-methylethyl)- | 536-66-3 | X    | ACTIVE                                        | -                           |

**Legend:**

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

-' - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)**

Not applicable

**TSCA 12(b)** - Notices of Export

Not applicable

**International Inventories**

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

| Component                        | CAS No   | DSL | NDL | EINECS    | PICCS | ENCS | ISHL | AICS | IECSC | KECL     |
|----------------------------------|----------|-----|-----|-----------|-------|------|------|------|-------|----------|
| Benzoic acid, 4-(1-methylethyl)- | 536-66-3 | -   | X   | 208-642-5 | -     | X    | X    | X    | -     | KE-21677 |

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)**U.S. Federal Regulations****SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

**SARA 311/312 Hazard Categories**

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

**CWA (Clean Water Act)**

Not applicable

**Clean Air Act**

Not applicable

**OSHA** - Occupational Safety and Health Administration

Not applicable

**CERCLA**

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

**California Proposition 65**

This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations**

Not applicable

**U.S. Department of Transportation**

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

**U.S. Department of Homeland**

This product does not contain any DHS chemicals.

## Security

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

| Component                        | CAS No   | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|----------------------------------|----------|---------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| Benzoic acid, 4-(1-methylethyl)- | 536-66-3 | -                                                                   | -                                                                             | -                                                                                                     |

## Safety, health and environmental regulations/legislation specific for the substance or mixture

| Component                        | CAS No   | OECD HPV       | Persistent Organic Pollutant | Ozone Depletion Potential | Restriction of Hazardous Substances (RoHS) |
|----------------------------------|----------|----------------|------------------------------|---------------------------|--------------------------------------------|
| Benzoic acid, 4-(1-methylethyl)- | 536-66-3 | Not applicable | Not applicable               | Not applicable            | Not applicable                             |

## Contains component(s) that meet a 'definition' of per &amp; poly fluoroalkyl substance (PFAS)?

Not applicable

## Other International Regulations

| Component                        | CAS No   | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements | Rotterdam Convention (PIC) | Basel Convention (Hazardous Waste) |
|----------------------------------|----------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|----------------------------|------------------------------------|
| Benzoic acid, 4-(1-methylethyl)- | 536-66-3 | Not applicable                                                                            | Not applicable                                                                           | Not applicable             | Not applicable                     |

## 16. Other information

Prepared By Health, Safety and Environmental Department  
Email: chem.techinfo@thermofisher.com  
www.thermofisher.com

Revision Date 25-Mar-2024  
Print Date 25-Mar-2024  
Revision Summary New emergency telephone response service provider.

## 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 SDS**