

## SAFETY DATA SHEET

Creation Date 09-Apr-2010

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Revision Number 3

### 1. Identification

**Product Name** 4-Methoxyphenyl isocyanate

**Cat No. :** A16805

**CAS No** 5416-93-3  
**Synonyms** No information available

**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)

|                                                  |            |
|--------------------------------------------------|------------|
| Acute oral toxicity                              | Category 4 |
| Acute dermal toxicity                            | Category 4 |
| Acute Inhalation Toxicity - Vapors               | Category 4 |
| Skin Corrosion/Irritation                        | Category 1 |
| Serious Eye Damage/Eye Irritation                | Category 1 |
| Specific target organ toxicity (single exposure) | Category 3 |
| Target Organs - Respiratory system.              |            |

#### Label Elements

##### **Signal Word**

Danger

**Hazard Statements**

Harmful if swallowed  
Harmful in contact with skin  
Causes severe skin burns and eye damage  
May cause respiratory irritation  
Harmful if inhaled

**Precautionary Statements****Prevention**

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

**Response**

Immediately call a POISON CENTER or doctor/physician

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

**Skin**

Wash contaminated clothing before reuse  
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

**Ingestion**

Rinse mouth  
Do NOT induce vomiting

**Storage**

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

**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 % |
|----------------------------------|-----------|----------|
| Benzene, 1-isocyanato-4-methoxy- | 5416-93-3 | 99       |

### 4. First-aid measures

**Eye Contact**

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

**Skin Contact**

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Immediate medical attention is required.

**Inhalation**

Remove from exposure, lie down. Remove to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Immediate medical attention is required.

|                                            |                                                                                                                                                                                                                                                                                                 |
|--------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Ingestion</b>                           | Call a physician immediately. Clean mouth with water.                                                                                                                                                                                                                                           |
| <b>Most important symptoms and effects</b> | Causes burns by all exposure routes. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation |
| <b>Notes to Physician</b>                  | Treat symptomatically                                                                                                                                                                                                                                                                           |

## 5. Fire-fighting measures

|                                         |                                                  |
|-----------------------------------------|--------------------------------------------------|
| <b>Suitable Extinguishing Media</b>     | Carbon dioxide (CO <sub>2</sub> ). Dry chemical. |
| <b>Unsuitable Extinguishing Media</b>   | No information available                         |
| <b>Flash Point</b>                      | 98 °C / 208.4 °F                                 |
| <b>Method -</b>                         | No information available                         |
| <b>Autoignition Temperature</b>         | No information available                         |
| <b>Explosion Limits</b>                 |                                                  |
| <b>Upper</b>                            | No data available                                |
| <b>Lower</b>                            | No data available                                |
| <b>Sensitivity to Mechanical Impact</b> | No information available                         |
| <b>Sensitivity to Static Discharge</b>  | No information available                         |

**Specific Hazards Arising from the Chemical**  
Flammable.

### Hazardous Combustion Products

Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen cyanide (hydrocyanic acid).

### 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

|               |                     |                    |                         |
|---------------|---------------------|--------------------|-------------------------|
| <b>Health</b> | <b>Flammability</b> | <b>Instability</b> | <b>Physical hazards</b> |
| 3             | 1                   | 0                  | N/A                     |

## 6. Accidental release measures

|                                             |                                                                                                                                                          |
|---------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Personal Precautions</b>                 | Ensure adequate ventilation. Use personal protective equipment as required.                                                                              |
| <b>Environmental Precautions</b>            | See Section 12 for additional Ecological Information.                                                                                                    |
| <b>Methods for Containment and Clean Up</b> | Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. |

## 7. Handling and storage

|                 |                                                                                                                                                                                                                     |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Handling</b> | Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Handle product only in closed system or provide appropriate exhaust ventilation.                                                     |
| <b>Storage.</b> | Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Incompatible Materials. Acids. Water. Strong oxidizing agents. Strong bases. Alcohols. Amines. |

## 8. Exposure controls / personal protection

|                            |                                                                                                                                               |
|----------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Exposure Guidelines</b> | This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies. |
|----------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|

**Engineering Measures** Ensure that eyewash stations and safety showers are close to the workstation location.

#### **Personal Protective Equipment**

**Eye/face Protection** 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.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure.

**Respiratory Protection** 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.

**Recommended Filter type:** Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

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

### **9. Physical and chemical properties**

|                                               |                                         |
|-----------------------------------------------|-----------------------------------------|
| <b>Physical State</b>                         | Liquid                                  |
| <b>Appearance</b>                             | Colorless                               |
| <b>Odor</b>                                   | No information available                |
| <b>Odor Threshold</b>                         | No information available                |
| <b>pH</b>                                     | No information available                |
| <b>Melting Point/Range</b>                    | No data available                       |
| <b>Boiling Point/Range</b>                    | 106 - 110 °C / 222.8 - 230 °F @ 16 mmHg |
| <b>Flash Point</b>                            | 98 °C / 208.4 °F                        |
| <b>Evaporation Rate</b>                       | No information available                |
| <b>Flammability (solid,gas)</b>               | Not applicable                          |
| <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>                          | No information available                |
| <b>Specific Gravity</b>                       | 1.150                                   |
| <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>                              | No information available                |
| <b>Molecular Formula</b>                      | C8 H7 N O2                              |
| <b>Molecular Weight</b>                       | 149.15                                  |

### **10. Stability and reactivity**

**Reactive Hazard** None known, based on information available

**Stability** Moisture sensitive.

**Conditions to Avoid** Burning produces obnoxious and toxic fumes. Excess heat. Incompatible products.

**Incompatible Materials** Acids, Water, Strong oxidizing agents, Strong bases, Alcohols, Amines

**Hazardous Decomposition Products** Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Hydrogen cyanide (hydrocyanic acid)

**Hazardous Polymerization** No information available.

**Hazardous Reactions** None under normal processing.

## 11. Toxicological information

### Acute Toxicity

**Product Information** No acute toxicity information is available for this product

**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     |
|-------------------------------------|-----------|------------|------------|------------|------------|------------|
| Benzene,<br>1-isocyanato-4-methoxy- | 5416-93-3 | 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** Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

**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** No information available

**Bioaccumulation/ Accumulation** No information available.

**Mobility** No information available.

## 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**

UN-No UN2206  
 Proper Shipping Name Isocyanates, toxic, n.o.s.  
 Technical Name Benzene, 1-isocyanato-4-methoxy-  
 Hazard Class 6.1  
 Packing Group II

**TDG**

UN-No UN2206  
 Proper Shipping Name Isocyanates, toxic, n.o.s.  
 Hazard Class 6.1  
 Packing Group II

**IATA**

UN-No UN2206  
 Proper Shipping Name Isocyanates, toxic, n.o.s.  
 Hazard Class 6.1  
 Packing Group II

**IMDG/IMO**

UN-No UN2206  
 Proper Shipping Name Isocyanates, toxic, n.o.s.  
 Hazard Class 6.1  
 Packing Group II

## 15. Regulatory information

**United States of America Inventory**

| Component                           | CAS No    | TSCA | TSCA Inventory notification -<br>Active-Inactive | TSCA - EPA Regulatory<br>Flags |
|-------------------------------------|-----------|------|--------------------------------------------------|--------------------------------|
| Benzene,<br>1-isocyanato-4-methoxy- | 5416-93-3 | X    | INACTIVE                                         | -                              |

**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 |
|-------------------------------------|-----------|-----|-----|-----------|-------|------|------|------|-------|------|
| Benzene,<br>1-isocyanato-4-methoxy- | 5416-93-3 | -   | X   | 226-513-1 | -     | -    |      | -    | -     | -    |

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 Security** This product does not contain any DHS chemicals.

#### **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) |
|----------------------------------|-----------|---------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| Benzene, 1-isocyanato-4-methoxy- | 5416-93-3 | -                                                                   | -                                                                             | -                                                                                                     |

#### **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) |
|----------------------------------|-----------|----------------|------------------------------|---------------------------|--------------------------------------------|
| Benzene, 1-isocyanato-4-methoxy- | 5416-93-3 | Not applicable | Not applicable               | Not applicable            | Not applicable                             |

**Contains component(s) that meet a 'definition' of per & 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) |
|----------------------------------|-----------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|----------------------------|------------------------------------|
| Benzene, 1-isocyanato-4-methoxy- | 5416-93-3 | 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

**Creation Date** 09-Apr-2010  
**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**