

## SAFETY DATA SHEET

Creation Date 06-Oct-2009

Revision Date 29-Mar-2024

Revision Number 4

### 1. Identification

**Product Name** 4'-(Trifluoromethoxy)acetophenone

**Cat No. :** A13928

**CAS No** 85013-98-5  
**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)

Flammable liquids	Category 4
Acute oral toxicity	Category 4
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**  
Combustible liquid  
Harmful if swallowed

Causes skin irritation  
Causes serious eye irritation  
May cause respiratory irritation

**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  
Avoid breathing dust/fume/gas/mist/vapors/spray  
Use only outdoors or in a well-ventilated area  
Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
Keep cool

**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

**Ingestion**

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
Rinse mouth

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam for extinction

**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 %
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one	85013-98-5	>95

### 4. First-aid measures

**General Advice**

If symptoms persist, call a physician. Show this safety data sheet to the doctor in attendance.

**Eye Contact**

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. Get medical attention.
<b>Inhalation</b>	Remove to fresh air. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Get medical attention. If not breathing, give artificial respiration.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Most important symptoms and effects</b>	Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
<b>Notes to Physician</b>	Treat symptomatically

## 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water spray, carbon dioxide (CO <sub>2</sub> ), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	87 °C / 188.6 °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

Combustible material. Containers may explode when heated.

### Hazardous Combustion Products

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

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

### NFPA

<b>Health</b>	<b>Flammability</b>	<b>Instability</b>	<b>Physical hazards</b>
2	2	0	N/A

## 6. Accidental release measures

<b>Personal Precautions</b>	Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	Should not be released into the environment. See Section 12 for additional Ecological Information.
<b>Methods for Containment and Clean Up</b>	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

## 7. Handling and storage

<b>Handling</b>	Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static
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discharges.

**Storage.**

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases.

## 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 that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment.

**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**

No protective equipment is needed under normal use conditions.

**Hygiene Measures**

When using do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

## 9. Physical and chemical properties

Physical State	Liquid
Appearance	No information available
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	100 - 102 °C / 212 - 215.6 °F
Flash Point	87 °C / 188.6 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	No information available
Specific Gravity	1.278
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C9 H7 F3 O2
Molecular Weight	204.15

## 10. Stability and reactivity

**Reactive Hazard**

None known, based on information available

<b>Stability</b>	Stable under normal conditions.
<b>Conditions to Avoid</b>	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.
<b>Incompatible Materials</b>	Strong oxidizing agents, Strong acids, Strong bases
<b>Hazardous Decomposition Products</b>	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Hydrogen fluoride
<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

<b>Irritation</b>	No information available
<b>Sensitization</b>	No information available
<b>Carcinogenicity</b>	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one	85013-98-5	Not listed	Not listed	Not listed	Not listed	Not listed

<b>Mutagenic Effects</b>	No information available
<b>Reproductive Effects</b>	No information available.
<b>Developmental Effects</b>	No information available.
<b>Teratogenicity</b>	No information available.
<b>STOT - single exposure</b>	Respiratory system
<b>STOT - repeated exposure</b>	None known
<b>Aspiration hazard</b>	No information available
<b>Symptoms / effects, both acute and delayed</b>	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
<b>Endocrine Disruptor Information</b>	No information available
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.

## 12. Ecological information

### Ecotoxicity

Do not empty into drains.

<b>Persistence and Degradability</b>	No information available
<b>Bioaccumulation/ Accumulation</b>	No information available.
<b>Mobility</b>	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**

COMBUSTIBLE LIQUID, NOT REGULATED FOR TRANSPORT IN THIS QUANTITY  
According to 49 CFR §173.150(f)(1), this material should be reclassified as NA1993, Combustible Liquid, NOS if it is shipped in bulk.

**UN-No**

NA1993

**Proper Shipping Name**

Combustible liquid, n.o.s.

**Packing Group**

III

**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
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one	85013-98-5	-	-	-

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

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one	85013-98-5	-	-	285-066-0	-	-		-	-	-

**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** Slight risk, Grade 1

**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)
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one	85013-98-5	-	-	-

**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)
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one	85013-98-5	Not applicable	Not applicable	Not applicable	Not applicable

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

See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin List)
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one (CAS #: 85013-98-5)	-	-	Listed	Listed	-

**PFAS Legend**

Listed = Meets the PFAS definition of the named authority

#### 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)
1-[4-(Trifluoromethoxy)phenyl]ethan-1-one	85013-98-5	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** 06-Oct-2009  
**Revision Date** 29-Mar-2024  
**Print Date** 29-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**