Chemical Safety Data Sheet MSDS / SDS

4'-(Trifluoromethoxy)acetophenone

Revision Date:2025-02-01 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name	: 4'-(Trifluoromethoxy)acetophenone				
CBnumber	: CB4714204				
CAS	: 85013-98-5				
EINECS Number	: 285-066-0				
Synonyms	: 4'-(Trifluoromethoxy)acetophenone				
Relevant identified uses of the substance or mixture and uses advised against					
Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.				
Uses advised against	: none				
Company Identification					
Company	: Chemicalbook				
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing				
Telephone	: 400-158-6606				

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Warning

Precautionary statements

P501 Dispose of contents/container to.....

P403+P235 Store in a well-ventilated place. Keep cool.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P264 Wash skin thouroughly after handling.

P264 Wash hands thoroughly after handling.

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Hazard statements

H319 Causes serious eye irritation

H315 Causes skin irritation

H227 Combustible liquid

1

SECTION 3: Composition/information on ingredients

Substance

Product name	: 4'-(Trifluoromethoxy)acetophenone
Synonyms	: 4'-(Trifluoromethoxy)acetophenone
CAS	: 85013-98-5
EC number	: 285-066-0
MF	: C9H7F3O2
MW	: 204.15

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen fluoride

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704

2	2 ×	0
HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. <u>diethyl</u> <u>ether</u> , ammonium phosphate, iodine)
FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, <u>sulfur</u>)
REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, <u>N2</u>)
SPEC. HAZ.	-	

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid breathing vapors, mist or gas. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

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

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it. Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

OdurNo data availableOdur ThresholdNo data availablepHNo data availableMelting point/freezing pointNo data availableInitial boiling range100 °CFlash point88 °C - closed cupEvaporation rateNo data availableFlammability (solid, gas)No data availableUpper/lower flammability or explosiveNo data availableInitisVapour pressureVapour pressureNo data availableRelative density1.278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableViscosityNo data availableExplositor temperatureNo data availableViscosityNo data availableViscosityNo data availableExplositor temperatureNo da	Appearance	liquid
PHNo data availableMelting point/freezing pointNo data availableInitial boiling point and boiling range100 °CFlash point88 °C - closed cupEvaporation rateNo data availableFlammability (solid, gas)No data availableUpper/lower flammability or explosiveNo data availableUpper/lower flammability or explosiveNo data availableVapour pressureNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableViscosityNo data availableViscosityNo data availableExplosive propertiesNo data available	Odour	No data available
Melting point/freezing pointNo data availableInitial boiling point and boiling range100 °CFlash point88 °C - closed cupEvaporation rateNo data availableFlammability (solid, gas)No data availableUpper/lower flammability or explosiveNo data availablelimitsVapour pressureNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableViscosityNo data availableViscosityNo data availableNo data availableNo data availablePartition coefficient: n-octanol/waterNo data availableDecomposition temperatureNo data availableViscosityNo data availableNo data available	Odour Threshold	No data available
Initial boiling point and boiling range100 °CFlash point88 °C - closed cupEvaporation rateNo data availableFlammability (solid, gas)No data availableUpper/lower flammability or explosiveNo data availableUpper/lower flammability or explosiveNo data availableVapour pressureNo data availableVapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableViscosityNo data availableViscosityNo data availableExplosive propertiesNo data available	рН	No data available
Flash point88 °C - closed cupEvaporation rateNo data availableFlammability (solid, gas)No data availableUpper/lower flammability or explosiveNo data availablelimitsVapour pressureVapour pressureNo data availableVapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableExplosive propertiesNo data available	Melting point/freezing point	No data available
Evaporation rateNo data availableFlammability (solid, gas)No data availableUpper/lower flammability or explosiveNo data availablelimitsVapour pressureNo data availableVapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableViscosityNo data availableViscosityNo data availableViscosityNo data availableViscosityNo data availableViscosityNo data availableExplosive propertiesNo data available	Initial boiling point and boiling range	100 °C
Flammability (solid, gas)No data availableUpper/lower flammability or explosiveNo data availablelimitsVapour pressureNo data availableVapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableExplosive propertiesNo data available	Flash point	88 °C - closed cup
Upper/lower flammability or explosiveNo data availablelimitsVapour pressureNo data availableVapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableViscosityNo data availableExplosive propertiesNo data available	Evaporation rate	No data available
limitsVapour pressureNo data availableVapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableViscosityNo data availableExplosive propertiesNo data available	Flammability (solid, gas)	No data available
Vapour pressureNo data availableVapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableExplosive propertiesNo data available	Upper/lower flammability or explosive	No data available
Vapour densityNo data availableRelative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableViscosityNo data availableExplosive propertiesNo data available	limits	
Relative density1,278 g/mL at 25 °CWater solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableExplosive propertiesNo data available	Vapour pressure	No data available
Water solubilityNo data availablePartition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableExplosive propertiesNo data available	Vapour density	No data available
Partition coefficient: n-octanol/waterNo data availableAutoignition temperatureNo data availableDecomposition temperatureNo data availableViscosityNo data availableExplosive propertiesNo data available	Relative density	1,278 g/mL at 25 °C
Autoignition temperature No data available Decomposition temperature No data available Viscosity No data available Explosive properties No data available	Water solubility	No data available
Decomposition temperature No data available Viscosity No data available Explosive properties No data available	Partition coefficient: n-octanol/water	No data available
Viscosity No data available Explosive properties No data available	Autoignition temperature	No data available
Explosive properties No data available	Decomposition temperature	No data available
	Viscosity	No data available
	Explosive properties	No data available
Uxidizing properties No data available	Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Strong oxidizing agents, Strong bases

Hazardous decomposition products

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity No data available Skin corrosion/irritation No data available Serious eye damage/eye irritation No data available Respiratory or skin sensitization No data available Germ cell mutagenicity No data available Carcinogenicity IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. **Reproductive toxicity** No data available Specific target organ toxicity - single exposure No data available Specific target organ toxicity - repeated exposure No data available Aspiration hazard No data available **Additional Information RTECS:** Not available To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Toxicity

No data available

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: - IMDG: - IATA: -

UN proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

Packaging group

ADR/RID: - IMDG: - IATA: -

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Not Listed. website: https://chemicaldata.gov.vn/

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: https://www.epa.gov/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: https://emb.gov.ph/

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: https://www.epa.govt.nz/

Korea Existing Chemicals List (KECL):Not Listed. website: http://ncis.nier.go.kr

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/ EC Inventory:Listed.

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

- CAS: Chemical Abstracts Service
- EC50: Effective Concentration 50%
- IATA: International Air Transportation Association
- IMDG: International Maritime Dangerous Goods
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- STEL: Short term exposure limit
- TWA: Time Weighted Average

References

- [1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- [2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- [3] ECHA European Chemicals Agency, website: https://echa.europa.eu/
- [4] eChemPortal The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

- [6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- [7] HSDB Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- [8] IARC International Agency for Research on Cancer, website: http://www.iarc.fr/
- [9] IPCS The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- [10] Sigma-Aldrich, website: https://www.sigmaaldrich.com/

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.