

Chemical Safety Data Sheet MSDS / SDS

2,3,6-TRIFLUOROPHENYLACETIC ACIDRevision Date:2025-02-01 Revision Number:1

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

Product name : 2,3,6-TRIFLUOROPHENYLACETIC ACID
CBnumber : CB3148770
CAS : 114152-23-7
Synonyms : 2-(2,3,6-trifluorophenyl)acetic acid,2,3,6-Trifluorophenylacetic acid

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 : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
Continuerinsing.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

H335 May cause respiratory irritation
H319 Causes serious eye irritation
H315 Causes skin irritation

SECTION 3: Composition/information on ingredients**Substance**

Product name	: 2,3,6-TRIFLUOROPHENYLACETIC ACID
Synonyms	: 2-(2,3,6-trifluorophenyl)acetic acid, 2,3,6-Trifluorophenylacetic acid
CAS	: 114152-23-7
MF	: C ₈ H ₅ F ₃ O ₂
MW	: 190.12

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this 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

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

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.

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

No data available

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

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

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatrill? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatrill? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	white powder
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 111 - 114 °C - lit.
Initial boiling point and boiling range	249.5±35.0 °C(Predicted)
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available

Relative density	No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive 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

No data available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen fluoride

Other decomposition products - No data available In the event of fire: see section 5

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 sensitisation

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component 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

Inhalation - May cause respiratory irritation.

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

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

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. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

SECTION 14: Transport information

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

IATA:

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 1993 IMDG: 1993 IATA: 1993

ADR/RID: - IMDG: - IATA: -

ADR/RID: 2811 IMDG: 2811 IATA: 2811

ADR/RID: 1578 IMDG: 1578 IATA: 1578

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: 3334

ADR/RID: 1993 IMDG: 1993 IATA: 1993

ADR/RID: 1162 IMDG: 1162 IATA: 1162

ADR/RID: 1502 IMDG: 1502 IATA: 1502

UN proper shipping name

ADR/RID: SODIUM PERCHLORATE IMDG: SODIUM PERCHLORATE IATA: Sodium perchlorate

ADR/RID: DIMETHYLDICHLOROSILANE IMDG: DIMETHYLDICHLOROSILANE IATA: Dimethyldichlorosilane Passenger Aircraft: Not permitted for transport

ADR/RID: FLAMMABLE LIQUID, N.O.S. (Perflunafene) IMDG: FLAMMABLE LIQUID, N.O.S. (Perflunafene) IATA: Flammable liquid, n.o.s. (Perflunafene)

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Aviation regulated liquid, n.o.s. (1-Undecanethiol)

ADR/RID: - IMDG: - IATA: -

ADR/RID: CHLORONITROBENZENES, SOLID IMDG: CHLORONITROBENZENES, SOLID IATA: Chloronitrobenzenes, solid

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (Vitamin D2) IMDG: TOXIC SOLID, ORGANIC, N.O.S. (Vitamin D2) IATA: Toxic solid, organic, n.o.s. (Vitamin D2)

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

ADR/RID: FLAMMABLE LIQUID, N.O.S. (2-Methoxythiophene) IMDG: FLAMMABLE LIQUID, N.O.S. (2-Methoxythiophene) IATA: Flammable liquid, n.o.s. (2-Methoxythiophene)

ADR/RID: III IMDG: III IATA: III

Environmental hazards

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

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: - IMDG: - IATA: -

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

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

ADR/RID: - IMDG: - IATA: 9

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 3 (8) IMDG: 3 (8) IATA: 3 (8)

ADR/RID: 5.1 IMDG: 5.1 IATA: 5.1

Packaging group

ADR/RID: II IMDG: II IATA: II

ADR/RID: II IMDG: II IATA: II

ADR/RID: - IMDG: - IATA: III

ADR/RID: III IMDG: III IATA: III

ADR/RID: II IMDG: II IATA: II

No data available

ADR/RID: - IMDG: - IATA: -

ADR/RID: III IMDG: III IATA: III

No data available

Environmental hazards

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

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

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

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

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

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

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

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

Special precautions for user

No data available

No data available

No data available

No data available

No data available

No data available

No data available

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

EC Inventory:Not Listed.

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):Not Listed. website: <https://echa.europa.eu/>

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

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

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/>

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

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

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】 ChemIDplus, 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.