



SAFETY DATA SHEET

2-Chloro-5-(trifluoromethyl)benzoic acid

According to Regulation (EC) No 1907/2006, Annex II, as amended. Commission Regulation (EU) No 2015/830 of 28 May 2015.

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

1.1. Product identifier

Product name	2-Chloro-5-(trifluoromethyl)benzoic acid
Product number	49574378
CAS number	657-06-7
EC number	629-974-0

1.2. Relevant identified uses of the substance or mixture and uses advised against

Uses advised against	For research and development purposes. Not suitable for human consumption or veterinary purposes.
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1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 1380 725952

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (EC 1272/2008)

Physical hazards	Not Classified
Health hazards	Skin Irrit. 2 - H315 Eye Irrit. 2 - H319 STOT SE 3 - H335
Environmental hazards	Not Classified

2.2. Label elements

EC number	629-974-0
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Hazard pictograms



Signal word	Warning
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Hazard statements	H315 Causes skin irritation. H319 Causes serious eye irritation. H335 May cause respiratory irritation.
Precautionary statements	P261 Avoid breathing dust. P264 Wash contaminated skin thoroughly after handling. P271 Use only outdoors or in a well-ventilated area. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P302+P352 IF ON SKIN: Wash with plenty of water. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P312 Call a POISON CENTRE/doctor if you feel unwell. P332+P313 If skin irritation occurs: Get medical advice/ attention. P337+P313 If eye irritation persists: Get medical advice/ attention. P362+P364 Take off contaminated clothing and wash it before reuse. P403+P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up. P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current EU criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	2-Chloro-5-(trifluoromethyl)benzoic acid
CAS number	657-06-7
EC number	629-974-0
Chemical formula	C ₁₀ H ₆ ClF ₃ O ₂

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
Inhalation	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention. Place unconscious person on their side in the recovery position and ensure breathing can take place.
Ingestion	Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on their side in the recovery position and ensure breathing can take place. Keep affected person under observation. Get medical attention if symptoms are severe or persist.
Skin contact	Rinse with water.
Eye contact	Rinse with water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Get medical attention if any discomfort continues.
Protection of first aiders	First aid personnel should wear appropriate protective equipment during any rescue.

4.2. Most important symptoms and effects, both acute and delayed

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General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Irritation of nose, throat and airway. Difficulty in breathing. Coughing.
Ingestion	May cause irritation.
Skin contact	Redness. Irritating to skin.
Eye contact	Irritating to eyes.

4.3. Indication of any immediate medical attention and special treatment needed

Notes for the doctor	Treat symptomatically.
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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards	None known.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO ₂). Hydrogen chloride (HCl). Hydrogen fluoride (HF).

5.3. Advice for firefighters

Protective actions during firefighting	Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.
Special protective equipment for firefighters	Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions	Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of dust. Use suitable respiratory protection if ventilation is inadequate.
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6.2. Environmental precautions

Environmental precautions	Avoid discharge into drains or watercourses or onto the ground.
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6.3. Methods and material for containment and cleaning up

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Methods for cleaning up

Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions

Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use.

Advice on general occupational hygiene

Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions

Store away from incompatible materials (see Section 10). Store locked up. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

Storage class

Chemical storage.

7.3. Specific end use(s)

Specific end use(s)

The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

STEL

TWA

8.2. Exposure controls

Protective equipment



Appropriate engineering controls

Provide adequate general and local exhaust ventilation. Ensure the ventilation system is regularly maintained and tested. Good general ventilation should be adequate to control worker exposure to airborne contaminants. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection

Wear tight-fitting, chemical splash goggles or face shield. If inhalation hazards exist, a full-face respirator may be required instead.

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Hand protection	Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacture, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, gloves should comply with European Standard EN374. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.
Other skin and body protection	Wear appropriate clothing to prevent repeated or prolonged skin contact.
Hygiene measures	Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.
Respiratory protection	Ensure all respiratory protective equipment is suitable for its intended use and is 'CE'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges should comply with European Standard EN14387. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.
Environmental exposure controls	Keep container tightly sealed when not in use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Powder.
Colour	White.
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	93 - 96°C/199.4 - 204.8°F
Initial boiling point and range	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	No information available.
Vapour density	No information available.
Relative density	No information available.
Solubility(ies)	No information available.
Partition coefficient	No information available.
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

9.2. Other information

Molecular weight	224.56
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SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity See the other subsections of this section for further details.

10.2. Chemical stability

Stability Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions No potentially hazardous reactions known.

10.4. Conditions to avoid

Conditions to avoid There are no known conditions that are likely to result in a hazardous situation.

10.5. Incompatible materials

Materials to avoid Avoid contact with strong oxidising agents.

10.6. Hazardous decomposition products

Hazardous decomposition products Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen chloride (HCl). Hydrogen fluoride (HF).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Summary Based on available data the classification criteria are not met.

Acute toxicity - dermal

Summary Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Summary Based on available data the classification criteria are not met.

Skin corrosion/irritation

Summary Causes skin irritation.

Serious eye damage/irritation

Summary Causes serious eye irritation.

Respiratory sensitisation

Summary Based on available data the classification criteria are not met.

Skin sensitisation

Summary Based on available data the classification criteria are not met.

Germ cell mutagenicity

Summary Based on available data the classification criteria are not met.

Carcinogenicity

Summary Based on available data the classification criteria are not met.

IARC carcinogenicity None of the ingredients are listed or exempt.

Reproductive toxicity

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Summary Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

Summary May cause respiratory irritation.

Target organs Respiratory system, lungs

Specific target organ toxicity - repeated exposure

Summary Based on available data the classification criteria are not met.

Aspiration hazard

Summary Not relevant. Solid.

General information The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation A single exposure may cause the following adverse effects: Irritation of nose, throat and airway. Difficulty in breathing. Coughing.

Ingestion May cause irritation.

Skin contact Redness. Irritating to skin.

Eye contact Irritating to eyes.

Route of exposure Ingestion Inhalation Skin and/or eye contact

Target organs Respiratory system, lungs

SECTION 12: Ecological information

Ecotoxicity Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity

Acute aquatic toxicity

Summary Based on available data the classification criteria are not met.

Chronic aquatic toxicity

Summary Based on available data the classification criteria are not met.

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient No information available.

12.4. Mobility in soil

Mobility No data available.

12.5. Results of PBT and vPvB assessment

12.6. Other adverse effects

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

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General information	The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.
Disposal methods	Do not empty into drains.

SECTION 14: Transport information

General	The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).
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14.1. UN number

Not applicable.

14.2. UN proper shipping name

Not applicable.

14.3. Transport hazard class(es)

No transport warning sign required.

14.4. Packing group

Not applicable.

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

14.6. Special precautions for user

Not applicable.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable.

SECTION 15: Regulatory information

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

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
EU legislation	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (as amended). Commission Regulation (EU) No 2015/830 of 28 May 2015. Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures (as amended).

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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Inventories

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
 ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
 RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
 IATA: International Air Transport Association.
 ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.
 IMDG: International Maritime Dangerous Goods.
 CAS: Chemical Abstracts Service.
 ATE: Acute Toxicity Estimate.
 LC₅₀: Lethal Concentration to 50 % of a test population.
 LD₅₀: Lethal Dose to 50% of a test population (Median Lethal Dose).
 EC₅₀: 50% of maximal Effective Concentration.
 PBT: Persistent, Bioaccumulative and Toxic substance.
 vPvB: Very Persistent and Very Bioaccumulative.

Classification abbreviations and acronyms

Eye Irrit. = Eye irritation
 Skin Irrit. = Skin irritation
 STOT SE = Specific target organ toxicity-single exposure

Classification procedures according to Regulation (EC) 1272/2008

STOT SE 3 - H335: Skin Irrit. 2 - H315: Eye Irrit. 2 - H319: : Expert judgement.

Training advice

Only trained personnel should use this material.

Revision date

22/10/2021

Revision

1

SDS number

416

Hazard statements in full

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

This 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. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.