



SAFETY DATA SHEET

Trichloroacetonitrile

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

1.1. Product identifier

Product name	Trichloroacetonitrile
CAS number	545-06-2
EC number	208-885-7

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

Identified uses	For research purposes only.
Uses advised against	No specific uses advised against are identified.

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) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Acute Tox. 3 - H301 Acute Tox. 3 - H311 Acute Tox. 3 - H331
Environmental hazards	Aquatic Chronic 2 - H411

2.2. Label elements

EC number	208-885-7
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Hazard pictograms



Signal word	Danger
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Hazard statements	H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled. H411 Toxic to aquatic life with long lasting effects.
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Precautionary statements	P261 Avoid breathing vapour/ spray. P264 Wash contaminated skin thoroughly after handling. P271 Use only outdoors or in a well-ventilated area. P273 Avoid release to the environment. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. P302+P352 IF ON SKIN: Wash with plenty of water. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P311 Call a POISON CENTER/ doctor. P312 Call a POISON CENTRE/doctor if you feel unwell. P330 Rinse mouth. P361+P364 Take off immediately all contaminated clothing and wash it before reuse. P391 Collect spillage. 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.
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2.3. Other hazards

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

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	Trichloroacetonitrile
CAS number	545-06-2
EC number	208-885-7
Chemical formula	C ₂ Cl ₃ N

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention immediately. 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	Get medical attention immediately. 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.
Skin contact	It is important to remove the substance from the skin immediately. Remove contamination with soap and water or recognised skin cleansing agent. Get medical attention.
Eye contact	Remove any contact lenses and open eyelids wide apart. Rinse with water. Get medical attention if any discomfort continues.
Protection of first aiders	It may be dangerous for first aid personnel to carry out mouth-to-mouth resuscitation.

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

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
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Inhalation	A single exposure may cause the following adverse effects: Drowsiness, dizziness, disorientation, vertigo. Unconsciousness. High concentrations may be fatal.
Ingestion	May cause stomach pain or vomiting. May cause severe internal injury.
Skin contact	A single exposure may cause the following adverse effects: Pain.
Eye contact	May be slightly irritating to eyes.

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

Notes for the doctor	Treat symptomatically. Keep affected person under observation.
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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.
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Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
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5.2. Special hazards arising from the substance or mixture

Specific hazards	Containers can burst violently or explode when heated, due to excessive pressure build-up. This product is toxic.
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Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Very toxic or corrosive gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO ₂). Oxides of nitrogen. Hydrogen chloride (HCl). Vapours are heavier than air and may travel along the floor and accumulate in the bottom of containers. Forms explosive mixtures with air on intense heating.
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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. If a leak or spill has not ignited, use water spray to disperse vapours and protect men stopping the leak. Avoid discharge to the aquatic environment. 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 chemical protective suit. Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing 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 vapours and spray/mists. Use suitable respiratory protection if ventilation is inadequate. Avoid contact with skin and eyes.
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6.2. Environmental precautions

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Environmental precautions Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.

6.3. Methods and material for containment and cleaning up

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. Provide adequate ventilation. Small Spillages: Collect spillage. Large Spillages: Absorb spillage with non-combustible, absorbent material. The contaminated absorbent may pose the same hazard as the spilled material. Collect and place in suitable waste disposal containers and seal securely. Label the containers containing waste and contaminated materials and remove from the area as soon as possible. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dangerous for the environment. Do not empty into drains. 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. Handle all packages and containers carefully to minimise spills. Keep container tightly sealed when not in use. Avoid the formation of mists. This product is toxic. Immediate first aid is imperative. Avoid discharge to the aquatic environment. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

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.

Store at temperatures between 2°C/35.6°F and 8°C/46.4°F.

Storage class Toxic 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

Occupational exposure limits

STEL:

TWA:

8.2. Exposure controls

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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

Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses.

Hand protection

Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacturer, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, wear gloves that are proven to be impervious to the chemical and resist degradation. 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 any possibility of 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 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.

Environmental exposure controls

Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Colourless liquid.
Colour	Transparent
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	-42°C/-43.6°F
Initial boiling point and range	83-84°C/181.4-183.2°F @ 760 mm Hg
Flash point	195°C/383°F Closed cup.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.

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Upper/lower flammability or explosive limits	No information available.
Vapour pressure	58 mm Hg @ 20°C/68°F
Vapour density	No information available.
Relative density	1.44 g/ml @ 25°C/77°F
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	144.39
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SECTION 10: Stability and reactivity

10.1. Reactivity

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

Stability	Stable under the prescribed storage conditions.
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10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	No potentially hazardous reactions known.
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10.4. Conditions to avoid

Conditions to avoid	Strong heating.
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10.5. Incompatible materials

Materials to avoid	Strong acids. Strong alkalis. Strong oxidising agents. Strong reducing agents.
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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: Toxic gases or vapours. Carbon dioxide (CO ₂). Carbon monoxide (CO). Oxides of: Nitrogen. Hydrogen chloride (HCl).
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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Summary	Toxic if swallowed.
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ATE oral (mg/kg)	100.0
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Acute toxicity - dermal

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Summary	Toxic in contact with skin.
ATE dermal (mg/kg)	300.0
<u>Acute toxicity - inhalation</u>	
Summary	Toxic if inhaled.
ATE inhalation (vapours mg/l)	3.0
<u>Skin corrosion/irritation</u>	
Summary	Based on available data the classification criteria are not met.
<u>Serious eye damage/irritation</u>	
Summary	Based on available data the classification criteria are not met.
<u>Respiratory sensitisation</u>	
Summary	Based on available data the classification criteria are not met.
<u>Skin sensitisation</u>	
Summary	Based on available data the classification criteria are not met.
<u>Germ cell mutagenicity</u>	
Summary	Based on available data the classification criteria are not met.
<u>Carcinogenicity</u>	
Summary	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.
<u>Reproductive toxicity</u>	
Summary	Based on available data the classification criteria are not met.
<u>Specific target organ toxicity - single exposure</u>	
Summary	Based on available data the classification criteria are not met.
<u>Specific target organ toxicity - repeated exposure</u>	
Summary	Based on available data the classification criteria are not met.
<u>Aspiration hazard</u>	
Summary	Based on available data the classification criteria are not met.
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: Drowsiness, dizziness, disorientation, vertigo. Unconsciousness. High concentrations may be fatal.
Ingestion	May cause stomach pain or vomiting. May cause severe internal injury.
Skin contact	A single exposure may cause the following adverse effects: Pain.
Eye contact	May be slightly irritating to eyes.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity

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

Chronic aquatic toxicity

Summary Toxic to aquatic life with long lasting effects.

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

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. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

SECTION 14: Transport information

General For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.

14.1. UN number

UN No. (ADR/RID) 3276

UN No. (IMDG) 3276

UN No. (ICAO) 3276

UN No. (ADN) 3276

14.2. UN proper shipping name

Proper shipping name (ADR/RID) NITRILES, LIQUID, TOXIC, N.O.S. (Trichloroacetonitrile)

Proper shipping name (IMDG) NITRILES, LIQUID, TOXIC, N.O.S. (Trichloroacetonitrile)

Proper shipping name (ICAO) NITRILES, LIQUID, TOXIC, N.O.S. (Trichloroacetonitrile)

Proper shipping name (ADN) NITRILES, LIQUID, TOXIC, N.O.S. (Trichloroacetonitrile)

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14.3. Transport hazard class(es)

ADR/RID class	6.1
ADR/RID classification code	T1
ADR/RID label	6.1
IMDG class	6.1
ICAO class/division	6.1
ADN class	6.1

Transport labels



14.4. Packing group

ADR/RID packing group	III
IMDG packing group	III
ICAO packing group	III
ADN packing group	III

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant



14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

EmS	F-A, S-A
ADR transport category	2
Emergency Action Code	2X
Hazard Identification Number (ADR/RID)	60
Tunnel restriction code	(E)

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.
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15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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).
	EC ₅₀ : 50% of maximal Effective Concentration.
	PBT: Persistent, Bioaccumulative and Toxic substance.
	vPvB: Very Persistent and Very Bioaccumulative.
Classification abbreviations and acronyms	Acute Tox. = Acute toxicity Aquatic Chronic = Hazardous to the aquatic environment (chronic)
Classification procedures according to SI 2019 No. 720	Acute Tox. 3 - H311: Acute Tox. 3 - H331: Acute Tox. 3 - H301: : Expert judgement. Aquatic Chronic 2 - H411: : Expert judgement.
Training advice	Only trained personnel should use this material.
Revision date	13/02/2023
Revision	1
SDS number	2119
Hazard statements in full	H301 Toxic if swallowed.
	H311 Toxic in contact with skin.
	H331 Toxic if inhaled.
	H411 Toxic to aquatic life with long lasting effects.

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.