

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

1.1. Product identifier

Product form	: Substance
Substance name	: 4-Chloro-3-cyanobenzotrifluoride
IUPAC name	: 4-Chloro-3-(trifluoromethyl)benzotrifluoride
EC-No.	: 671-867-6
CAS-No.	: 1735-54-2
Product code	: 74623204
Formula	: C ₈ H ₃ ClF ₃ N
Product group	: Raw material

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

1.2.1. Relevant identified uses

Main use category	: Laboratory use, Industrial use, Professional use
Industrial/Professional use spec	: For professional use only
Use of the substance/mixture	: For analytical purposes Scientific research and development Not for human consumption or veterinary purposes.

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Supplier

Scafell Organics
Molekula Ltd
Lingfield Way
Darlington - England
T +44 (0) 1949 823777 / +44 (0) 7590 545705
info@molekula.com / kbowen@molekula.com - www.molekula.com

1.4. Emergency telephone number

Emergency number : +44 (0) 7590 545705

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute toxicity (oral), Category 4	H302
Acute toxicity (dermal), Category 3	H311
Acute toxicity (inhalation:dust,mist) Category 4	H332
Skin corrosion/irritation, Category 2	H315
Serious eye damage/eye irritation, Category 2	H319
Full text of H statements : see section 16	

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS06

Signal word (CLP) :

Danger

Hazard statements (CLP) :

H302+H332 - Harmful if swallowed or if inhaled.
H311 - Toxic in contact with skin.
H315 - Causes skin irritation.
H319 - Causes serious eye irritation.

Precautionary statements (CLP) :

P260 - Do not breathe dusts or mists.
P264 - Wash hands, forearms and face thoroughly after handling.
P280 - Wear protective clothing, eye protection, face protection, protective gloves.
P301+P312 - IF SWALLOWED: Call a POISON CENTRE or doctor if you feel unwell.
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

4-Chloro-3-cyanobenzotrifluoride

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

2.3. Other hazards

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

SECTION 3: Composition/information on ingredients

3.1. Substances

Name	Product identifier	%
4-Chloro-3-cyanobenzotrifluoride	(CAS-No.) 1735-54-2 (EC-No.) 671-867-6	100

Full text of H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: If possible show this sheet, if not available show packaging or label. Never give anything by mouth to an unconscious person. Do not leave affected person unattended.
First-aid measures after inhalation	: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. Give oxygen or artificial respiration if necessary. If breathing difficulties persist : Get medical advice/attention.
First-aid measures after skin contact	: After contact with skin, take off immediately all contaminated clothing, and wash immediately with plenty of water. Do not remove clothing if it sticks to the skin. If irritation persists, consult a doctor.
First-aid measures after eye contact	: Rinse immediately with plenty of water. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Rinse mouth out with water. Do not induce vomiting. Get medical advice/attention.

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

Symptoms/effects	: Toxic in contact with skin. Harmful if inhaled. Harmful if swallowed.
Symptoms/effects after inhalation	: May cause irritation to the respiratory tract, sneezing, coughing, burning sensation of throat with constricting sensation of the larynx and difficulty in breathing. Headache. More severe symptoms are also possible.
Symptoms/effects after skin contact	: May cause skin irritation. Redness, pain. More severe symptoms are also possible.
Symptoms/effects after eye contact	: May cause severe irritation. redness, itching, tears. Blurred vision. More severe symptoms are also possible.
Symptoms/effects after ingestion	: Swallowing this material may result in health hazard. Symptoms of ingestion include drowsiness, weakness, headache, dizziness, nausea, vomiting. More severe symptoms are also possible.

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

Immediately call a POISON CENTER/doctor.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	: Foam. Dry powder. Carbon dioxide. Water spray. Sand.
Unsuitable extinguishing media	: Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Hazardous decomposition products in case of fire : Carbon oxides (CO, CO₂). hydrogen chloride. hydrogen fluoride. Nitrogen oxides.

5.3. Advice for firefighters

Precautionary measures fire	: Keep container tightly closed and away from heat, sparks and flame. Keep away from combustible materials.
Firefighting instructions	: Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire. Prevent fire fighting water from entering the environment.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.
Other information	: Warn all persons of toxic hazard.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Isolate from fire, if possible, without unnecessary risk. Avoid dust formation. No flames, no sparks. Eliminate all sources of ignition.

6.1.1. For non-emergency personnel

Protective equipment	: Wear recommended personal protective equipment.
Emergency procedures	: Evacuate unnecessary personnel. Mark out the contaminated area with signs and prevent access to unauthorized personnel. Do not touch or walk on the spilled product. Avoid contact with skin, eyes and clothing.

4-Chloro-3-cyanobenzotrifluoride

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

Measures in case of dust release : Keep upwind. Avoid creating or spreading dust. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc).

6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection. Use self-contained breathing apparatus and chemically protective clothing.

Emergency procedures : Ventilate area.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : On land, sweep or shovel into suitable containers. Shovel or sweep up and put in a closed container for disposal.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Avoid creating or spreading dust. Provide local exhaust or general room ventilation.

Hygiene measures : Take off immediately all contaminated clothing and wash it before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not eat, drink or smoke when using this product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Ensure adequate ventilation, especially in confined areas.

Storage conditions : Keep only in the original container in a cool, well ventilated place away from : Heat sources, Direct sunlight. Keep container closed when not in use.

Incompatible products : Strong oxidizing agents.

Incompatible materials : Sources of ignition. Direct sunlight. Heat sources.

Heat and ignition sources : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Storage area : Store below 20 °C. Store in a dry place. Store in a closed container.

7.3. Specific end use(s)

For analytical purposes. Scientific research and development. Not for human consumption or veterinary purposes.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls:

Handle in accordance with good industrial hygiene and safety procedures.

Personal protective equipment:

Avoid all unnecessary exposure.

Materials for protective clothing:

Wear suitable protective clothing, gloves and eye/face protection

Hand protection:

The protective gloves to be used must comply with the specifications of the regulation 2016/425 and the resultant standard EN 374

Type	Material	Permeation	Thickness (mm)	Penetration	Standard
Disposable gloves	Nitrile rubber (NBR)	6 (> 480 minutes)	0.11		EN 374

Eye protection:

Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure. Use eye protection according to EN 166, designed to protect against powders and dusts.

Type	Use	Characteristics	Standard
Safety goggles, Face shield	Fine dust, Dust	tightly fitting safety goggles, With side shields	EN 166

Skin and body protection:

Emergency safety showers should be available in the immediate vicinity of any potential exposure. Keep suitable chemically resistant protective clothing readily available for emergency use

4-Chloro-3-cyanobenzotrifluoride

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

Type	Standard		
Total impervious protective suits, gloves, and boots must be worn to prevent any contact with the product	EN ISO 13982		
Respiratory protection:			
Keep self contained breathing apparatus readily available for emergency use. Where exposure through inhalation may occur from use, respiratory protection equipment is recommended			
Device	Filter type	Condition	Standard
Respiratory protective device with a particle filter	Type P3	Dust protection	EN 143

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Crystals. Crystalline powder.
Molecular mass	: 205.56 g/mol
Colour	: Off-white.
Odour	: No data available.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: 64 - 68 °C
Freezing point	: No data available
Boiling point	: 100 - 105 °C
Flash point	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Non flammable.
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: No data available
Solubility	: No data available
Log Pow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under recommended handling and storage conditions (see section 7).

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Protect from sunlight. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

10.5. Incompatible materials

Strong oxidizers.

10.6. Hazardous decomposition products

No hazardous decomposition products known at room temperature. Thermal decomposition generates : Carbon oxides (CO, CO₂). hydrogen chloride. hydrogen fluoride. Nitrogen oxides.

4-Chloro-3-cyanobenzotrifluoride

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral)	: Oral: Harmful if swallowed.
Acute toxicity (dermal)	: Dermal: Toxic in contact with skin.
Acute toxicity (inhalation)	: Inhalation:dust,mist: Harmful if inhaled.
Skin corrosion/irritation	: Causes skin irritation.
Additional information	: Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Causes serious eye irritation.
Additional information	: Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Potential adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity	: Not classified
Chronic aquatic toxicity	: Not classified

12.2. Persistence and degradability

4-Chloro-3-cyanobenzotrifluoride (1735-54-2)

Persistence and degradability	No data available.
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12.3. Bioaccumulative potential

4-Chloro-3-cyanobenzotrifluoride (1735-54-2)

Bioaccumulative potential	No data available.
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12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

4-Chloro-3-cyanobenzotrifluoride (1735-54-2)

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

12.6. Other adverse effects

Additional information : Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations	: Dispose in a safe manner in accordance with local/national regulations.
Ecology - waste materials	: Avoid release to the environment. Hazardous waste due to toxicity.

SECTION 14: Transport information






In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
3439	3439	3439	3439	3439

4-Chloro-3-cyanobenzotrifluoride

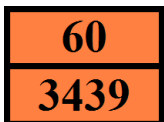
Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

14.2. UN proper shipping name				
NITRILES, SOLID, TOXIC, N.O.S.	NITRILES, SOLID, TOXIC, N.O.S.	Nitriles, toxic, solid, n.o.s.	NITRILES, SOLID, TOXIC, N.O.S.	NITRILES, SOLID, TOXIC, N.O.S.
Transport document description				
UN 3439 NITRILES, SOLID, TOXIC, N.O.S. (4-Chloro-3-cyanobenzotrifluoride), 6.1, III, (E)	UN 3439 NITRILES, SOLID, TOXIC, N.O.S. (4-Chloro-3-cyanobenzotrifluoride), 6.1, III	UN 3439 Nitriles, toxic, solid, n.o.s. (4-Chloro-3-cyanobenzotrifluoride), 6.1, III	UN 3439 NITRILES, SOLID, TOXIC, N.O.S. (4-Chloro-3-cyanobenzotrifluoride), 6.1, III	UN 3439 NITRILES, SOLID, TOXIC, N.O.S. (4-Chloro-3-cyanobenzotrifluoride), 6.1, III
14.3. Transport hazard class(es)				
6.1	6.1	6.1	6.1	6.1
				
14.4. Packing group				
III	III	III	III	III
14.5. Environmental hazards				
Dangerous for the environment : No	Dangerous for the environment : No Marine pollutant : No	Dangerous for the environment : No	Dangerous for the environment : No	Dangerous for the environment : No
No supplementary information available				

14.6. Special precautions for user

Overland transport

Classification code (ADR)	: T2
Special provisions (ADR)	: 274
Limited quantities (ADR)	: 5kg
Excepted quantities (ADR)	: E1
Packing instructions (ADR)	: P002, IBC08, LP02, R001
Special packing provisions (ADR)	: B3
Mixed packing provisions (ADR)	: MP10
Portable tank and bulk container instructions (ADR)	: T1
Portable tank and bulk container special provisions (ADR)	: TP33
Tank code (ADR)	: SGAH, L4BH
Tank special provisions (ADR)	: TU15, TE19
Vehicle for tank carriage	: AT
Transport category (ADR)	: 2
Special provisions for carriage - Bulk (ADR)	: VC1, VC2, AP7
Special provisions for carriage - Loading, unloading and handling (ADR)	: CV13, CV28
Special provisions for carriage - Operation (ADR)	: S9
Hazard identification number (Kemler No.)	: 60
Orange plates	: 

Tunnel restriction code (ADR) : E

Transport by sea

Special provisions (IMDG)	: 223, 274
Packing instructions (IMDG)	: P002, LP02
IBC packing instructions (IMDG)	: IBC08
IBC special provisions (IMDG)	: B3
Tank instructions (IMDG)	: T1
Tank special provisions (IMDG)	: TP33

4-Chloro-3-cyanobenzotrifluoride

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

EmS-No. (Fire)	: F-A
EmS-No. (Spillage)	: S-A
Stowage category (IMDG)	: A
Segregation (IMDG)	: SG35
Properties and observations (IMDG)	: Solid, evolving toxic vapours. Reacts with acids or acid fumes, evolving hydrogen cyanide, a highly toxic and flammable gas. Soluble in water. Toxic if swallowed, by skin contact or by inhalation.

Air transport

PCA Excepted quantities (IATA)	: E1
PCA Limited quantities (IATA)	: Y645
PCA limited quantity max net quantity (IATA)	: 10kg
PCA packing instructions (IATA)	: 670
PCA max net quantity (IATA)	: 100kg
CAO packing instructions (IATA)	: 677
CAO max net quantity (IATA)	: 200kg
Special provisions (IATA)	: A3, A5
ERG code (IATA)	: 6L

Inland waterway transport

Classification code (ADN)	: T2
Special provisions (ADN)	: 274, 802
Limited quantities (ADN)	: 5 kg
Excepted quantities (ADN)	: E1
Equipment required (ADN)	: PP, EP
Number of blue cones/lights (ADN)	: 0

Rail transport

Classification code (RID)	: T2
Special provisions (RID)	: 274
Excepted quantities (RID)	: E1
Packing instructions (RID)	: P002, IBC08, LP02, R001
Special packing provisions (RID)	: B3
Mixed packing provisions (RID)	: MP10
Portable tank and bulk container instructions (RID)	: T1
Portable tank and bulk container special provisions (RID)	: TP33
Tank codes for RID tanks (RID)	: SGAH, L4BH
Special provisions for RID tanks (RID)	: TU15
Transport category (RID)	: 2
Special provisions for carriage – Bulk (RID)	: VC1, VC2, AP7
Special provisions for carriage - Loading, unloading and handling (RID)	: CW13, CW28, CW31
Colis express (express parcels) (RID)	: CE11
Hazard identification number (RID)	: 60

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

Not applicable

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

No REACH Annex XVII restrictions
4-Chloro-3-cyanobenzotrifluoride is not on the REACH Candidate List
Directive 2012/18/EU (SEVESO III)

15.1.2. National regulations

No additional information available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out for the substance or the mixture by the supplier

4-Chloro-3-cyanobenzotrifluoride

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

SECTION 16: Other information

Data sources : 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, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Other information : None.

Full text of H- and EUH-statements:	
Acute Tox. 3 (Dermal)	Acute toxicity (dermal), Category 3
Acute Tox. 4 (Inhalation:dust,mist)	Acute toxicity (inhalation:dust,mist) Category 4
Acute Tox. 4 (Oral)	Acute toxicity (oral), Category 4
Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
Skin Irrit. 2	Skin corrosion/irritation, Category 2
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

SDS EU (REACH Annex II)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.