



3,5-Bis(trifluoromethyl)phenylacetonitrile

Apollo Scientific

Chemwatch Hazard Alert Code: 2

Part Number: PC3114G

Version No: 3.3

Safety Data Sheet

Issue Date: 29/06/2023

Print Date: 29/06/2023

S.GHS.GB-NIR.EN

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

Product Identifier

Product name	3,5-Bis(trifluoromethyl)phenylacetonitrile
Chemical Name	3,5-bis(trifluoromethyl)phenylacetonitrile
Synonyms	Not Available
Proper shipping name	NITRILES, LIQUID, TOXIC, N.O.S.
Chemical formula	C10-H5-F6-N
Other means of identification	Not Available
CAS number	85068-32-2*

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

Relevant identified uses	Not Available
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Details of the manufacturer or supplier of the safety data sheet

Registered company name	Apollo Scientific	Apollo Scientific Ltd
Address	Whitefield Road, Bredbury SK62QR United Kingdom	Whitefield Road, Bredbury SK6 2QR United Kingdom (NI)
Telephone	01614060505	+44(0) 161 406 0505
Fax	0161 406 0506	Not Available
Website	http://www.apolloscientific.co.uk/	apolloscientific.co.uk
Email	sales@apolloscientific.co.uk	sales@apolloscientific.co.uk

Emergency telephone number

Association / Organisation	Not Available
Emergency telephone numbers	Not Available
Other emergency telephone numbers	Not Available

SECTION 2 Hazards identification


Classification of the substance or mixture

Classification according to regulation (EC) No 1272/2008 [CLP] and amendments [1]	H312 - Acute Toxicity (Dermal) Category 4, H332 - Acute Toxicity (Inhalation) Category 4, H335 - Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3, H302 - Acute Toxicity (Oral) Category 4, H315 - Skin Corrosion/Irritation Category 2, H319 - Serious Eye Damage/Eye Irritation Category 2
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3,5-Bis(trifluoromethyl)phenylacetonitrile

Legend: 1. Classified by Chemwatch; 2. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI

Label elements

Hazard pictogram(s)	
Signal word	Warning

Hazard statement(s)

H312	Harmful in contact with skin.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.

Precautionary statement(s) Prevention

P271	Use only outdoors or in a well-ventilated area.
P261	Avoid breathing mist/vapours/spray.
P264	Wash all exposed external body areas thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P280	Wear protective gloves, protective clothing, eye protection and face protection.

Precautionary statement(s) Response

P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313	If eye irritation persists: Get medical advice/attention.
P301+P312	IF SWALLOWED: Call a POISON CENTER/doctor/physician/first aider if you feel unwell.
P302+P352	IF ON SKIN: Wash with plenty of water.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P330	Rinse mouth.
P332+P313	If skin irritation occurs: Get medical advice/attention.
P362+P364	Take off contaminated clothing and wash it before reuse.

Precautionary statement(s) Storage

P405	Store locked up.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.

Precautionary statement(s) Disposal

P501	Dispose of contents/container to authorised hazardous or special waste collection point in accordance with any local regulation.
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SECTION 3 Composition / information on ingredients

Substances

CAS No	%[weight]	Name	Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	SCL / M-Factor
85068-32-2*	100	<u>3,5-Bis(trifluoromethyl)phenylacetonitrile</u>	Acute Toxicity (Dermal) Category 4, Acute Toxicity (Inhalation) Category 4, Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3 , Acute Toxicity (Oral) Category 4, Skin Corrosion/Irritation Category 2, Serious Eye Damage/Eye Irritation Category 2; H312, H332, H335, H302, H315, H319 [1]	Not Available

3,5-Bis(trifluoromethyl)phenylacetonitrile

Legend: 1. Classified by Chemwatch; 2. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI; 3. Classification drawn from C&L; * EU IOELVs available; [e] Substance identified as having endocrine disrupting properties

Mixtures

See section above for composition of Substances

SECTION 4 First aid measures

Description of first aid measures

Eye Contact	<p>If this product comes in contact with the eyes:</p> <ul style="list-style-type: none"> ▶ Wash out immediately with fresh running water. ▶ Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids. ▶ Seek medical attention without delay; if pain persists or recurs seek medical attention. ▶ Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.
Skin Contact	<p>If skin or hair contact occurs:</p> <ul style="list-style-type: none"> ▶ Flush skin and hair with running water (and soap if available). ▶ Seek medical attention in event of irritation.
Inhalation	<ul style="list-style-type: none"> ▶ If fumes or combustion products are inhaled remove from contaminated area. ▶ Lay patient down. Keep warm and rested. ▶ Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures. ▶ Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary. ▶ Transport to hospital, or doctor.
Ingestion	<ul style="list-style-type: none"> ▶ If swallowed do NOT induce vomiting. ▶ If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration. ▶ Observe the patient carefully. ▶ Never give liquid to a person showing signs of being sleepy or with reduced awareness; i.e. becoming unconscious. ▶ Give water to rinse out mouth, then provide liquid slowly and as much as casualty can comfortably drink. ▶ Seek medical advice.

Indication of any immediate medical attention and special treatment needed

As in all cases of suspected poisoning, follow the ABCDEs of emergency medicine (airway, breathing, circulation, disability, exposure), then the ABCDEs of toxicology (antidotes, basics, change absorption, change distribution, change elimination).

For poisons (where specific treatment regime is absent):

BASIC TREATMENT

- ▶ Establish a patent airway with suction where necessary.
- ▶ Watch for signs of respiratory insufficiency and assist ventilation as necessary.
- ▶ Administer oxygen by non-rebreather mask at 10 to 15 L/min.
- ▶ Monitor and treat, where necessary, for pulmonary oedema.
- ▶ Monitor and treat, where necessary, for shock.
- ▶ Anticipate seizures.
- ▶ **DO NOT** use emetics. Where ingestion is suspected rinse mouth and give up to 200 ml water (5 ml/kg recommended) for dilution where patient is able to swallow, has a strong gag reflex and does not drool.

ADVANCED TREATMENT

- ▶ Consider orotracheal or nasotracheal intubation for airway control in unconscious patient or where respiratory arrest has occurred.
- ▶ Positive-pressure ventilation using a bag-valve mask might be of use.
- ▶ Monitor and treat, where necessary, for arrhythmias.
- ▶ Start an IV D5W TKO. If signs of hypovolaemia are present use lactated Ringers solution. Fluid overload might create complications.
- ▶ Drug therapy should be considered for pulmonary oedema.
- ▶ Hypotension with signs of hypovolaemia requires the cautious administration of fluids. Fluid overload might create complications.
- ▶ Treat seizures with diazepam.
- ▶ Proparacaine hydrochloride should be used to assist eye irrigation.

BRONSTEIN, A.C. and CURRANCE, P.L.

EMERGENCY CARE FOR HAZARDOUS MATERIALS EXPOSURE: 2nd Ed. 1994

SECTION 5 Firefighting measures

3,5-Bis(trifluoromethyl)phenylacetonitrile

Extinguishing media

- There is no restriction on the type of extinguisher which may be used.
- Use extinguishing media suitable for surrounding area.

Special hazards arising from the substrate or mixture

Fire Incompatibility	None known.
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Advice for firefighters

Fire Fighting	<ul style="list-style-type: none">▸ Alert Fire Brigade and tell them location and nature of hazard.▸ Wear breathing apparatus plus protective gloves in the event of a fire.▸ Prevent, by any means available, spillage from entering drains or water courses.▸ Use fire fighting procedures suitable for surrounding area.▸ DO NOT approach containers suspected to be hot.▸ Cool fire exposed containers with water spray from a protected location.▸ If safe to do so, remove containers from path of fire.▸ Equipment should be thoroughly decontaminated after use.
Fire/Explosion Hazard	<ul style="list-style-type: none">▸ Non combustible.▸ Not considered a significant fire risk, however containers may burn. May emit poisonous fumes.

SECTION 6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

See section 8

Environmental precautions

See section 12

Methods and material for containment and cleaning up

Minor Spills	<ul style="list-style-type: none">▸ Clean up all spills immediately.▸ Avoid breathing vapours and contact with skin and eyes.▸ Control personal contact with the substance, by using protective equipment.▸ Contain and absorb spill with sand, earth, inert material or vermiculite.▸ Wipe up.▸ Place in a suitable, labelled container for waste disposal.
Major Spills	<ul style="list-style-type: none">▸ Clear area of personnel and move upwind.▸ Alert Fire Brigade and tell them location and nature of hazard.▸ Wear breathing apparatus plus protective gloves.▸ Prevent, by any means available, spillage from entering drains or water course.▸ Stop leak if safe to do so.▸ Contain spill with sand, earth or vermiculite.▸ Collect recoverable product into labelled containers for recycling.▸ Neutralise/decontaminate residue (see Section 13 for specific agent).▸ Collect solid residues and seal in labelled drums for disposal.▸ Wash area and prevent runoff into drains.▸ After clean up operations, decontaminate and launder all protective clothing and equipment before storing and re-using.▸ If contamination of drains or waterways occurs, advise emergency services.

Personal Protective Equipment advice is contained in Section 8 of the SDS.

SECTION 7 Handling and storage

Precautions for safe handling

Safe handling	<ul style="list-style-type: none">▸ Avoid all personal contact, including inhalation.▸ Wear protective clothing when risk of exposure occurs.▸ Use in a well-ventilated area.▸ Prevent concentration in hollows and sumps.▸ DO NOT enter confined spaces until atmosphere has been checked.▸ DO NOT allow material to contact humans, exposed food or food utensils.▸ Avoid contact with incompatible materials.▸ When handling, DO NOT eat, drink or smoke.
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3,5-Bis(trifluoromethyl)phenylacetonitrile

	<ul style="list-style-type: none"> ▶ Keep containers securely sealed when not in use. ▶ Avoid physical damage to containers. ▶ Always wash hands with soap and water after handling. ▶ Work clothes should be laundered separately. Launder contaminated clothing before re-use. ▶ Use good occupational work practice. ▶ Observe manufacturer's storage and handling recommendations contained within this SDS. ▶ Atmosphere should be regularly checked against established exposure standards to ensure safe working conditions are maintained.
Other information	<ul style="list-style-type: none"> ▶ Store in original containers. ▶ Keep containers securely sealed. ▶ Store in a cool, dry, well-ventilated area. ▶ Store away from incompatible materials and foodstuff containers. ▶ Protect containers against physical damage and check regularly for leaks. ▶ Observe manufacturer's storage and handling recommendations contained within this SDS.

Conditions for safe storage, including any incompatibilities

Suitable container	<ul style="list-style-type: none"> ▶ Lined metal can, lined metal pail/ can. ▶ Plastic pail. ▶ Polyliner drum. ▶ Packing as recommended by manufacturer. ▶ Check all containers are clearly labelled and free from leaks. <p>For low viscosity materials</p> <ul style="list-style-type: none"> ▶ Drums and jerricans must be of the non-removable head type. ▶ Where a can is to be used as an inner package, the can must have a screwed enclosure. <p>For materials with a viscosity of at least 2680 cSt. (23 deg. C) and solids (between 15 C deg. and 40 deg C.):</p> <ul style="list-style-type: none"> ▶ Removable head packaging; ▶ Cans with friction closures and ▶ low pressure tubes and cartridges <p>may be used.</p> <p>-</p> <p>Where combination packages are used, and the inner packages are of glass, there must be sufficient inert cushioning material in contact with inner and outer packages *.</p> <p>-</p> <p>In addition, where inner packagings are glass and contain liquids of packing group I and II there must be sufficient inert absorbent to absorb any spillage *.</p> <p>-</p> <p>* unless the outer packaging is a close fitting moulded plastic box and the substances are not incompatible with the plastic.</p>
Storage incompatibility	<p>None known</p> <ul style="list-style-type: none"> ▶ Nitriles may polymerise in the presence of metals and some metal compounds. ▶ They are incompatible with acids; mixing nitriles with strong oxidising acids can lead to extremely violent reactions. ▶ Nitriles are generally incompatible with other oxidising agents such as peroxides and epoxides. ▶ The combination of bases and nitriles can produce hydrogen cyanide. Nitriles are hydrolysed exothermally in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids). ▶ Nitriles can react vigorously with reducing agents. ▶ The covalent cyano group is endothermic and many organic nitriles are reactive under certain conditions; N-cyano derivatives are reactive or unstable. ▶ The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation. ▶ Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds. <p>BREThERICK L.: Handbook of Reactive Chemical Hazards</p>

SECTION 8 Exposure controls / personal protection

Control parameters

Occupational Exposure Limits (OEL)

INGREDIENT DATA

Not Available

Emergency Limits

Ingredient	TEEL-1	TEEL-2	TEEL-3
3,5-Bis(trifluoromethyl)phenylacetonitrile	Not Available	Not Available	Not Available

Ingredient	Original IDLH	Revised IDLH

3,5-Bis(trifluoromethyl)phenylacetonitrile

Ingredient	Original IDLH	Revised IDLH
3,5-Bis(trifluoromethyl)phenylacetonitrile	Not Available	Not Available

Occupational Exposure Banding

Ingredient	Occupational Exposure Band Rating	Occupational Exposure Band Limit
3,5-Bis(trifluoromethyl)phenylacetonitrile	E	≤ 0.1 ppm

Notes:

Occupational exposure banding is a process of assigning chemicals into specific categories or bands based on a chemical's potency and the adverse health outcomes associated with exposure. The output of this process is an occupational exposure band (OEB), which corresponds to a range of exposure concentrations that are expected to protect worker health.

Exposure controls

Appropriate engineering controls	<p>Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.</p> <p>The basic types of engineering controls are:</p> <p>Process controls which involve changing the way a job activity or process is done to reduce the risk.</p> <p>Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment. Ventilation can remove or dilute an air contaminant if designed properly. The design of a ventilation system must match the particular process and chemical or contaminant in use. Employers may need to use multiple types of controls to prevent employee overexposure.</p> <p>Local exhaust ventilation usually required. If risk of overexposure exists, wear approved respirator. Correct fit is essential to obtain adequate protection. Supplied-air type respirator may be required in special circumstances. Correct fit is essential to ensure adequate protection.</p> <p>An approved self contained breathing apparatus (SCBA) may be required in some situations.</p> <p>Provide adequate ventilation in warehouse or closed storage area. Air contaminants generated in the workplace possess varying "escape" velocities which, in turn, determine the "capture velocities" of fresh circulating air required to effectively remove the contaminant.</p>										
	<table border="1"> <thead> <tr> <th>Type of Contaminant:</th> <th>Air Speed:</th> </tr> </thead> <tbody> <tr> <td>solvent, vapours, degreasing etc., evaporating from tank (in still air).</td> <td>0.25-0.5 m/s (50-100 f/min.)</td> </tr> <tr> <td>aerosols, fumes from pouring operations, intermittent container filling, low speed conveyer transfers, welding, spray drift, plating acid fumes, pickling (released at low velocity into zone of active generation)</td> <td>0.5-1 m/s (100-200 f/min.)</td> </tr> <tr> <td>direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)</td> <td>1-2.5 m/s (200-500 f/min.)</td> </tr> <tr> <td>grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).</td> <td>2.5-10 m/s (500-2000 f/min.)</td> </tr> </tbody> </table>	Type of Contaminant:	Air Speed:	solvent, vapours, degreasing etc., evaporating from tank (in still air).	0.25-0.5 m/s (50-100 f/min.)	aerosols, fumes from pouring operations, intermittent container filling, low speed conveyer transfers, welding, spray drift, plating acid fumes, pickling (released at low velocity into zone of active generation)	0.5-1 m/s (100-200 f/min.)	direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)	1-2.5 m/s (200-500 f/min.)	grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).	2.5-10 m/s (500-2000 f/min.)
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<p>Within each range the appropriate value depends on:</p> <table border="1"> <thead> <tr> <th>Lower end of the range</th> <th>Upper end of the range</th> </tr> </thead> <tbody> <tr> <td>1: Room air currents minimal or favourable to capture</td> <td>1: Disturbing room air currents</td> </tr> <tr> <td>2: Contaminants of low toxicity or of nuisance value only.</td> <td>2: Contaminants of high toxicity</td> </tr> <tr> <td>3: Intermittent, low production.</td> <td>3: High production, heavy use</td> </tr> <tr> <td>4: Large hood or large air mass in motion</td> <td>4: Small hood-local control only</td> </tr> </tbody> </table>	Lower end of the range	Upper end of the range	1: Room air currents minimal or favourable to capture	1: Disturbing room air currents	2: Contaminants of low toxicity or of nuisance value only.	2: Contaminants of high toxicity	3: Intermittent, low production.	3: High production, heavy use	4: Large hood or large air mass in motion	4: Small hood-local control only	
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<p>Simple theory shows that air velocity falls rapidly with distance away from the opening of a simple extraction pipe. Velocity generally decreases with the square of distance from the extraction point (in simple cases). Therefore the air speed at the extraction point should be adjusted, accordingly, after reference to distance from the contaminating source. The air velocity at the extraction fan, for example, should be a minimum of 1-2 m/s (200-400 f/min) for extraction of solvents generated in a tank 2 meters distant from the extraction point. Other mechanical considerations, producing performance deficits within the extraction apparatus, make it essential that theoretical air velocities are multiplied by factors of 10 or more when extraction systems are installed or used.</p>											

Individual protection measures, such as personal protective equipment



Eye and face protection

- ▶ Safety glasses with side shields.
- ▶ Chemical goggles. [AS/NZS 1337.1, EN166 or national equivalent]
- ▶ Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lenses or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience.

3,5-Bis(trifluoromethyl)phenylacetonitrile

	Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59].
Skin protection	See Hand protection below
Hands/feet protection	<p>The selection of suitable gloves does not only depend on the material, but also on further marks of quality which vary from manufacturer to manufacturer. Where the chemical is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.</p> <p>The exact break through time for substances has to be obtained from the manufacturer of the protective gloves and has to be observed when making a final choice.</p> <p>Personal hygiene is a key element of effective hand care. Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.</p> <p>Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include:</p> <ul style="list-style-type: none"> - frequency and duration of contact, - chemical resistance of glove material, - glove thickness and - dexterity <p>Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739, AS/NZS 2161.1 or national equivalent).</p> <ul style="list-style-type: none"> - When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374, AS/NZS 2161.10.1 or national equivalent) is recommended. - When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374, AS/NZS 2161.10.1 or national equivalent) is recommended. - Some glove polymer types are less affected by movement and this should be taken into account when considering gloves for long-term use. - Contaminated gloves should be replaced. <p>As defined in ASTM F-739-96 in any application, gloves are rated as:</p> <ul style="list-style-type: none"> - Excellent when breakthrough time > 480 min - Good when breakthrough time > 20 min - Fair when breakthrough time < 20 min - Poor when glove material degrades <p>For general applications, gloves with a thickness typically greater than 0.35 mm, are recommended.</p> <p>It should be emphasised that glove thickness is not necessarily a good predictor of glove resistance to a specific chemical, as the permeation efficiency of the glove will be dependent on the exact composition of the glove material. Therefore, glove selection should also be based on consideration of the task requirements and knowledge of breakthrough times.</p> <p>Glove thickness may also vary depending on the glove manufacturer, the glove type and the glove model. Therefore, the manufacturers technical data should always be taken into account to ensure selection of the most appropriate glove for the task.</p> <p>Note: Depending on the activity being conducted, gloves of varying thickness may be required for specific tasks. For example:</p> <ul style="list-style-type: none"> - Thinner gloves (down to 0.1 mm or less) may be required where a high degree of manual dexterity is needed. However, these gloves are only likely to give short duration protection and would normally be just for single use applications, then disposed of. - Thicker gloves (up to 3 mm or more) may be required where there is a mechanical (as well as a chemical) risk i.e. where there is abrasion or puncture potential <p>Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.</p> <ul style="list-style-type: none"> ▸ Wear chemical protective gloves, e.g. PVC. ▸ Wear safety footwear or safety gumboots, e.g. Rubber
Body protection	See Other protection below
Other protection	<ul style="list-style-type: none"> ▸ Overalls. ▸ Eyewash unit. ▸ Barrier cream. ▸ Skin cleansing cream.

SECTION 9 Physical and chemical properties

Information on basic physical and chemical properties

Appearance	Not Available		
Physical state	Liquid	Relative density (Water = 1)	Not Available
Odour	Not Available	Partition coefficient n-octanol / water	Not Available
Odour threshold	Not Available	Auto-ignition temperature (°C)	Not Available
pH (as supplied)	Not Available	Decomposition temperature (°C)	Not Available

3,5-Bis(trifluoromethyl)phenylacetonitrile

Melting point / freezing point (°C)	Not Available	Viscosity (cSt)	Not Available
Initial boiling point and boiling range (°C)	Not Available	Molecular weight (g/mol)	Not Available
Flash point (°C)	Not Available	Taste	Not Available
Evaporation rate	Not Available	Explosive properties	Not Available
Flammability	Not Available	Oxidising properties	Not Available
Upper Explosive Limit (%)	Not Available	Surface Tension (dyn/cm or mN/m)	Not Available
Lower Explosive Limit (%)	Not Available	Volatile Component (%vol)	Not Available
Vapour pressure (kPa)	Not Available	Gas group	Not Available
Solubility in water	Not Available	pH as a solution (1%)	Not Available
Vapour density (Air = 1)	Not Available	VOC g/L	Not Available

SECTION 10 Stability and reactivity

Reactivity	See section 7
Chemical stability	<ul style="list-style-type: none"> ▶ Unstable in the presence of incompatible materials. ▶ Product is considered stable. ▶ Hazardous polymerisation will not occur.
Possibility of hazardous reactions	See section 7
Conditions to avoid	See section 7
Incompatible materials	See section 7
Hazardous decomposition products	See section 5

SECTION 11 Toxicological information

Information on toxicological effects

Inhaled	<p>The material is not thought to produce respiratory irritation (as classified by EC Directives using animal models). Nevertheless inhalation of vapours, fumes or aerosols, especially for prolonged periods, may produce respiratory discomfort and occasionally, distress.</p> <p>Inhalation of vapours or aerosols (mists, fumes), generated by the material during the course of normal handling, may be damaging to the health of the individual.</p>
Ingestion	<p>Accidental ingestion of the material may be damaging to the health of the individual.</p> <p>Nitrile poisoning exhibits similar symptoms to poisoning due to hydrogen cyanide. The substances irritate the eyes and skin, and are absorbed quickly and completely through the skin.</p>
Skin Contact	<p>The material is not thought to produce adverse health effects or skin irritation following contact (as classified by EC Directives using animal models). Nevertheless, good hygiene practice requires that exposure be kept to a minimum and that suitable gloves be used in an occupational setting.</p> <p>Open cuts, abraded or irritated skin should not be exposed to this material</p> <p>Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.</p>
Eye	This material can cause eye irritation and damage in some persons.
Chronic	Long-term exposure to the product is not thought to produce chronic effects adverse to the health (as classified by EC Directives using animal models); nevertheless exposure by all routes should be minimised as a matter of course.
Legend:	1. Value obtained from Europe ECHA Registered Substances - Acute toxicity 2. Value obtained from manufacturer's SDS. Unless otherwise specified data extracted from RTECS - Register of Toxic Effect of chemical Substances

3,5-Bis(trifluoromethyl)phenylacetone nitrile

Acute Toxicity	✓	Carcinogenicity	✗
Skin Irritation/Corrosion	✓	Reproductivity	✗
Serious Eye Damage/Irritation	✓	STOT - Single Exposure	✓
Respiratory or Skin sensitisation	✗	STOT - Repeated Exposure	✗
Mutagenicity	✗	Aspiration Hazard	✗

Legend: ✗ – Data either not available or does not fill the criteria for classification
 ✓ – Data available to make classification

SECTION 12 Ecological information

Toxicity

Legend:	Extracted from 1. IUCLID Toxicity Data 2. Europe ECHA Registered Substances - Ecotoxicological Information - Aquatic Toxicity 4. US EPA, Ecotox database - Aquatic Toxicity Data 5. ECETOC Aquatic Hazard Assessment Data 6. NITE (Japan) - Bioconcentration Data 7. METI (Japan) - Bioconcentration Data 8. Vendor Data
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DO NOT discharge into sewer or waterways.

Persistence and degradability

Ingredient	Persistence: Water/Soil	Persistence: Air
3,5-Bis(trifluoromethyl)phenylacetone nitrile	HIGH	HIGH

Bioaccumulative potential

Ingredient	Bioaccumulation
3,5-Bis(trifluoromethyl)phenylacetone nitrile	LOW (LogKOW = 3.4883)

Mobility in soil

Ingredient	Mobility
3,5-Bis(trifluoromethyl)phenylacetone nitrile	LOW (KOC = 9218)

SECTION 13 Disposal considerations

Waste treatment methods

Product / Packaging disposal	<p>Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.</p> <p>A Hierarchy of Controls seems to be common - the user should investigate:</p> <ul style="list-style-type: none"> ▶ Reduction ▶ Reuse ▶ Recycling ▶ Disposal (if all else fails) <p>This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.</p> <ul style="list-style-type: none"> ▶ DO NOT allow wash water from cleaning or process equipment to enter drains. ▶ It may be necessary to collect all wash water for treatment before disposal. ▶ In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first. ▶ Where in doubt contact the responsible authority.
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SECTION 14 Transport information

Labels Required

3,5-Bis(trifluoromethyl)phenylacetonitrile

Marine Pollutant	NO

Land transport (ADR-RID)

UN number or ID number	3276	
UN proper shipping name	NITRILES, LIQUID, TOXIC, N.O.S.	
Transport hazard class(es)	Class	6.1
	Subsidiary risk	Not Applicable
Packing group	III	
Environmental hazard	Not Applicable	
Special precautions for user	Hazard identification (Kemler)	60
	Classification code	T1
	Hazard Label	6.1
	Special provisions	274
	Limited quantity	5 L
	Tunnel Restriction Code	2 (E)

Air transport (ICAO-IATA / DGR)

UN number	3276	
UN proper shipping name	Nitriles, liquid, toxic, n.o.s. *	
Transport hazard class(es)	ICAO/IATA Class	6.1
	ICAO / IATA Subrisk	Not Applicable
	ERG Code	6L
Packing group	III	
Environmental hazard	Not Applicable	
Special precautions for user	Special provisions	A3 A4 A137
	Cargo Only Packing Instructions	663
	Cargo Only Maximum Qty / Pack	220 L
	Passenger and Cargo Packing Instructions	655
	Passenger and Cargo Maximum Qty / Pack	60 L
	Passenger and Cargo Limited Quantity Packing Instructions	Y642
	Passenger and Cargo Limited Maximum Qty / Pack	2 L

Sea transport (IMDG-Code / GGVSee)

UN number	3276	
UN proper shipping name	NITRILES, LIQUID, TOXIC, N.O.S.	
Transport hazard class(es)	IMDG Class	6.1
	IMDG Subrisk	Not Applicable
Packing group	III	
Environmental hazard	Not Applicable	
Special precautions for user	EMS Number	F-A, S-A
	Special provisions	223 274
	Limited Quantities	5 L

Inland waterways transport (ADN)

3,5-Bis(trifluoromethyl)phenylacetonitrile

UN number	3276	
UN proper shipping name	NITRILES, LIQUID, TOXIC, N.O.S.	
Transport hazard class(es)	6.1	Not Applicable
Packing group	III	
Environmental hazard	Not Applicable	
Special precautions for user	Classification code	T1
	Special provisions	274; 802
	Limited quantity	5 L
	Equipment required	PP, EP, TOX, A
	Fire cones number	0

Transport in bulk according to Annex II of MARPOL and the IBC code

Not Applicable

Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

Product name	Group
3,5-Bis(trifluoromethyl)phenylacetonitrile	Not Available

Transport in bulk in accordance with the IGC Code

Product name	Ship Type
3,5-Bis(trifluoromethyl)phenylacetonitrile	Not Available

SECTION 15 Regulatory information

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

3,5-Bis(trifluoromethyl)phenylacetonitrile is found on the following regulatory lists

Europe EC Inventory

European Union - European Inventory of Existing Commercial Chemical Substances (EINECS)

National Inventory Status

National Inventory	Status
Australia - AIIIC / Australia Non-Industrial Use	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Canada - DSL	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Canada - NDSL	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
China - IECSC	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Europe - EINEC / ELINCS / NLP	Yes
Japan - ENCS	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Korea - KECI	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
New Zealand - NZIoC	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Philippines - PICCS	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
USA - TSCA	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Taiwan - TCSI	Yes
Mexico - INSQ	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Vietnam - NCI	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Russia - FBEPH	No (3,5-Bis(trifluoromethyl)phenylacetonitrile)
Legend:	Yes = All CAS declared ingredients are on the inventory No = One or more of the CAS listed ingredients are not on the inventory. These ingredients may be exempt or will require registration.

SECTION 16 Other information

3,5-Bis(trifluoromethyl)phenylacetonitrile

Revision Date	29/06/2023
Initial Date	30/06/2023

SDS Version Summary

Version	Date of Update	Sections Updated
2.3	29/06/2023	Korean MSDS Number, Identification of the substance / mixture and of the company / undertaking - Supplier Information

Other information

Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

The SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

For detailed advice on Personal Protective Equipment, refer to the following EU CEN Standards:

EN 166 Personal eye-protection

EN 340 Protective clothing

EN 374 Protective gloves against chemicals and micro-organisms

EN 13832 Footwear protecting against chemicals

EN 133 Respiratory protective devices

Definitions and abbreviations

PC - TWA: Permissible Concentration-Time Weighted Average

PC - STEL: Permissible Concentration-Short Term Exposure Limit

IARC: International Agency for Research on Cancer

ACGIH: American Conference of Governmental Industrial Hygienists

STEL: Short Term Exposure Limit

TEEL: Temporary Emergency Exposure Limit,

IDLH: Immediately Dangerous to Life or Health Concentrations

ES: Exposure Standard

OSF: Odour Safety Factor

NOAEL :No Observed Adverse Effect Level

LOAEL: Lowest Observed Adverse Effect Level

TLV: Threshold Limit Value

LOD: Limit Of Detection

OTV: Odour Threshold Value

BCF: BioConcentration Factors

BEI: Biological Exposure Index

AIIC: Australian Inventory of Industrial Chemicals

DSL: Domestic Substances List

NDSL: Non-Domestic Substances List

IECSC: Inventory of Existing Chemical Substance in China

EINECS: European INventory of Existing Commercial chemical Substances

ELINCS: European List of Notified Chemical Substances

NLP: No-Longer Polymers

ENCS: Existing and New Chemical Substances Inventory

KECI: Korea Existing Chemicals Inventory

NZIoC: New Zealand Inventory of Chemicals

PICCS: Philippine Inventory of Chemicals and Chemical Substances

TSCA: Toxic Substances Control Act

TCSI: Taiwan Chemical Substance Inventory

INSQ: Inventario Nacional de Sustancias Químicas

NCI: National Chemical Inventory

FBEPH: Russian Register of Potentially Hazardous Chemical and Biological Substances

Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]

Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	Classification Procedure
Acute Toxicity (Dermal) Category 4, H312	Expert judgement
Acute Toxicity (Inhalation) Category 4, H332	Expert judgement

3,5-Bis(trifluoromethyl)phenylacetonitrile

Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	Classification Procedure
Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3 , H335	Expert judgement
Acute Toxicity (Oral) Category 4, H302	Expert judgement
Skin Corrosion/Irritation Category 2, H315	Expert judgement
Serious Eye Damage/Eye Irritation Category 2, H319	Expert judgement

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