



## 3,5-Bis(trifluoromethyl)phenyl isocyanate

### Apollo Scientific

Chemwatch Hazard Alert Code: 2

Part Number: PC3115A

Version No: 3.2

Safety Data Sheet

Issue Date: 29/06/2023

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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)phenyl isocyanate
Chemical Name	3,5-bis(trifluoromethyl)phenyl isocyanate
Synonyms	Not Available
Proper shipping name	ISOCYANATES, TOXIC, N.O.S. or ISOCYANATE SOLUTION, TOXIC, N.O.S.
Other means of identification	Not Available
CAS number	16588-74-2*

##### 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	<a href="http://www.apolloscientific.co.uk/">http://www.apolloscientific.co.uk/</a>	<a href="http://apolloscientific.co.uk">apolloscientific.co.uk</a>
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
Legend:	1. Classified by Chemwatch; 2. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI

**3,5-Bis(trifluoromethyl)phenyl isocyanate**

**Label elements**

<b>Hazard pictogram(s)</b>	
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<b>Signal word</b>	<b>Warning</b>
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**Hazard statement(s)**

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

**Precautionary statement(s) Prevention**

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

**Precautionary statement(s) Response**

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

**Precautionary statement(s) Storage**

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

**Precautionary statement(s) Disposal**

<b>P501</b>	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
16588-74-2*	100	<u>3,5-Bis(trifluoromethyl)phenyl isocyanate</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 <sup>[1]</sup>	Not Available

**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**

3,5-Bis(trifluoromethyl)phenyl isocyanate

See section above for composition of Substances

**SECTION 4 First aid measures**

**Description of first aid measures**

<b>Eye Contact</b>	<p>If this product comes in contact with the eyes:</p> <ul style="list-style-type: none"><li>▶ Wash out immediately with fresh running water.</li><li>▶ 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.</li><li>▶ Seek medical attention without delay; if pain persists or recurs seek medical attention.</li><li>▶ Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.</li></ul>
<b>Skin Contact</b>	<p>If skin contact occurs:</p> <ul style="list-style-type: none"><li>▶ Immediately remove all contaminated clothing, including footwear.</li><li>▶ Flush skin and hair with running water (and soap if available).</li><li>▶ Seek medical attention in event of irritation.</li></ul>
<b>Inhalation</b>	<ul style="list-style-type: none"><li>▶ If fumes or combustion products are inhaled remove from contaminated area.</li><li>▶ Lay patient down. Keep warm and rested.</li><li>▶ Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.</li><li>▶ 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.</li><li>▶ Transport to hospital, or doctor.</li></ul>
<b>Ingestion</b>	<ul style="list-style-type: none"><li>▶ <b>IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY.</b></li><li>▶ For advice, contact a Poisons Information Centre or a doctor.</li><li>▶ Urgent hospital treatment is likely to be needed.</li><li>▶ In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition.</li><li>▶ If the services of a medical officer or medical doctor are readily available, the patient should be placed in his/her care and a copy of the SDS should be provided. Further action will be the responsibility of the medical specialist.</li><li>▶ If medical attention is not available on the worksite or surroundings send the patient to a hospital together with a copy of the SDS.</li></ul> <p><b>Where medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed otherwise:</b></p> <ul style="list-style-type: none"><li>▶ <b>INDUCE</b> vomiting with fingers down the back of the throat, <b>ONLY IF CONSCIOUS</b>. Lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.</li></ul> <p><b>NOTE:</b> Wear a protective glove when inducing vomiting by mechanical means.</p>

**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.

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BRONSTEIN, A.C. and CURRANCE, P.L.  
EMERGENCY CARE FOR HAZARDOUS MATERIALS EXPOSURE: 2nd Ed. 1994

## SECTION 5 Firefighting measures

### 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

<b>Fire Incompatibility</b>	None known.
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### Advice for firefighters

<b>Fire Fighting</b>	<ul style="list-style-type: none"><li>▸ Alert Fire Brigade and tell them location and nature of hazard.</li><li>▸ Wear breathing apparatus plus protective gloves in the event of a fire.</li><li>▸ Prevent, by any means available, spillage from entering drains or water courses.</li><li>▸ Use fire fighting procedures suitable for surrounding area.</li><li>▸ <b>DO NOT</b> approach containers suspected to be hot.</li><li>▸ Cool fire exposed containers with water spray from a protected location.</li><li>▸ If safe to do so, remove containers from path of fire.</li><li>▸ Equipment should be thoroughly decontaminated after use.</li></ul>
<b>Fire/Explosion Hazard</b>	<ul style="list-style-type: none"><li>- Combustible.</li><li>- Moderate fire hazard when exposed to heat or flame.</li><li>- When heated to high temperatures decomposes rapidly generating vapour which pressures and may then rupture containers with release of flammable and highly toxic isocyanate vapour.</li><li>- Burns with acrid black smoke and poisonous fumes.</li><li>- Due to reaction with water producing CO<sub>2</sub>-gas, a hazardous build-up of pressure could result if contaminated containers are re-sealed.</li><li>- Combustion yields traces of highly toxic hydrogen cyanide HCN, plus toxic nitrogen oxides NO<sub>x</sub> and carbon monoxide.</li></ul> Decomposition may produce toxic fumes of: nitrogen oxides (NO <sub>x</sub> )

## 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

<b>Minor Spills</b>	<ul style="list-style-type: none"><li>▸ Clean up all spills immediately.</li><li>▸ Avoid breathing vapours and contact with skin and eyes.</li><li>▸ Control personal contact with the substance, by using protective equipment.</li><li>▸ Contain and absorb spill with sand, earth, inert material or vermiculite.</li><li>▸ Wipe up.</li><li>▸ Place in a suitable, labelled container for waste disposal.</li></ul>
<b>Major Spills</b>	<ul style="list-style-type: none"><li>▸ Clear area of personnel and move upwind.</li><li>▸ Alert Fire Brigade and tell them location and nature of hazard.</li><li>▸ Wear breathing apparatus plus protective gloves.</li><li>▸ Prevent, by any means available, spillage from entering drains or water course.</li><li>▸ Stop leak if safe to do so.</li><li>▸ Contain spill with sand, earth or vermiculite.</li><li>▸ Collect recoverable product into labelled containers for recycling.</li><li>▸ Neutralise/decontaminate residue (see Section 13 for specific agent).</li><li>▸ Collect solid residues and seal in labelled drums for disposal.</li><li>▸ Wash area and prevent runoff into drains.</li><li>▸ After clean up operations, decontaminate and launder all protective clothing and equipment before storing and re-using.</li><li>▸ If contamination of drains or waterways occurs, advise emergency services.</li></ul> For isocyanate spills of less than 40 litres (2 m <sup>2</sup> ): <ul style="list-style-type: none"><li>▸ Evacuate area from everybody not dealing with the emergency, keep them upwind and prevent further access, remove ignition sources and, if inside building, ventilate area as well as possible.</li><li>▸ Notify supervision and others as necessary.</li></ul>

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- ▶ Put on personal protective equipment (suitable respiratory protection, face and eye protection, protective suit, gloves and impermeable boots).
- ▶ Control source of leakage (where applicable).
- ▶ Dike the spill to prevent spreading and to contain additions of decontaminating solution.
- ▶ Prevent the material from entering drains.
- ▶ Estimate spill pool volume or area.
- ▶ Absorb and decontaminate. - Completely cover the spill with wet sand, wet earth, vermiculite or other similar absorbent. - Add neutraliser (for suitable formulations: see below) to the adsorbent materials (equal to that of estimated spill pool volume). Intensify contact between spill, absorbent and neutraliser by carefully mixing with a rake and allow to react for 15 minutes
- ▶ Shovel absorbent/decontaminant solution mixture into a steel drum.
- ▶ Decontaminate surface. - Pour an equal amount of neutraliser solution over contaminated surface. - Scrub area with a stiff bristle brush, using moderate pressure. - Completely cover decontaminant with vermiculite or other similar absorbent. - After 5 minutes, shovel absorbent/decontamination solution mixture into the same steel drum used above.
- ▶ Monitor for residual isocyanate. If surface is decontaminated, proceed to next step. If contamination persists, repeat decontaminate procedure immediately above
- ▶ Place loosely covered drum (release of carbon dioxide) outside for at least 72 hours. Label waste-containing drum appropriately. Remove waste materials for incineration.
- ▶ Decontaminate and remove personal protective equipment.
- ▶ Return to normal operation.
- ▶ Conduct accident investigation and consider measures to prevent reoccurrence.

#### Decontamination:

Treat isocyanate spills with sufficient amounts of isocyanate decontaminant preparation ("neutralising fluid"). Isocyanates and polyisocyanates are generally not miscible with water. Liquid surfactants are necessary to allow better dispersion of isocyanate and neutralising fluids/ preparations. Alkaline neutralisers react faster than water/surfactant mixtures alone.

Typically, such a preparation may consist of:

Sawdust: 20 parts by weight Kieselguhr 40 parts by weight plus a mixture of {ammonia (s.g. 0.880) 8% v/v non-ionic surfactant 2% v/v water 90% v/v}.

Let stand for 24 hours

Three commonly used neutralising fluids each exhibit advantages in different situations.

#### Formulation A :

liquid surfactant 0.2-2%

sodium carbonate 5-10%

water to 100%

#### Formulation B

liquid surfactant 0.2-2%

concentrated ammonia 3-8%

water to 100%

#### Formulation C

ethanol, isopropanol or butanol 50%

concentrated ammonia 5%

water to 100%

After application of any of these formulae, let stand for 24 hours.

Formulation B reacts faster than Formulation A. However, ammonia-based neutralisers should be used only under well-ventilated conditions to avoid overexposure to ammonia or if members of the emergency team wear suitable respiratory protection.

Formulation C is especially suitable for cleaning of equipment from unreacted isocyanate and neutralizing under freezing conditions. Regard has to be taken to the flammability of the alcoholic solution.

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

## SECTION 7 Handling and storage

### Precautions for safe handling

#### Safe handling

- ▶ 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.**
- ▶ 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

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	<p>maintained.</p> <ul style="list-style-type: none"> <li>▶ <b>DO NOT</b> allow clothing wet with material to stay in contact with skin</li> </ul>
Other information	<ul style="list-style-type: none"> <li>▶ Store in original containers.</li> <li>▶ Keep containers securely sealed.</li> <li>▶ Store in a cool, dry, well-ventilated area.</li> <li>▶ Store away from incompatible materials and foodstuff containers.</li> <li>▶ Protect containers against physical damage and check regularly for leaks.</li> <li>▶ Observe manufacturer's storage and handling recommendations contained within this SDS.</li> </ul>

## Conditions for safe storage, including any incompatibilities

Suitable container	<ul style="list-style-type: none"> <li>▶ Lined metal can, lined metal pail/ can.</li> <li>▶ Plastic pail.</li> <li>▶ Polyliner drum.</li> <li>▶ Packing as recommended by manufacturer.</li> <li>▶ Check all containers are clearly labelled and free from leaks.</li> </ul> <p>For low viscosity materials</p> <ul style="list-style-type: none"> <li>▶ Drums and jerricans must be of the non-removable head type.</li> <li>▶ Where a can is to be used as an inner package, the can must have a screwed enclosure.</li> </ul> <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"> <li>▶ Removable head packaging;</li> <li>▶ Cans with friction closures and</li> <li>▶ low pressure tubes and cartridges</li> </ul> <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	<ul style="list-style-type: none"> <li>· Avoid reaction with water, alcohols and detergent solutions. Isocyanates are electrophiles, and as such they are reactive toward a variety of nucleophiles including alcohols, amines, and even water. Upon treatment with an alcohol, an isocyanate forms a urethane linkage. If a di-isocyanate is treated with a compound containing two or more hydroxyl groups, such as a diol or a polyol, polymer chains are formed, which are known as polyurethanes. Reaction between a di-isocyanate and a compound containing two or more amine groups, produces long polymer chains known as polyureas.</li> <li>· Isocyanates and thioisocyanates are incompatible with many classes of compounds, reacting exothermically to release toxic gases. Reactions with amines, strong bases, aldehydes, alcohols, alkali metals, ketones, mercaptans, strong oxidisers, hydrides, phenols, and peroxides can cause vigorous releases of heat. Acids and bases initiate polymerisation reactions in these materials.</li> <li>· Isocyanates also can react with themselves. Aliphatic di-isocyanates can form trimers, which are structurally related to cyanuric acid. Isocyanates participate in Diels-Alder reactions, functioning as dienophiles</li> <li>· Isocyanates easily form adducts with carbodiimides, isothiocyanates, ketenes, or with substrates containing activated CC or CN bonds.</li> <li>· Some isocyanates react with water to form amines and liberate carbon dioxide. This reaction may also generate large volumes of foam and heat. Foaming spaces may produce pressure in confined spaces or containers. Gas generation may pressurise drums to the point of rupture.</li> <li>· Do NOT reseal container if contamination is expected</li> <li>· Open all containers with care</li> <li>· Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence,</li> <li>· Isocyanates will attack and embrittle some plastics and rubbers.</li> <li>· The isocyanate anion is a pseudohalide (syn pseudohalogen) whose chemistry, resembling that of the true halogens, allows it to substitute for halogens in several classes of chemical compounds.. The behavior and chemical properties of the several pseudohalides are identical to that of the true halide ions. <ul style="list-style-type: none"> <li>▶ A range of exothermic decomposition energies for isocyanates is given as 20-30 kJ/mol.</li> <li>▶ The relationship between energy of decomposition and processing hazards has been the subject of discussion; it is suggested that values of energy released per unit of mass, rather than on a molar basis (J/g) be used in the assessment.</li> <li>▶ For example, in "open vessel processes" (with man-hole size openings, in an industrial setting), substances with exothermic decomposition energies below 500 J/g are unlikely to present a danger, whilst those in "closed vessel processes" (opening is a safety valve or bursting disk) present some danger where the decomposition energy exceeds 150 J/g.</li> </ul> </li> </ul> <p>BREThERICK: Handbook of Reactive Chemical Hazards, 4th Edition</p> <ul style="list-style-type: none"> <li>▶ Store at 2-8°C</li> <li>▶ Lachrymatory</li> <li>▶ Moisture sensitive</li> <li>▶ Store under argon</li> </ul>

## SECTION 8 Exposure controls / personal protection

**3,5-Bis(trifluoromethyl)phenyl isocyanate**

**Control parameters**

**Occupational Exposure Limits (OEL)**

**INGREDIENT DATA**


Source	Ingredient	Material name	TWA	STEL	Peak	Notes
UK Workplace Exposure Limits (WELs)	3,5-Bis(trifluoromethyl)phenyl isocyanate	Isocyanates, all (as -NCO) Except methyl isocyanate	0.02 mg/m3	0.07 mg/m3	Not Available	Sen

**Emergency Limits**

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

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

**Exposure controls**

<b>Appropriate engineering controls</b>	<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.</p> <p>Employers may need to use multiple types of controls to prevent employee overexposure.</p> <ul style="list-style-type: none"> <li>▸ Spraying of material or material in admixture with other components must be carried out in conditions conforming to local state regulations (AS/NZS 4114, UNI EN 12215:2010, ANSI/AIHA Z9.3-2007 or national equivalent).</li> <li>▸ Local exhaust ventilation with full face positive-pressure air supplied breathing apparatus (hood or helmet type) is required.</li> <li>▸ Spraying should be performed in a spray booth fitted with an effective exhaust system which complies with local environmental legislation.</li> <li>▸ The spray booth area must be isolated from unprotected personnel whilst spraying is in progress and until all spraying mist has cleared.</li> </ul> <p><b>NOTE:</b> Isocyanate vapours will not be adequately absorbed by organic vapour respirators. 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" style="width: 100%;"> <thead> <tr> <th>Type of Contaminant:</th> <th>Air Speed:</th> </tr> </thead> <tbody> <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> </tbody> </table> <p>Within each range the appropriate value depends on:</p> <table border="1" style="width: 100%;"> <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> <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 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 4-10 m/s (800-2000 f/min.) for extraction of solvents generated by spraying at a point 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>	Type of Contaminant:	Air Speed:	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.)	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
Type of Contaminant:	Air Speed:														
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4: Large hood or large air mass in motion	4: Small hood-local control only														
<b>Individual protection measures, such as personal protective equipment</b>															
<b>Eye and face protection</b>	<ul style="list-style-type: none"> <li>▸ Safety glasses with side shields.</li> <li>▸ Chemical goggles. [AS/NZS 1337.1, EN166 or national equivalent]</li> <li>▸ 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</li> </ul>														

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	<p>include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience. 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].</p>
<b>Skin protection</b>	See Hand protection below
<b>Hands/feet protection</b>	<ul style="list-style-type: none"> <li>▶ Wear chemical protective gloves, e.g. PVC.</li> <li>▶ Wear safety footwear or safety gumboots, e.g. Rubber</li> </ul> <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"> <li>· frequency and duration of contact,</li> <li>· chemical resistance of glove material,</li> <li>· glove thickness and</li> <li>· dexterity</li> </ul> <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"> <li>· 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.</li> <li>· 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.</li> <li>· Some glove polymer types are less affected by movement and this should be taken into account when considering gloves for long-term use.</li> <li>· Contaminated gloves should be replaced.</li> </ul> <p>As defined in ASTM F-739-96 in any application, gloves are rated as:</p> <ul style="list-style-type: none"> <li>· Excellent when breakthrough time &gt; 480 min</li> <li>· Good when breakthrough time &gt; 20 min</li> <li>· Fair when breakthrough time &lt; 20 min</li> <li>· Poor when glove material degrades</li> </ul> <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"> <li>· 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.</li> <li>· 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</li> </ul> <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>
<b>Body protection</b>	See Other protection below
<b>Other protection</b>	<ul style="list-style-type: none"> <li>▶ Overalls.</li> <li>▶ Eyewash unit.</li> <li>▶ Barrier cream.</li> <li>▶ Skin cleansing cream.</li> </ul>

## Respiratory protection

Type A Filter of sufficient capacity. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

Where the concentration of gas/particulates in the breathing zone, approaches or exceeds the "Exposure Standard" (or ES), respiratory protection is required. Degree of protection varies with both face-piece and Class of filter; the nature of protection varies with Type of filter.

Required Minimum Protection Factor	Half-Face Respirator	Full-Face Respirator	Powered Air Respirator
up to 10 x ES	A-AUS	-	A-PAPR-AUS / Class 1
up to 50 x ES	-	A-AUS / Class 1	-
up to 100 x ES	-	A-2	A-PAPR-2 ^

^ - Full-face

A(All classes) = Organic vapours, B AUS or B1 = Acid gasses, B2 = Acid gas or hydrogen cyanide(HCN), B3 = Acid gas or hydrogen cyanide(HCN), E = Sulfur dioxide(SO<sub>2</sub>), G = Agricultural chemicals, K = Ammonia(NH<sub>3</sub>), Hg = Mercury, NO = Oxides of nitrogen, MB = Methyl bromide, AX = Low boiling point organic compounds(below 65 degC)



## 3,5-Bis(trifluoromethyl)phenyl isocyanate

## SECTION 9 Physical and chemical properties

## Information on basic physical and chemical properties

<b>Appearance</b>	Not Available		
<b>Physical state</b>	Liquid	<b>Relative density (Water = 1)</b>	Not Available
<b>Odour</b>	Not Available	<b>Partition coefficient n-octanol / water</b>	Not Available
<b>Odour threshold</b>	Not Available	<b>Auto-ignition temperature (°C)</b>	Not Available
<b>pH (as supplied)</b>	Not Available	<b>Decomposition temperature (°C)</b>	Not Available
<b>Melting point / freezing point (°C)</b>	Not Available	<b>Viscosity (cSt)</b>	Not Available
<b>Initial boiling point and boiling range (°C)</b>	62/2mm	<b>Molecular weight (g/mol)</b>	Not Available
<b>Flash point (°C)</b>	Not Available	<b>Taste</b>	Not Available
<b>Evaporation rate</b>	Not Available	<b>Explosive properties</b>	Not Available
<b>Flammability</b>	Not Available	<b>Oxidising properties</b>	Not Available
<b>Upper Explosive Limit (%)</b>	Not Available	<b>Surface Tension (dyn/cm or mN/m)</b>	Not Available
<b>Lower Explosive Limit (%)</b>	Not Available	<b>Volatile Component (%vol)</b>	Not Available
<b>Vapour pressure (kPa)</b>	Not Available	<b>Gas group</b>	Not Available
<b>Solubility in water</b>	Not Available	<b>pH as a solution (1%)</b>	Not Available
<b>Vapour density (Air = 1)</b>	Not Available	<b>VOC g/L</b>	Not Available

## SECTION 10 Stability and reactivity

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

## SECTION 11 Toxicological information

## Information on toxicological effects

<b>Inhaled</b>	Inhalation of aerosols (mists, fumes), generated by the material during the course of normal handling, may be harmful. 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.
<b>Ingestion</b>	Accidental ingestion of the material may be harmful; animal experiments indicate that ingestion of less than 150 gram may be fatal or may produce serious damage to the health of the individual.
<b>Skin Contact</b>	Skin contact with the material may be harmful; systemic effects may result following absorption. This material can cause inflammation of the skin on contact in some persons. The material may accentuate any pre-existing dermatitis condition

## 3,5-Bis(trifluoromethyl)phenyl isocyanate

	Open cuts, abraded or irritated skin should not be exposed to this material 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.
<b>Eye</b>	This material can cause eye irritation and damage in some persons.
<b>Chronic</b>	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

<b>3,5-Bis(trifluoromethyl)phenyl isocyanate</b>	Isocyanate vapours are irritating to the airways and can cause their inflammation, with wheezing, gasping, severe distress, even loss of consciousness and fluid in the lungs. Nervous system symptoms that may occur include headache, sleep disturbance, euphoria, inco-ordination, anxiety, depression and paranoia.
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<b>Acute Toxicity</b>	✓	<b>Carcinogenicity</b>	✗
<b>Skin Irritation/Corrosion</b>	✓	<b>Reproductivity</b>	✗
<b>Serious Eye Damage/Irritation</b>	✓	<b>STOT - Single Exposure</b>	✓
<b>Respiratory or Skin sensitisation</b>	✗	<b>STOT - Repeated Exposure</b>	✗
<b>Mutagenicity</b>	✗	<b>Aspiration Hazard</b>	✗

**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

**DO NOT** discharge into sewer or waterways.

## Persistence and degradability

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

## Bioaccumulative potential

Ingredient	Bioaccumulation
3,5-Bis(trifluoromethyl)phenyl isocyanate	HIGH (LogKOW = 4.519)

## Mobility in soil

Ingredient	Mobility
3,5-Bis(trifluoromethyl)phenyl isocyanate	LOW (KOC = 48640)

## SECTION 13 Disposal considerations

## Waste treatment methods


<b>Product / Packaging disposal</b>	<ul style="list-style-type: none"> <li>▸ Containers may still present a chemical hazard/ danger when empty.</li> <li>▸ Return to supplier for reuse/ recycling if possible.</li> </ul> Otherwise:
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**3,5-Bis(trifluoromethyl)phenyl isocyanate**

	<ul style="list-style-type: none"> <li>▸ If container can not be cleaned sufficiently well to ensure that residuals do not remain or if the container cannot be used to store the same product, then puncture containers, to prevent re-use, and bury at an authorised landfill.</li> <li>▸ Where possible retain label warnings and SDS and observe all notices pertaining to the product.</li> </ul> <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"> <li>▸ Reduction</li> <li>▸ Reuse</li> <li>▸ Recycling</li> <li>▸ Disposal (if all else fails)</li> </ul> <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"> <li>▸ <b>DO NOT allow wash water from cleaning or process equipment to enter drains.</b></li> <li>▸ It may be necessary to collect all wash water for treatment before disposal.</li> <li>▸ In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first.</li> <li>▸ Where in doubt contact the responsible authority.</li> </ul>
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**SECTION 14 Transport information**

**Labels Required**

	
<b>Marine Pollutant</b>	NO

**Land transport (ADR-RID)**

<b>UN number or ID number</b>	2206	
<b>UN proper shipping name</b>	ISOCYANATES, TOXIC, N.O.S. or ISOCYANATE SOLUTION, TOXIC, N.O.S.	
<b>Transport hazard class(es)</b>	Class	6.1
	Subsidiary risk	Not Applicable
<b>Packing group</b>	III	
<b>Environmental hazard</b>	Not Applicable	
<b>Special precautions for user</b>	Hazard identification (Kemler)	60
	Classification code	T1
	Hazard Label	6.1
	Special provisions	274 551
	Limited quantity	5 L
	Tunnel Restriction Code	2 (E)

**Air transport (ICAO-IATA / DGR)**

<b>UN number</b>	2206	
<b>UN proper shipping name</b>	Isocyanates, toxic, n.o.s. *; Isocyanate solution, toxic, n.o.s. *	
<b>Transport hazard class(es)</b>	ICAO/IATA Class	6.1
	ICAO / IATA Subrisk	Not Applicable
	ERG Code	6L
<b>Packing group</b>	III	
<b>Environmental hazard</b>	Not Applicable	
<b>Special precautions for user</b>	Special provisions	A3
	Cargo Only Packing Instructions	663
	Cargo Only Maximum Qty / Pack	220 L
	Passenger and Cargo Packing Instructions	655

**3,5-Bis(trifluoromethyl)phenyl isocyanate**

	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)**

<b>UN number</b>	2206	
<b>UN proper shipping name</b>	ISOCYANATES, TOXIC, N.O.S. or ISOCYANATE SOLUTION, TOXIC, N.O.S.	
<b>Transport hazard class(es)</b>	IMDG Class	6.1
	IMDG Subrisk	Not Applicable
<b>Packing group</b>	III	
<b>Environmental hazard</b>	Not Applicable	
<b>Special precautions for user</b>	EMS Number	F-A, S-A
	Special provisions	223 274
	Limited Quantities	5 L

**Inland waterways transport (ADN)**

<b>UN number</b>	2206	
<b>UN proper shipping name</b>	ISOCYANATES, TOXIC, N.O.S. or ISOCYANATE SOLUTION, TOXIC, N.O.S.	
<b>Transport hazard class(es)</b>	6.1	Not Applicable
<b>Packing group</b>	III	
<b>Environmental hazard</b>	Not Applicable	
<b>Special precautions for user</b>	Classification code	T1
	Special provisions	274; 551; 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)phenyl isocyanate	Not Available

**Transport in bulk in accordance with the IGC Code**

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

**SECTION 15 Regulatory information**

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

**3,5-Bis(trifluoromethyl)phenyl isocyanate is found on the following regulatory lists**

Not Applicable

**National Inventory Status**

National Inventory	Status
Australia - AIIIC / Australia Non-Industrial Use	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)

**3,5-Bis(trifluoromethyl)phenyl isocyanate**

National Inventory	Status
Canada - DSL	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Canada - NDSSL	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
China - IECSC	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Europe - EINEC / ELINCS / NLP	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Japan - ENCS	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Korea - KECI	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
New Zealand - NZIoC	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Philippines - PICCS	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
USA - TSCA	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Taiwan - TCSI	Yes
Mexico - INSQ	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Vietnam - NCI	Yes
Russia - FBEPH	No (3,5-Bis(trifluoromethyl)phenyl isocyanate)

**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**

<b>Revision Date</b>	29/06/2023
<b>Initial Date</b>	30/06/2023

**SDS Version Summary**

Version	Date of Update	Sections Updated
1.2	29/06/2023	Toxicological information - Acute Health (inhaled), Toxicological information - Acute Health (skin), Toxicological information - Acute Health (swallowed), Physical and chemical properties - Appearance, CAS Number, Disposal considerations - Disposal, Firefighting measures - Fire Fighter (extinguishing media), Firefighting measures - Fire Fighter (fire/explosion hazard), Firefighting measures - Fire Fighter (fire incompatibility), First Aid measures - First Aid (skin), First Aid measures - First Aid (swallowed), Handling and storage - Handling Procedure, Composition / information on ingredients - Ingredients, Korean MSDS Number, Exposure controls / personal protection - Personal Protection (Respirator), Exposure controls / personal protection - Personal Protection (hands/feet), Accidental release measures - Spills (minor), Handling and storage - Storage (storage incompatibility), Identification of the substance / mixture and of the company / undertaking - Supplier Information, Identification of the substance / mixture and of the company / undertaking - Synonyms

**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

## 3,5-Bis(trifluoromethyl)phenyl isocyanate

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	On basis of test data
Acute Toxicity (Inhalation) Category 4, H332	On basis of test data
Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3 , H335	Expert judgement
Acute Toxicity (Oral) Category 4, H302	On basis of test data
Skin Corrosion/Irritation Category 2, H315	Calculation method
Serious Eye Damage/Eye Irritation Category 2, H319	Calculation method