

ALFAAL09448

3-(Trifluoromethyl)phenyl isocyanate

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: Product Description:	3-(三氟甲基)苯基异氰酸苯酯 3-(Trifluoromethyl)phenyl isocyanate
Cat No. :	L09448
Synonyms	3-(Trifluoromethyl)phenyl isocyanate
CAS No	329-01-1
Molecular Formula	C ₈ H ₄ F ₃ N O
Supplier	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
Emergency Telephone Number	For information US call: 001-800-227-6701 / Europe call: +32 14 57 52 11 Emergency Number US :001-201-796-7100 / Europe : +32 14 57 52 99 CHEMTREC Tel. No. US :001-800-424-9300 / Europe :001-703-527-3887
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State Liquid	Appearance Colorless	Odor No information available
Emergency Overview May cause allergy or asthma symptoms or breathing difficulties if inhaled. Toxic to aquatic life with long lasting effects. Combustible liquid. Toxic in contact with skin. Causes skin irritation. Causes serious eye damage. Fatal if inhaled. May cause respiratory irritation. Moisture sensitive.		

Classification of the substance or mixture

Flammable liquids.	Category 3 Category 4
Acute Dermal Toxicity	Category 3
Acute Inhalation Toxicity - Vapors	Category 1
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 1
Respiratory Sensitization	Category 1
Specific target organ toxicity - (single exposure)	Category 3
Acute aquatic toxicity	Category 2
Chronic aquatic toxicity	Category 2

Label Elements

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**Signal Word****Danger****Hazard Statements**

H226 - Flammable liquid and vapor
 H227 - Combustible liquid
 H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled
 H411 - Toxic to aquatic life with long lasting effects
 H311 - Toxic in contact with skin
 H315 - Causes skin irritation
 H318 - Causes serious eye damage
 H330 - Fatal if inhaled
 H335 - May cause respiratory irritation

Precautionary Statements**Prevention**

P241 - Use explosion-proof electrical/ ventilating/ lighting equipment
 P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
 P264 - Wash face, hands and any exposed skin thoroughly after handling
 P270 - Do not eat, drink or smoke when using this product
 P271 - Use only outdoors or in a well-ventilated area
 P272 - Contaminated work clothing should not be allowed out of the workplace
 P280 - Wear protective gloves/protective clothing/eye protection/face protection
 P284 - In case of inadequate ventilation wear respiratory protection

Response

P310 - Immediately call a POISON CENTER or doctor
 P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
 P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
 P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
 P330 - Rinse mouth
 P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
 P361 + P364 - Take off immediately all contaminated clothing and wash it before reuse

Storage

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

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

Vapors may cause flash fire or explosion. Combustible material.

Health Hazards

May cause allergy or asthma symptoms or breathing difficulties if inhaled. Toxic in contact with skin. Causes skin irritation. Fatal if inhaled. May cause respiratory irritation.

Environmental hazards

Toxic to aquatic life with long lasting effects. Will likely be mobile in the environment due to its volatility. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Benzene, 1-isocyanato-3-(trifluoromethyl)-	329-01-1	>95

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SECTION 4. FIRST AID MEASURES

General Advice

If symptoms persist, call a physician. Show this safety data sheet to the doctor in attendance.

Eye Contact

Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Rinse thoroughly with plenty of water for at least 15 minutes, lifting lower and upper eyelids. Consult a physician. Immediately flush with plenty of water. After initial flushing, remove any contact lenses and continue flushing for at least 15 minutes. Keep eye wide open while rinsing. If symptoms persist, call a physician.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Immediate medical attention is required. Call a physician immediately. SPEEDY ACTION IS CRITICAL, GET MEDICAL AID IMMEDIATELY. If symptoms persist, call a physician. Wash off immediately with plenty of water for at least 15 minutes. Remove and wash contaminated clothing and gloves, including the inside, before re-use. If skin irritation persists, call a physician. Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

Inhalation

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required. Artificial respiration and/or oxygen may be necessary. Consult a physician if necessary. Oxygen or artificial respiration if needed. Immediate medical attention is not required. Move to fresh air in case of accidental inhalation of vapors. If symptoms persist, call a physician. Move to fresh air in case of accidental inhalation of vapors or decomposition products.

Ingestion

Call a physician immediately. Clean mouth with water. Clean mouth with water and drink afterwards plenty of water. Do not induce vomiting without medical advice. Never give anything by mouth to an unconscious person. Consult a physician if necessary.

Most important symptoms and effects

May cause allergy or asthma symptoms or breathing difficulties if inhaled. Causes eye burns. Difficulty in breathing. May cause allergic skin reaction. Causes severe eye damage. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing: Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

Use personal protective equipment as required.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES

Suitable Extinguishing Media

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers. Use: Alcohol resistant foam.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Combustible material. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Keep product and empty container away from heat and sources of ignition. Risk of ignition.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6. ACCIDENTAL RELEASE MEASURES

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Personal Precautions

Remove all sources of ignition. Take precautionary measures against static discharges. Use personal protective equipment as required. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Pay attention to flashback.

Environmental Precautions

Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean Up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Wear self-contained breathing apparatus and protective suit. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Do not let this chemical enter the environment.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

Handling

Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Handle product only in closed system or provide appropriate exhaust ventilation. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges. Pay attention to flashback. No information available. Do not take internally. Contents under pressure. Avoid contact with skin and clothing.

Storage

Keep in a dry place. Keep away from heat, sparks and flame. Keep refrigerated. Keep in properly labeled containers. Keep away from heat. Keep containers tightly closed in a dry, cool and well-ventilated place. Store under an inert atmosphere.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
Benzene, 1-isocyanato-3-(trifluoromethyl)-				STEL: 0.07 mg/m ³ 15 min TWA: 0.02 mg/m ³ 8 hr Resp. Sens.	

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

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Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Nitrile rubber	recommendations			
Neoprene				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.
(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure Apron Impervious gloves Chemical resistant apron Antistatic boots

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141
When RPE is used a face piece Fit Test should be conducted

Hygiene Measures When using do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

Environmental exposure controls Prevent product from entering drains. Do not allow material to contaminate ground water system.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Colorless	
Physical State	Liquid	
Odor	No information available	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	-26 °C / -14.8 °F	
Softening Point	No data available	
Boiling Point/Range	54 °C / 129.2 °F	@ 11 mmHg
Flash Point	66 °C / 150.8 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	126 mmHg @ 20 °C	
Vapor Density	No data available	(Air = 1.0)
Specific Gravity / Density	1.336	

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Bulk Density	Not applicable	Liquid
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	600 - °C / 1112 - °F	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C8 H4 F3 N O	
Molecular Weight	187.12	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions. Moisture sensitive.
Hazardous Reactions	No information available.
Hazardous Polymerization	No information available.
Conditions to Avoid	Excess heat. Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition. Heating in air.
Materials to avoid	Acids. Water. Strong oxidizing agents. Strong bases. Alcohols. Amines.
Hazardous Decomposition Products	Nitrogen oxides (NO _x). Carbon monoxide (CO). Carbon dioxide (CO ₂). Hydrogen cyanide (hydrocyanic acid). Gaseous hydrogen fluoride (HF).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, 1-isocyanato-3-(trifluoromethyl)-	975 mg/kg (Rat) 6604 mg/kg (Rat)	>210 mg/kg (Rat)	>0.036 mg/L (Rat) 4h <0.087 mg/L (Rat) 4h

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;

Respiratory	Category 1
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

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Results / Target organs	Respiratory system
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	No data available
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects, both acute and delayed	Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing: Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.
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Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
Benzene, 1-isocyanato-3-(trifluoromethyl)-	LC50: = 4.2 mg/L, 96h static (Brachydanio rerio)			

Persistence and Degradability	No information available
Persistence	Persistence is unlikely, based on information available.
Degradation in sewage treatment plant	Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential	Bioaccumulation is unlikely
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Mobility in soil	The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.
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Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
Contaminated Packaging	Dispose of this container to hazardous or special waste collection point.
Other Information	Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

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UN-No UN3382
Proper Shipping Name TOXIC BY INHALATION LIQUID, N.O.S.
Technical Shipping Name α,α,α -Trifluoro-m-tolyl isocyanate
Hazard Class 6.1
Packing Group I

IMDG/IMO

UN-No UN3382
Proper Shipping Name TOXIC BY INHALATION LIQUID, N.O.S.
Technical Shipping Name α,α,α -Trifluoro-m-tolyl isocyanate
Hazard Class 6.1
Packing Group I

IATA

FORBIDDEN FOR IATA TRANSPORT

UN-No UN3382
Proper Shipping Name TOXIC BY INHALATION LIQUID, N.O.S. FORBIDDEN FOR IATA TRANSPORT
Technical Shipping Name α,α,α -Trifluoro-m-tolyl isocyanate
Hazard Class 6.1
Packing Group I

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Benzene, 1-isocyanato-3-(trifluoromethyl)-	X	-	X	-	206-341-3	X	-	-	-		-	-

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 01-May-2012
Revision Date 22-Apr-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

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Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet