

Creation Date 19-Oct-2009

Revision Date 02-Mar-2016

Revision Number 3

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identification

Product Description: **3,5-Difluorophenyl isocyanate**  
 Cat No. : **428230000; 428230010; 428230050**  
 CAS-No **83594-83-6**  
 Molecular Formula **C7 H3 F2 N O**

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

Recommended Use Laboratory chemicals.  
 Uses advised against No Information available

### 1.3. Details of the supplier of the safety data sheet

Company Acros Organics BVBA  
 Janssen Pharmaceuticaaan 3a  
 2440 Geel, Belgium  
 E-mail address [begel.sdsdesk@thermofisher.com](mailto:begel.sdsdesk@thermofisher.com)

### 1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - Regulation (EC) No 1272/2008

##### Physical hazards

Flammable liquids Category 3

##### Health hazards

Acute oral toxicity	Category 3
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Respiratory Sensitization	Category 1
Skin Sensitization	Category 1
Specific target organ toxicity - (single exposure)	Category 3

##### Environmental hazards

Based on available data, the classification criteria are not met

### 2.2. Label elements

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Signal Word

Danger

## Hazard Statements

H226 - Flammable liquid and vapor  
H301 - Toxic if swallowed  
H312 - Harmful in contact with skin  
H332 - Harmful if inhaled  
H315 - Causes skin irritation  
H317 - May cause an allergic skin reaction  
H319 - Causes serious eye irritation  
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H335 - May cause respiratory irritation

## Precautionary Statements

P210 - Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection  
P303 + P361 + P353 - IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower  
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician  
P304 + P340 - IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing  
P333 + P313 - If skin irritation or rash occurs: Get medical advice/ attention

## 2.3. Other hazards

Lachrymator (substance which increases the flow of tears)

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008
3,5-Difluorophenyl isocyanate	83594-83-6		>95	Flam. Liq. 3 (H226) Acute Tox. 3 (H301) Acute Tox. 4 (H312) Skin Irrit. 2 (H315) Skin Sens. 1 (H317) Eye Irrit. 2 (H319) Acute Tox. 4 (H332) Resp. Sens. 1 (H334) STOT SE 3 (H335)

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

#### General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

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<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Ingestion</b>	Do not induce vomiting. Call a physician or Poison Control Center immediately.
<b>Inhalation</b>	Move to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
<b>Protection of First-aiders</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: 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

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

**Notes to Physician** Treat symptomatically.

## **SECTION 5: FIREFIGHTING MEASURES**

### **5.1. Extinguishing media**

#### **Suitable Extinguishing Media**

Carbon dioxide (CO<sub>2</sub>). Foam. Dry powder. Cool closed containers exposed to fire with water spray.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

### **5.2. Special hazards arising from the substance or mixture**

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), Hydrogen fluoride.

### **5.3. Advice for firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

### **6.1. Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Ensure adequate ventilation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.

### **6.2. Environmental precautions**

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Should not be released into the environment.

## **6.3. Methods and material for containment and cleaning up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

## **6.4. Reference to other sections**

Refer to protective measures listed in Sections 8 and 13.

## **SECTION 7: HANDLING AND STORAGE**

### **7.1. Precautions for safe handling**

Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe vapors or spray mist. Do not ingest. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing before re-use. Wash hands before breaks and at the end of workday.

### **7.2. Conditions for safe storage, including any incompatibilities**

Flammables area. Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place. To maintain product quality. Keep refrigerated. Store under an inert atmosphere.

### **7.3. Specific end use(s)**

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1. Control parameters**

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies.

#### **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

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chromatography

**Derived No Effect Level (DNEL)** No information available

Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral Dermal Inhalation				

**Predicted No Effect Concentration (PNEC)** No information available.

## 8.2. Exposure controls

### Engineering Measures

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure adequate ventilation, especially in confined areas. 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

**Eye Protection** Goggles (European standard - EN 166)  
**Hand Protection** Protective gloves

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

**Skin and body protection** Long sleeved clothing

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.

### 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

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

#### Appearance

**Physical State** Liquid

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Odor	No information available	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	159 °C / 318.2 °F	Based on available literature
Flash Point	54 °C / 129.2 °F	<b>Method</b> - Closed cup
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	No data available	(Air = 1.0)
Specific Gravity / Density	1.31	
Bulk Density	Not applicable	Liquid
Water Solubility	hydrolyses	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties	No information available	explosive air/vapour mixtures possible
Oxidizing Properties	No information available	

## 9.2. Other information

Molecular Formula	C7 H3 F2 N O
Molecular Weight	155.10

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

Yes

### 10.2. Chemical stability

Stable under recommended storage conditions: Moisture sensitive: Decomposes in contact with water

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

### 10.4. Conditions to avoid

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition. Exposure to moist air or water.

### 10.5. Incompatible materials

Strong oxidizing agents. Water. Alcohols. Amines.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</sub>). Hydrogen fluoride.

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on toxicological effects

#### Product Information

(a) acute toxicity;	
Oral	Category 3
Dermal	Category 4

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Inhalation	Category 4
(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization;	
Respiratory	Category 1
Skin	Category 1
(e) germ cell mutagenicity;	No information available 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
Results / Target organs	Respiratory system.
(i) STOT-repeated exposure;	No data available
Target Organs	None known.
(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 overexposure may be headache, dizziness, tiredness, nausea and vomiting: 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

## SECTION 12: ECOLOGICAL INFORMATION

**12.1. Toxicity**  
**Ecotoxicity effects** Do not empty into drains. Reacts with water so no ecotoxicity data for the substance is available.

**12.2. Persistence and degradability**  
**Persistence** Persistence is unlikely, based on information available.  
**Degradability** Decomposes in contact with water.  
**Degradation in sewage treatment plant** Decomposes in contact with water.

**12.3. Bioaccumulative potential** Product does not bioaccumulate due to reaction with water

**12.4. Mobility in soil** Hydrolyses Is not likely mobile in the environment.

**12.5. Results of PBT and vPvB assessment** No data available for assessment.

**12.6. Other adverse effects**  
**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

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## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

#### 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. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

#### European Waste Catalogue (EWC)

According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.

#### Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not dispose of waste into sewer. Can be incinerated, when in compliance with local regulations.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

#### 14.1. UN number

UN2478

#### 14.2. UN proper shipping name

ISOCYANATES, FLAMMABLE, TOXIC, N.O.S

#### 14.3. Transport hazard class(es)

3

##### Subsidiary Hazard Class

6.1

#### 14.4. Packing group

III

### ADR

#### 14.1. UN number

UN2478

#### 14.2. UN proper shipping name

ISOCYANATES, FLAMMABLE, TOXIC, N.O.S

#### 14.3. Transport hazard class(es)

3

##### Subsidiary Hazard Class

6.1

#### 14.4. Packing group

III

### IATA

#### 14.1. UN number

UN2478

#### 14.2. UN proper shipping name

ISOCYANATES, FLAMMABLE, TOXIC, N.O.S

#### 14.3. Transport hazard class(es)

3

##### Subsidiary Hazard Class

6.1

#### 14.4. Packing group

III

#### 14.5. Environmental hazards

No hazards identified

#### 14.6. Special precautions for user

No special precautions required

#### 14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

Complete Regulatory Information contained in following SDS's X = listed The product is classified and labeled according to EC directives or corresponding national laws The product is classified and labeled in accordance with Directive 1999/45/EC



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## National Regulations

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment.

Take note of Dir 94/33/EC on the protection of young people at work

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full Text of H-/EUH-Statements Referred to Under Section 3

H301 - Toxic if swallowed

H312 - Harmful in contact with skin

H332 - Harmful if inhaled

H315 - Causes skin irritation

H317 - May cause an allergic skin reaction

H319 - Causes serious eye irritation

H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled

H335 - May cause respiratory irritation

H226 - Flammable liquid and vapor

### 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

**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

**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

**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

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

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

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

### Key literature references and sources for data

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

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

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - Volatile Organic Compounds

### 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.

**Creation Date** 19-Oct-2009

**Revision Date** 02-Mar-2016

**Revision Summary** SDS sections updated, 2, 3, 4, 5, 7, 8, 10, 11, 12.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006**

Disclaimer

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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**