Safety Data Sheet

fluorochem.

1. Identification of Substance / Mixture

Product Identifier

Product Name	**3,5,5-Trimethylhexanoyl chloride**
Other Names	**Isononanoyl chloride**
Product Code	174700
CAS	36727-29-4
MDL	MFCD00044028
EINECS	253-168-4
REACH Registration Number	
Relevant Uses	Research and Development
Uses Advised Against	No uses advised against.

Supplier Details

Company	Fluorochem Limited
Address	Unit 14, Graphite Way, Hadfield. SK13 1QH. UK
Telephone	+44(0)1457 860111
Email	sds@fluorochem.co.uk
Emergency Telephone	+44(0)1457 860111 (08:00 - 17:30)

2. Hazards Identification

Classification

Skin Corr. 1A
Skin Sens. 1
Acute Tox. 1
Acute Tox. 3
Aquatic Chronic 3

Signal Word

Danger

Pictograms

GHS05

GHS06

GHS07

Hazards

H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.
H330 Fatal if inhaled.
H301+H311 Toxic if swallowed or in contact with skin.
H412 Harmful to aquatic life with long lasting effects.
EUH071 Corrosive to the respiratory tract.

Precautions

P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P272 Contaminated work clothing should not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear face protection.
P284 Wear respiratory protection.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302+P352 IF ON SKIN: Wash with plenty of water.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with 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.
P310 Immediately call a POISON CENTER/doctor.
P311 Call a POISON CENTER/doctor.
P320 Specific treatment is urgent.
P321 Specific treatment.
P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
P362+P364 Take off contaminated clothing and wash it before reuse.
P363 Wash contaminated clothing before reuse.
P391 Collect spillage.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.

Other Classification Hazards

Fatal By Inhalation

3. Composition of Ingredients

SUBSTANCE

Name	CAS	Einecs	Composition	Hazards
3,5,5-Trimethylhexanoyl chloride	36727-29-4	253-168-4	<= 100%	H314 Skin Corr. 1A H317 Skin Sens. 1 H330 Acute Tox. 1 H301+H311 Acute Tox. 3 H412 Aquatic Chronic 3 EUH071

4. First Aid Measures

Eye contact
In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing and seek immediate medical attention.

Ingestion
If swallowed rinse the mouth with plenty of water (only if the person is conscious) and immediately contact a poison centre.

Inhalation
Remove person to fresh air and keep comfortable for breathing. Immediately call a poison centre or physician. If breathing is irregular or stopped, administer artificial respiration.

Skin Contact
After contact with skin or hair, wash immediately with plenty of water and soap. Remove contaminated clothing immediately. Immediately seek medical attention.

General Advice
No additional advice.

Most Important Symptoms and Effects
Corrosive to the respiratory tract.
Severe burns may occur.

Immediate First Aid Measures
No additional first aid measures required.

5. Fire Fighting Measures

Suitable Fire Extinguishing Media
Carbon dioxide, dry chemical powder or sand.

Unsuitable Fire Extinguishing Media
Water.

Special Hazards
Corrosive.
In combustion toxic fumes may form.

Advice for Fire Fighters
As in any fire, wear self-contained breathing apparatus and full protective gear.

6. Accidental Release Measures

Personal Precautions
Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Keep personnel away from spill/leak.

Environmental Precautions
Prevent further leakage if safe to do so. Prevent product from entering drains. Do not let product enter waterways or sewer systems. Discharge into the environment must be avoided.

Containment - Methods and Materials
Spill Response should only be carried out by trained or qualified personnel.

Referenced SDS Sections
For personal protection see section 8. For disposal see section 13.

7. Handling and Storage

Personal Precautions

Safe Handling
Wear appropriate personal protective equipment. Use only under a chemical fume hood ensuring adequate ventilation, especially if dust, aerosol or fumes will be generated. Avoid contact with skin, eyes and clothing. For precautions see section 2.2.

Protection Against Explosion and Fire
Where possible, use anti static and spark proof equipment when handling.

General Occupational Hygiene
Handle in accordance with good industrial hygiene and safety practice. Wash hands before and after use. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing before re-use.

Conditions for Safe Storage and Incompatabilities

Managing Storage Risks
Water or moisture.
Do not pack in metal.

Storage Controls
No special requirements

Maintaining Integrity
Keep container tightly closed in a cool area away from sunlight or heat sources.

Other Advice
No other specific advice available.

Specific End Use(s)
No specific end uses are advised. The products supplied are for research purposes only.

8. Exposure Controls / Personal Protection

Control Parameters

Country	Info	Long Term (ppm)	Long Term (mgm3)	Short Term (ppm)	Short Term (mgm3)	Ceiling (ppm)	Ceiling (mgm3)	Other Unit	Remarks

Engineering Measures
Use only under a chemical fume hood ensuring adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are

	close to the workstation location.
Face Protection	Wear tightly fitting safety goggles which adhere to European standard EN 166. Ensure eye bath is to hand.
Hand Proection	Handle with impermeable gloves. Inspect gloves before use. Gloves must satisfy the specifications of EU Directive 89/686/EEC and the standard EN374 derived from it. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.
Skin Protection	Wear appropriate protective clothing ensuring all skin is covered. Wear safety shoes that meet at least S1 standards. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
Respiratory Protection	Product should be handled in a fume cupboard with adequate extraction. No respiratory equipment is needed under normal use conditions.
Hygiene Protection	Ensure hair or skin particles cannot enter the chemical container.
Environment Exposure Controls	Avoid discharge into the environment, see section 6.2.

9. Physical and Chemical Properties

State	Liquid
Appearance	No data available.
Odour	No data available.
Odour Threshold	No data available.
pH	No data available.
Melting Point / Freezing Point	<-50Â°C
Initial Boiling Point	190.3Â°C
Boiling Range	No data available.
Flash Point	74Â°C Method: Closed Cup
Evaporation Rate	No data available.
Flammability	No data available.
Upper / Lower Flammability or Explosion Limits	No data available.
Vapour Pressure	0.68hPa at 20Â°C
Vapour Density	No data available.
Relative Density	0.937g/cm3 at 20Â°C
Solubility	No data available.
Partion Coefficient	No data available.
Auto Ignition Temperature	372Â°C
Decomposition Temperature	No data available.
Viscosity	No data available.
Explosive Properties	No data available.
Oxidising Properties	No data available.
Other information	

10. Stability and Reactivity

Reactivity	Corrosive effect on metals Reacts with water.
Stability	Stable under recommended storage conditions.
Possibility of Hazardous Reactions	Fatal if inhaled.
Conditions To Avoid	Moisture.
Incompatible Materials	Strong oxidising agents. Metals. Water. Alcohols. Amines. Bases. Water. Do not pack in metal.
Hazardous Decomposition Products	In combustion emits toxic fumes of carbon dioxide / carbon monoxide. In combustion emits toxic fumes of nitrogen oxides. In combustion emits toxic fumes of hydrogen chloride / phosgene.

11. Toxicology Information

Acute Toxicity	Oral LD50, Rat, 1700mg/kg Inhalation LC50 , Rat, 0.24mg/l/1 h
Skin Corrosion / Irritation	Strong corrosive effect on skin and mucous membranes.
Serious Eye Damage / Irritation	Lachrymator Strong corrosive effect.

Respiratory or Skin Sensitisation	Corrosive to the respiratory tract. May cause an allergic skin reaction. Toxic if swallowed or in contact with skin . Fatal if inhaled.
Germ Cell Mutagenicity	No Toxicology data available for this product.
Carcinogencity	No Toxicology data available for this product.
Reproductive Toxicity	No Toxicology data available for this product.
STOT-single Exposure	Fatal if inhaled.
STOT-repeated Exposure	No Toxicology data available for this product.
Aspiration Hazard	No Toxicology data available for this product.
Additional Toxicology Information	No Toxicology data available for this product.

12. Ecological Information

Toxicity	Toxicity to fish: Danio rerio LC50 - >120mg/l/96 h Toxicity to aquatic invertebrates: Daphnia magna EC50 - 68mg/l/48 h Toxicity to aquatic algae and cyanobacteria: Desmodesmus subspicatus ErC50 - 40.8mg/l/72 h
Persistence and Degradability	No Ecological data available for this product.
Bio-Accumulative Potential	No Ecological data available for this product.
Mobility in Soil	No Ecological data available for this product.
Results of PBT and vPvB assessment	No Ecological data available for this product.
Endocrine Disrupting Properties	Harmful to aquatic life with long lasting effects.
Other Adverse Effects	Avoid release to the environment.

13. Disposal Considerations

Disposal Operations	Ensure product is disposed of by licensed waste carriers.
Disposal of Packaging	Ensure INNER PACKAGING is disposed of by licensed waste carriers. Some OUTER PACKAGING MAY be recyclable if not contaminated.

14. Transport Information

IATA UN Number	2927	**ADR UN Number**	2927	**IMDG UN Number**	2927
IATA Proper Shipping Name	TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S. (3,5,5-Trimethylhexanoyl chloride)	**ADR Proper Shipping Name**	TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S. (3,5,5-Trimethylhexanoyl chloride)	**IMDG Proper Shipping Name**	TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S. (3,5,5-Trimethylhexanoyl chloride)
IATA Packing Group	II	**ADR Packing Group**	II	**IMDG Packing Group**	II
IATA Hazard Class	6.1	**ADR Hazard Class**	6.1	**IMDG Hazard Class**	6.1
IATA Sub Class	8	**ADR Sub Class**	8	**IMDG Sub Class**	8
				IMDG Special Provisions	
				IMDG IBS Instructions	
				IMDG IBC Instructions	IBC02
				IMDG Tank Instructions	T11
				IMDG Tank Provisions	TP2, TP27

15. Regulatory Information

Regulatory Information	As far as Fluorochem is aware, there are no further regulations controlling this product.
Chemical Safety Assessment	No Chemical Safety Assessment available for this product.

16. Other Information

Information Not Covered in Other Sections	ADR: Accord Europeen sur le transport des merchandises Dangereuses par Route(European Agreement concerning the International Carriage of Dangerous Goods by road) RID:Reglement International concernant le transport des merchandises dangereuses par chemin de fer (Regulations concerning the International transport of Dangerous Goods by Rail) IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association
IATA-DGR: Dangerous Goods Regulations by the International Air Transport Association ICAO:International Civil Aviation Organization
ICAO-TI: Technical Instructions by the ICAO
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
CAS:Chemical Abstracts Service

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Disclaimer	The product listed is for research and development purposes only and not for human or animal use. As such, in most cases, the toxicological, ecological and physicochemical properties have not been fully determined and the product should be treated with respect and always handled under suitable conditions by appropriately qualified personnel. The responsible party shall use this datasheet only in conjunction with other sources of information gathered by them, and should make an independent judgement of suitability, to ensure proper use and protect the health and safety of employees. This information is furnished without warranty and any use of the product not in conformance with this material safety data sheet, or in combination with any other product or process, is the responsibility of the user. This SDS adheres to Regulation (EC) No 1907/2006.