

SAFETY DATA SHEET

Version 5.4
Revision Date 07/02/2014
Print Date 11/20/2018

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : 3,5,5-Trimethylhexanoyl chloride

Product Number : 422959

Brand : Aldrich

CAS-No. : 36727-29-4

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Corrosive to metals (Category 1), H290

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 1), H330

Skin corrosion (Category 1A), H314

Serious eye damage (Category 1), H318

Skin sensitisation (Category 1), H317

Acute aquatic toxicity (Category 3), H402

Chronic aquatic toxicity (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H290

May be corrosive to metals.

H302

Harmful if swallowed.

H314

Causes severe skin burns and eye damage.

H317

May cause an allergic skin reaction.

H330

Fatal if inhaled.

H412

Harmful to aquatic life with long lasting effects.

Precautionary statement(s)	
P234	Keep only in original container.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash 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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P284	Wear respiratory protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.
P301 + P330 + P331	IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position 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 or doctor/ physician.
P320	Specific treatment is urgent (see supplemental first aid instructions on this label).
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P390	Absorb spillage to prevent material damage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P406	Store in corrosive resistant stainless steel container with a resistant inner liner.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Reacts violently with water.
Lachrymator.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	: Isononanoyl chloride
Formula	: C ₉ H ₁₇ ClO
Molecular Weight	: 176.68 g/mol
CAS-No.	: 36727-29-4
EC-No.	: 253-168-4

Hazardous components

Component	Classification	Concentration
3,5,5-Trimethylhexanoyl chloride	Met. Corr. 1; Acute Tox. 4; Acute Tox. 1; Skin Corr. 1A; Eye Dam. 1; Skin Sens. 1; Aquatic Acute 3; Aquatic Chronic 3; H290, H302, H314, H317, H330, H412	90 - 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Dry powder

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen chloride gas

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Do not flush with water. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Never allow product to get in contact with water during storage.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. 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.

Body Protection

Complete suit protecting against chemicals, Flame retardant protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|--|---|
| a) Appearance | Form: liquid
Colour: colourless |
| b) Odour | no data available |
| c) Odour Threshold | no data available |
| d) pH | no data available |
| e) Melting point/freezing point | Melting point/freezing point: < -50 °C (< -58 °F) |
| f) Initial boiling point and boiling range | 188 - 190 °C (370 - 374 °F) - lit. |
| g) Flash point | 140 °C (284 °F) - closed cup |
| h) Evaporation rate | no data available |
| i) Flammability (solid, gas) | no data available |
| j) Upper/lower | no data available |

flammability or
explosive limits

- | | |
|---|---|
| k) Vapour pressure | 2 hPa (2 mmHg) at 36.22 °C (97.20 °F) - OECD Test Guideline 104 |
| l) Vapour density | no data available |
| m) Relative density | 0.93 g/cm ³ at 25 °C (77 °F) - lit. |
| n) Water solubility | no data available |
| o) Partition coefficient: n-octanol/water | no data available |
| p) Auto-ignition temperature | 372 °C (702 °F) at 1,012 - 1,016 hPa (759 - 762 mmHg) |
| q) Decomposition temperature | no data available |
| r) Viscosity | no data available |
| s) Explosive properties | no data available |
| t) Oxidizing properties | no data available |

9.2 Other safety information

no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Reacts violently with water.

10.4 Conditions to avoid

Exposure to moisture.

10.5 Incompatible materials

Strong oxidizing agents Water, Strong oxidizing agents, Alcohols, Alkali metals, Amines

10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - rat - male and female - 1,700 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - rat - male and female - 4 h - 0.1 mg/l

Dermal: no data available

no data available

Skin corrosion/irritation

Skin - rabbit

Result: Causes severe burns. - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

Ames test

S. typhimurium

Result: negative

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

no data available

no data available

Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

no data available

Additional Information

RTECS: MP4560000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

Toxicity to algae static test EC50 - *Desmodesmus subspicatus* (*Scenedesmus subspicatus*) - 40.8 mg/l - 72 h

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 50 % - Partially biodegradable.
(OECD Test Guideline 301C)

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 2922 Class: 8 (6.1) Packing group: I
Proper shipping name: Corrosive liquids, toxic, n.o.s. (3,5,5-Trimethylhexanoyl chloride)
Reportable Quantity (RQ):
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN number: 2922 Class: 8 (6.1) Packing group: I EMS-No: F-A, S-B
Proper shipping name: CORROSIVE LIQUID, TOXIC, N.O.S. (3,5,5-Trimethylhexanoyl chloride)
Marine pollutant: No

IATA

UN number: 2922 Class: 8 (6.1) Packing group: I
Proper shipping name: Corrosive liquid, toxic, n.o.s. (3,5,5-Trimethylhexanoyl chloride)

15. REGULATORY INFORMATION

SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3,5,5-Trimethylhexanoyl chloride	36727-29-4	

New Jersey Right To Know Components

	CAS-No.	Revision Date
3,5,5-Trimethylhexanoyl chloride	36727-29-4	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity

Aquatic Chronic	Chronic aquatic toxicity
Eye Dam.	Serious eye damage
H290	May be corrosive to metals.
H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H330	Fatal if inhaled.

HMIS Rating

Health hazard:	4
Chronic Health Hazard:	
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	4
Fire Hazard:	1
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.4

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