

SAFETY DATA SHEET

Version 5.2
Revision Date 07/08/2014
Print Date 11/15/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 3,5,5-Trimethylhexanoic acid

Product Number : S415006

Brand : Aldrich

CAS-No. : 3302-10-1

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)

Acute toxicity, Oral (Category 4), H302

Skin irritation (Category 2), H315

Serious eye damage (Category 1), H318

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)

H302

Harmful if swallowed.

H315

Causes skin irritation.

H318

Causes serious eye damage.

Precautionary statement(s)

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P280

Wear protective gloves/ eye protection/ face protection.

P301 + P312

IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.

P302 + P352

IF ON SKIN: Wash with plenty of soap and water.

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.
P321	Specific treatment (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula	: C ₉ H ₁₈ O ₂
Molecular Weight	: 158.24 g/mol
CAS-No.	: 3302-10-1
EC-No.	: 221-975-0

Hazardous components

Component	Classification	Concentration
3,5,5-Trimethylhexanoic acid		
	Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; H302, H315, H318	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

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

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

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

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

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. 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.

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

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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, 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

Do not let product enter drains.

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	4.4 at 0.1 g/l at 25 °C (77 °F)
e) Melting point/freezing point	Melting point/freezing point: -77 °C (-107 °F)
f) Initial boiling point and boiling range	236 °C (457 °F) at 1,013 hPa (760 mmHg) - OECD Test Guideline 103
g) Flash point	117 °C (243 °F) - closed cup
h) Evaporation rate	no data available
i) Flammability (solid, gas)	no data available
j) Upper/lower flammability or explosive limits	no data available
k) Vapour pressure	0.0046 hPa (0.0035 mmHg) at 20 °C (68 °F)
l) Vapour density	no data available
m) Relative density	0.8996 g/cm ³ at 20 °C (68 °F)
n) Water solubility	0.7 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - slightly soluble
o) Partition coefficient: n-octanol/water	log Pow: 2.833log Pow: 3.2 at 25 °C (77 °F)
p) Auto-ignition temperature	415 °C (779 °F) at 1,009 hPa (757 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

Surface tension	35.3 mN/m at 0.63 at 20 °C (68 °F)
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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

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - rat - male and female - 1,160 mg/kg
(OECD Test Guideline 401)

Inhalation: no data available

Dermal: no data available

no data available

Skin corrosion/irritation

Skin - rabbit

Result: Irritating to skin. - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - rabbit

Result: Risk of serious damage to eyes. - 72 h
(OECD Test Guideline 405)

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

Hamster

fibroblast

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

Repeated dose toxicity - rat - male and female - 28 d - No observed adverse effect level - 50 mg/kg - Lowest observed adverse effect level - 200 mg/kg

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 122 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - 68 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	Growth inhibition EC50 - Pseudokirchneriella subcapitata (green algae) - 81 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - 470 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 21 d Result: 96 % - Readily biodegradable. (OECD Test Guideline 301A)
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12.3 Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 1 mg/l Bioconcentration factor (BCF): 0.5 - 1.7 (OECD Test Guideline 305)
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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

no data available

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.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

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-Trimethylhexanoic acid	3302-10-1	

New Jersey Right To Know Components

	CAS-No.	Revision Date
3,5,5-Trimethylhexanoic acid	3302-10-1	

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
Eye Dam.	Serious eye damage
H302	Harmful if swallowed.
H315	Causes skin irritation.
H318	Causes serious eye damage.
Skin Irrit.	Skin irritation

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	2
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

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