SIGMA-ALDRICH

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SAFETY DATA SHEET

Version 3.8 Revision Date 07/02/2014 Print Date 11/11/2015

1. PRODUCT AND COMPANY IDENTIFICATION

| 1.1 | Product identifiers Product name | : | Etiocholanone solution | |
|-----|---|-----|--|--|
| | Product Number Brand Index-No. | : | 32833 Fluka 608-001-00-3 | |
| | CAS-No. | : | 53-42-9 | |
| 1.2 | Relevant identified uses of the substance or mixture and uses advised against | | | |
| | Identified uses | : | Laboratory chemicals, Manufacture of substances | |
| 1.3 | 3 Details of the supplier of the safety data sheet | | | |
| | Company | : | Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA | |
| | Telephone Fax | : | +1 800-325-5832 +1 800-325-5052 | |
| 1.4 | Emergency telephone num | nbe | r | |

1.4 Emergency telephone numbe

| Emergency Phone # | : | (314) 776-6555 |
|-------------------|---|----------------|
| | | |

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 2), H225 Acute toxicity, Oral (Category 4), H302 Acute toxicity, Inhalation (Category 4), H332 Acute toxicity, Dermal (Category 4), H312 Eye irritation (Category 2A), H319

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) H225 H302 + H312 + H332 H319 | Highly flammable liquid and vapour. Harmful if swallowed, in contact with skin or if inhaled Causes serious eye irritation. |
| Precautionary statement(s) P210 P233 P240 P241 P242 | Keep away from heat/sparks/open flames/hot surfaces No smoking. Keep container tightly closed. Ground/bond container and receiving equipment. Use explosion-proof electrical/ ventilating/ lighting/ equipment. Use only non-sparking tools. |

| P243 | Take precautionary measures against static discharge. |
|--------------------|--|
| P261 | Avoid breathing 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. |
| P280 | Wear protective gloves/ protective clothing/ eye protection/ face protection. |
| P301 + P312 | IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell. |
| 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. |
| P312 | Call a POISON CENTER or doctor/ physician if you feel unwell. |
| P322 | Specific measures (see supplemental first aid instructions on this label). |
| P330 | Rinse mouth. |
| P337 + P313 | If eye irritation persists: Get medical advice/ attention. |
| P363 | Wash contaminated clothing before reuse. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction. |
| P403 + P235 | Store in a well-ventilated place. Keep cool. |
| 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

3.2 Mixtures

| Synonyms | : | 5β-Androsterone 3α-Hydroxy-5β-androstan-17-one Etiocholan-3α-ol-17-one |
|------------------|---|--|
| Formula | : | C ₁₉ H ₃₀ O ₂ |
| Molecular Weight | : | 290.44 g/mol |

Hazardous components

| Component | | Classification | Concentration | |
|---|-----------------------|---------------------------------|---------------|--|
| Acetonitrile | | | | |
| CAS-No. | 75-05-8 | Flam. Liq. 2; Acute Tox. 4; Eye | 90 - 100 % | |
| EC-No. | 200-835-2 | Irrit. 2A; H225, H302 + H312 + | | |
| Index-No. | 608-001-00-3 | H332, H319 | | |
| Registration number | 01-2119471307-38-XXXX | | | |
| For the full text of the H-Statements mentioned in this Section, see Section 16 | | | | |

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

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

5.2 Special hazards arising from the substance or mixture no data available

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

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. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low 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.

6.3 Methods and materials for containment and cleaning up Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

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. Use explosion-proof equipment.Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge. 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.

Recommended storage temperature: 2 - 8 °C

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

| Component | CAS-No. | Value | Control parameters | Basis |
|--------------|---------|---------------|--------------------------|--|
| Acetonitrile | 75-05-8 | TWA | 20 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Lower Resp | iratory Tract irritation | on |
| | | Not classifia | ble as a human ca | rcinogen |
| | | Danger of cu | utaneous absorptio | n |
| | | TWA 20 ppm | | USA. NIOSH Recommended |
| | | | 34 mg/m3 | Exposure Limits |
| | | Forms cyani | de in the body. | |
| | | TWA 40 ppm | | USA. Occupational Exposure Limits |
| | | | 70 mg/m3 | (OSHA) - Table Z-1 Limits for Air |
| | | | _ | Contaminants |
| | | The value in | mg/m3 is approxir | mate. |
| | | TWA | 40 ppm | USA. OSHA - TABLE Z-1 Limits for |
| | | | 70 mg/m3 | Air Contaminants - 1910.1000 |
| | | STEL | 60 ppm | USA. OSHA - TABLE Z-1 Limits for |
| | | | 105 mg/m3 | Air Contaminants - 1910.1000 |

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, Flame retardant antistatic 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 multipurpose 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

| a) | Appearance | Form: liquid, clear |
|----|---|-----------------------------------|
| b) | Odour | pungent |
| c) | Odour Threshold | no data available |
| d) | рН | no data available |
| e) | Melting point/freezing point | -48.0 °C (-54.4 °F) |
| f) | Initial boiling point and boiling range | 81.0 - 82.0 °C (177.8 - 179.6 °F) |

| | g) | Flash point | 2.0 °C (35.6 °F) - closed cup | | |
|----|--------------------------|--|---|--|--|
| | h) | Evapouration rate | 5.8 | | |
| | i) | Flammability (solid, gas) | no data available | | |
| | j) | Upper/lower flammability or explosive limits | Upper explosion limit: 16 %(V) Lower explosion limit: 4.4 %(V) | | |
| | k) | Vapour pressure | 97.1 hPa (72.8 mmHg) at 20.0 °C (68.0 °F) | | |
| | I) | Vapour density | no data available | | |
| | m) | Relative density | 0.78 g/cm3 | | |
| | n) | Water solubility | soluble | | |
| | o) | Partition coefficient: n- octanol/water | log Pow: -0.34 | | |
| | p) | Auto-ignition temperature | 523.0 °C (973.4 °F) | | |
| | q) | Decomposition temperature | no data available | | |
| | r) | Viscosity | no data available | | |
| | s) | Explosive properties | no data available | | |
| | t) | Oxidizing properties | no data available | | |
| | Oth | ner safety information | | | |
| | | Surface tension | 29.0 mN/m at 20.0 °C (68.0 °F) | | |
| SI | STABILITY AND REACTIVITY | | | | |
| 1 | Dor | octivity | | | |

10. 5

10.1 Reactivity

9.2

no data available

10.2 Chemical stability Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions Vapours may form explosive mixture with air.

10.4 Conditions to avoid Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials acids, Bases, Oxidizing agents, Reducing agents, Alkali metals

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 - 1,320 - 6,690 mg/kg

LC50 Inhalation - mouse - 4 h - 3587 ppm (OECD Test Guideline 403)

LC50 Inhalation - rat - 4 h - 26.8 mg/l

LD50 Dermal - rabbit - male and female - > 2,000 mg/kg (OECD Test Guideline 402)

no data available

Skin corrosion/irritation

Skin - rabbit Result: No skin irritation (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - rabbit Result: Irritating to eyes. (OECD Test Guideline 405)

Respiratory or skin sensitisation

Buehler Test - guinea pig Did not cause sensitisation on laboratory animals. (OECD Test Guideline 406)

Germ cell mutagenicity

Hamster ovary Result: negative Mutation in mammalian somatic cells.

Ames test S. typhimurium Result: Not mutagenic in Ames Test.

Hamster ovary Result: Equivocal evidence. Sister chromatid exchange

Mutagenicity (micronucleus test) mouse Result: Positive results were obtained in some in vivo tests.

Carcinogenicity

No evidence of carcinogenicity in animal studies (when indicated)

- 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.
- 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

Animal testing did not show any effects on fertility.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

Additional Information

RTECS: Not available

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death

Lungs - Lung oedema - Based on Human Evidence - Fever (3α-Hydroxy-5β-androstan-17-one)

12. ECOLOGICAL INFORMATION

12.1 Toxicity

| Toxicity to fish | LC50 - Pimephales promelas (fathead minnow) - 1,640.00 mg/l - 96 h | | |
|---|--|--|--|
| | NOEC - Oryzias latipes - 102 mg/l - 21 d | | |
| Toxicity to daphnia and other aquatic invertebrates | EC50 - Daphnia magna (Water flea) - 3,600 mg/l - 48 h (OECD Test Guideline 202) | | |
| | | | |

NOEC - Daphnia magna (Water flea) - 160 mg/l - 21 d

12.2 Persistence and degradability Result: 84 % - Readily biodegradable. Biodegradability (OECD Test Guideline 301C)

12.3 Bioaccumulative potential No bioaccumulation is to be expected (log Pow <= 4).

12.4 Mobility in soil

Not expected to adsorb on soil.

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

Avoid release to the environment.

Stability in water

Remarks: Hydrolyses slowly.

13. DISPOSAL CONSIDERATIONS

Waste treatment methods 13.1

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. 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)

| UN number: 1648 Proper shipping name Marine pollutant: No Poison Inhalation Haz | Class: 3 e: Acetonitrile, solution eard: No | Packing group: II | |
|--|---|---------------------------|------------------|
| IMDG UN number: 1648 Proper shipping name Marine pollutant: No | Class: 3 e: ACETONITRILE, SOLU | Packing group: II TION | EMS-No: F-E, S-D |
| ΙΑΤΑ | | | |

Packing group: II

UN number: 1648 Class: 3

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

The following components are subject to reporting levels established by SARA Title III, Section 313:

| | CAS-No. | Revision Date |
|---|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01 |
| SARA 311/312 Hazards Fire Hazard, Acute Health Hazard, Chronic Health Hazard | | |
| Massachusetts Right To Know Components | | |
| | CAS-No. | Revision Date |
| Acetonitrile | 75-05-8 | 2007-07-01 |
| Pennsylvania Right To Know Components | | |
| | CAS-No. | Revision Date |
| Acetonitrile | 75-05-8 | 2007-07-01 |
| New Jersey Right To Know Components | | |
| | CAS-No. | Revision Date |
| Acetonitrile | 75-05-8 | 2007-07-01 |
| | | |

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 Irrit. | Eye irritation |
| Flam. Liq. | Flammable liquids |
| H225 | Highly flammable liquid and vapour. |
| H302 | Harmful if swallowed. |
| H302 + H312 + | Harmful if swallowed, in contact with skin or if inhaled |
| H332 | |
| H312 | Harmful in contact with skin. |
| H319 | Causes serious eye irritation. |
| H332 | Harmful if inhaled. |
| HMIS Rating | |

HMIS Rating

| Health hazard: | 3 | |
|------------------------|---|--|
| Chronic Health Hazard: | * | |
| Flammability: | 3 | |
| Physical Hazard | 0 | |
| NFPA Rating | | |
| Health hazard: | | |

| Health hazard: | 2 |
|--------------------|---|
| Fire Hazard: | 3 |
| 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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