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 : 32833
Brand : Fluka
Index-No. : 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 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 # : (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 Highly flammable liquid and vapour.
H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled
H319 Causes serious eye irritation.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 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 Irrit. 2A; H225, H302 + H312 + H332, H319	90 - 100 %
EC-No.	200-835-2		
Index-No.	608-001-00-3		
Registration number	01-2119471307-38-XXXX		

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 Respiratory Tract irritation Not classifiable as a human carcinogen Danger of cutaneous absorption		
		TWA	20 ppm 34 mg/m3	USA. NIOSH Recommended Exposure Limits
		Forms cyanide in the body.		
		TWA	40 ppm 70 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	40 ppm 70 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	60 ppm 105 mg/m3	USA. OSHA - TABLE Z-1 Limits for 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 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.

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)	pH	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)
l)	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

9.2 Other safety information

Surface tension	29.0 mN/m at 20.0 °C (68.0 °F)

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
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

Biodegradability: Result: 84 % - Readily biodegradable. (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

13.1 Waste treatment methods

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 Class: 3 Packing group: II
Proper shipping name: Acetonitrile, solution
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 1648 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: ACETONITRILE, SOLUTION
Marine pollutant: No

IATA
UN number: 1648 Class: 3 Packing group: II

Proper shipping name: Acetonitrile, solution

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 + H332	Harmful if swallowed, in contact with skin or if inhaled
H312	Harmful in contact with skin.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

HMIS Rating

Health hazard:	3
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	0

NFPA Rating

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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