

Revision Date 28-Nov-2013

**Revision Number 3** 

# SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

#### 1.1. Product identifier

Product Description: (S)-3-Amino-3-phenylpropanoic acid ethyl ester hydrochloride

Cat No.: 362040000; 362040010; 362040050, 362040250

Synonyms None.

CAS-No 167834-24-4

Molecular Formula C11 H15 N O2 . H Cl

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

Recommended Use Laboratory chemicals Uses advised against No Information available

### 1.3. Details of the supplier of the safety data sheet

**Company** Acros Organics BVBA

Janssen Pharmaceuticalaan 3a

2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99 **CHEMTREC** Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

### **SECTION 2: HAZARDS IDENTIFICATION**

#### 2.1. Classification of the substance or mixture

### CLP Classification - Regulation (EC) No 1272/2008

Based on available data, the classification criteria are not met

Physical hazards

Based on available data, the classification criteria are not met

#### Health hazards

Based on available data, the classification criteria are not met

#### **Environmental hazards**

Based on available data, the classification criteria are not met

#### Classification according to EU Directives 67/548/EEC or 1999/45/EC

R-phrase(s) none

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

#### 2.2. Label elements

**Hazard Statements** 

**Precautionary Statements** 

2.3. Other hazards

No information available.

### **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### 3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008	DSD Classification - 67/548/EEC
(S)-3-Amino-3-phenylpropanoic acid ethyl ester hydrochloride	167834-24-4		>95	-	-

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

### **SECTION 4: FIRST AID MEASURES**

#### 4.1. Description of first aid measures

**Eye Contact** Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Obtain

medical attention.

Skin Contact Wash off immediately with soap and plenty of water while removing all contaminated clothes

and shoes. Obtain medical attention.

**Ingestion** Clean mouth with water. Get medical attention.

**Inhalation** Remove from exposure, lie down. Move to fresh air. If breathing is difficult, give oxygen. If not

breathing, give artificial respiration. Obtain medical attention.

**Protection of First-aiders** No special precautions required.

4.2. Most important symptoms and effects, both acute and delayed

No information available

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically

### **SECTION 5: FIREFIGHTING MEASURES**

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Substance is nonflammable; use agent most appropriate to extinguish surrounding fire..

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### Extinguishing media which must not be used for safety reasons

No information available.

#### 5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors

#### **Hazardous Combustion Products**

None under normal use conditions.

#### 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

### **SECTION 6: ACCIDENTAL RELEASE MEASURES**

#### 6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation

### 6.2. Environmental precautions

See Section 12 for additional ecological Information.

#### 6.3. Methods and material for containment and cleaning up

Sweep up or vacuum up spillage and collect in suitable container for disposal. Do not let this chemical enter the environment.

#### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

### **SECTION 7: HANDLING AND STORAGE**

### 7.1. Precautions for safe handling

Avoid contact with skin and eyes. Do not breathe dust. Do not ingest.

### 7.2. Conditions for safe storage, including any incompatibilities

Keep in a dry, cool and well-ventilated place. Keep container tightly closed.

#### 7.3. Specific end use(s)

Use in laboratories

### **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

#### 8.1. Control parameters

### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies.

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Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

Derived No Effect Level (DNEL) No information available.

Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral				
Dermal				
Inhalation				

Predicted No Effect Concentration

(PNEC)

No information available.

8.2. Exposure controls

**Engineering Measures** 

None under normal use conditions..

Personal protective equipment

**Eye Protection** Safety glasses with side-shields (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber Nitrile rubber Neoprene PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. Remove gloves with care avoiding skin contamination.

**Skin and body protection**Wear appropriate protective gloves and clothing to prevent skin exposure

**Respiratory Protection** No protective equipment is needed under normal use conditions.

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are

exceeded or if irritation or other symptoms are experienced..

Recommended Filter type: Particle filter.

Small scale/Laboratory use Maintain adequate ventilation

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice

**Environmental exposure controls** No information available.

### **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

#### 9.1. Information on basic physical and chemical properties

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### (S)-3-Amino-3-phenylpropanoic acid ethyl ester hydrochloride

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**Appearance** White

Physical State Powder, Solid.

Odor No information available
Odor Threshold No data available
pH No information available.

Melting Point/Range117°C / 242.6°FSoftening PointNo data available

Boiling Point/Range No information available.

Flash Point No information available. Method - No information available.

Evaporation Rate Not applicable Solid

Flammability (solid,gas) No information available. Explosion Limits No data available.

Explosion Limits

Vapor PressureNo data availableVapor DensityNot applicable

Specific Gravity / DensityNo data availableBulk DensityNo data availableWater SolubilityNo information available.Solubility in other solventsNo information available.

Partition Coefficient (n-

octanol/water)

Autoignition Temperature Not applicable

Decomposition temperature No data available

Viscosity

Not applicable

No information available

**Explosive Properties**No information available. **Oxidizing Properties**No information available.

9.2. Other information

Molecular Formula C11 H15 N O2 . H Cl

Molecular Weight 229.71

### **SECTION 10: STABILITY AND REACTIVITY**

Solid

Solid

10.1. Reactivity

None known, based on information available.

10.2. Chemical stability

Stable under normal conditions

10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions No information available.

10.4. Conditions to avoid

Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases.

10.6. Hazardous decomposition products

None under normal use conditions.

### **SECTION 11: TOXICOLOGICAL INFORMATION**

### 11.1. Information on toxicological effects

#### **Product Information**

(a) acute toxicity:

Based on available data, the classification criteria are not met Oral

**Dermal** No data available Inhalation No data available

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
(S)-3-Amino-3-phenylpropanoic acid ethyl	>2500 mg/kg (Rat)		
ester hydrochloride			

(b) skin corrosion/irritation; No data available

No data available (c) serious eye damage/irritation;

(d) respiratory or skin sensitization;

No data available Respiratory Skin No data available

(e) germ cell mutagenicity; No data available

No data available (f) carcinogenicity;

There are no known carcinogenic chemicals in this product

No data available (g) reproductive toxicity; No data available (h) STOT-single exposure;

(i) STOT-repeated exposure; No data available

> **Target Organs** No information available.

(j) aspiration hazard; Not applicable

Solid

Other Adverse Effects Symptoms / effects, both acute and delayed The toxicological properties have not been fully investigated.

No information available.

### **SECTION 12: ECOLOGICAL INFORMATION**

12.1. Toxicity

**Ecotoxicity effects** Do not empty into drains. No information available 12.2. Persistence and degradability No information available. 12.3. Bioaccumulative potential

12.5. Results of PBT and vPvB

assessment

12.4. Mobility in soil

No data available for assessment

No information available.

12.6. Other adverse effects

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**Endocrine Disruptor Information Persistent Organic Pollutant** 

**Ozone Depletion Potential** 

This product does not contain any known or suspected endocrine disruptors

This product does not contain any known or suspected substance This product does not contain any known or suspected substance

### **SECTION 13: DISPOSAL CONSIDERATIONS**

13.1. Waste treatment methods

Waste from Residues / Unused

**Products** 

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure

complete and accurate classification.

Contaminated Packaging Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use

empty containers.

**European Waste Catalogue (EWC)** 

According to the European Waste Catalogue, Waste Codes are not product specific, but

application specific

Other Information Waste codes should be assigned by the user based on the application for which the product

was used

### **SECTION 14: TRANSPORT INFORMATION**

IMDG/IMO Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

ADR Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

IATA Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required

14.7. Transport in bulk according to Annex II of MARPOL73/78 and the

Not applicable, packaged goods

**IBC Code** 

### **SECTION 15: REGULATORY INFORMATION**

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

**International Inventories** X = listed

#### **National Regulations**

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment Take note of Dir 94/33/EC on the protection of young people at work

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Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work

#### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

### **SECTION 16: OTHER INFORMATION**

#### Full text of R-phrases referred to under sections 2 and 3

Not applicable

Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical

Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - China Inventory of Existing Chemical Substances

**KECL** - Existing and Evaluated Chemical Substances

WEL - Workplace Exposure Limit

**ACGIH** - American Conference of Industrial Hygiene

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent. Bioaccumulative. Toxic

ADR - European Agreement Concerning the International Carriage of

Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime

Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

Key literature references and sources for data

Suppliers safety data sheet,

Chemadvisor - LOLI,

Merck index.

**RTECS** 

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic

Substances List

**ENCS** - Japan Existing and New Chemical Substances AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air

Transport Association

MARPOL - International Convention for the Prevention of Pollution from

Ships

ATE - Acute Toxicity Estimate

VOC - Volatile Organic Compounds

### **Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

28-Nov-2013 **Revision Date** 

**Revision Summary** 

Reason for revision Not applicable

### This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

#### **Disclaimer**

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

# **End of Safety Data Sheet**