

## Efavirenz Related Compound A

### SECTION 1: Identification of the substance/mixture and of the company/undertaking

#### 1.1 Product identifiers

Product name : Efavirenz Related Compound A

Product Number : 1234125  
Brand : US Pharmacopeia  
CAS-No. : 209414-27-7

#### 1.2 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich (Shanghai) Trading Co.Ltd.  
509 Renqing Road  
Zhangjiang High Tech East Park, Pudong  
SHANGHAI  
201201 SHANGHAI  
CHINA

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Merck KGaA  
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Phone: +49 6151 72-0

Telephone : +86 21 6141-5566  
Fax : +86 21 6141-5567

#### 1.3 Emergency telephone

Emergency Phone # : +86 532 83889090

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

Identified uses : For R&D use only. Not for pharmaceutical, household or other uses.

### SECTION 2: Hazards identification

#### Summary of emergency

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



Wash off with soap and plenty of water. Flush eyes with water as a precaution. Never give anything by mouth to an unconscious person., Rinse mouth with water.

## 2.1 GHS Classification

Not a hazardous substance or mixture.

## 2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

## 2.3 Physical and chemical hazards

Referring to current information, no physical or chemical hazard.

## 2.4 Health hazards

Referring to current information, no health hazard.

## 2.5 Environmental hazards

Referring to current information, no environmental hazard.

## 2.6 Other hazards

Possible sensitizer.

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## SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

### 3.1 Substances

Synonyms : (S)-1-(2-Amino-5-chlorophenyl)-1-(trifluoromethyl)-3-cyclopropyl-2-propyn-1-ol, (S)-2-(2-Amino-5-chlorophenyl)-4-cyclopropyl

Formula : C<sub>13</sub>H<sub>11</sub>ClF<sub>3</sub>NO

Molecular weight : 289.68 g/mol

CAS-No. : 209414-27-7

No components need to be disclosed according to the applicable regulations.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### If inhaled

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

#### In case of skin contact

Wash off with soap and plenty of water.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water.

### 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



#### 4.4 Notes to physician

No data available

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### SECTION 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  
Nitrogen oxides (NO<sub>x</sub>)  
Hydrogen chloride gas  
Hydrogen fluoride

#### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

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### SECTION 6: Accidental release measures

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

Avoid dust formation. Avoid breathing vapors, mist or gas.  
For personal protection see section 8.

#### 6.2 Environmental precautions

No special environmental precautions required.

#### 6.3 Methods and materials for containment and cleaning up

Sweep up and shovel. Keep in suitable, closed containers for disposal.

#### 6.4 Reference to other sections

For disposal see section 13.

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### SECTION 7: Handling and storage

#### 7.1 Precautions for safe handling

##### Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.

##### Hygiene measures

General industrial hygiene practice.  
For precautions see section 2.2.

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

##### Storage conditions

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

##### Storage stability

Recommended storage temperature  
2 - 8 °C

##### Storage class

Storage class (TRGS 510): 11: Combustible Solids



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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **8.2 Exposure controls**

#### **Appropriate engineering controls**

General industrial hygiene practice.

#### **Personal protective equipment**

##### **Eye/face protection**

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### **Body Protection**

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### **Respiratory protection**

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### **Control of environmental exposure**

No special environmental precautions required.

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## **SECTION 9: Physical and chemical properties**

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

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| a) Physical state                          | solid                                      |
| b) Color                                   | No data available                          |
| c) Odor                                    | No data available                          |
| d) Melting point/freezing point            | Melting point/freezing point: 139 - 141 °C |
| e) Initial boiling point and boiling range | No data available                          |
| f) Flammability (solid, gas)               | No data available                          |
| g) Upper/lower                             | No data available                          |



|    |  |  |
|----|--|--|
|    | flammability or explosive limits       |  |
| h) | Flash point                            | No data available  |
| i) | Autoignition temperature               | No data available  |
| j) | Decomposition temperature              | No data available  |
| k) | pH                                     | No data available  |
| l) | Viscosity                              | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) | Water solubility                       | No data available  |
| n) | Partition coefficient: n-octanol/water | No data available  |
| o) | Vapor pressure                         | No data available  |
| p) | Density                                | No data available  |
|    | Relative density                       | No data available  |
| q) | Relative vapor density                 | No data available  |
| r) | Particle characteristics               | No data available  |
| s) | Explosive properties                   | No data available  |
| t) | Oxidizing properties                   | No data available  |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Chemical stability

Stable under recommended storage conditions.

### 10.2 Possibility of hazardous reactions

No data available

### 10.3 Conditions to avoid

No data available

### 10.4 Incompatible materials

Strong oxidizing agents

### 10.5 Hazardous decomposition products

In the event of fire: see section 5



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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

Oral: No data available

Inhalation: No data available

Dermal: No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitization**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

No data available

#### **Reproductive toxicity**

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

### **11.2 Additional Information**

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

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

No data available

### **12.2 Persistence and degradability**

No data available

### **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 Endocrine disrupting properties**

No data available

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The life science business of Merck operates as MilliporeSigma in the US and Canada



## 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: -

IMDG: -

IATA-DGR: -

### 14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA-DGR: Not dangerous goods

### 14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA-DGR: -

### 14.4 Packaging group

ADR/RID: -

IMDG: -

IATA-DGR: -

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

### 14.6 Special precautions for user

### 14.7 Incompatible materials

Strong oxidizing agents

#### Further information

Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15: Regulatory information

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

#### National regulatory information

#### Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

: B1A222212749

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.



**Other regulations**

Please pay attention on the waste treatment should also comply with local regulations requirement.

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**SECTION 16: Other information****Further information**

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