

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 4.0 Revision Date 26.12.2010

Print Date 25.09.2011

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING**1.1 Product identifiers**

Product name : [6,6]-Phenyl C₈₅ butyric acid methyl ester, mixture of isomers

Product Number : 684473
Brand : Aldrich
CAS-No. : 905843-95-0

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 (Shanghai) Trading Co.,Ltd
41F K. Wah Centre
1010 Huai Hai Zhong Road
200031 SHANGHAI
CHINA

Telephone : +86 21-61415566
Fax : +86 21-61415567
E-mail address : china@sial.com

1.4 Emergency telephone number

Emergency Phone # : +8615021113336

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture****Classification according to Regulation (EC) No 1272/2008 [EU-GHS/CLP]**

Skin irritation (Category 2)

Eye irritation (Category 2)

Specific target organ toxicity - single exposure (Category 3)

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

Irritating to eyes, respiratory system and skin.

2.2 Label elements**Labelling according Regulation (EC) No 1272/2008 [CLP]**

Pictogram



Signal word

Warning

Hazard statement(s)

H315

Causes skin irritation.

H319

Causes serious eye irritation.

H335

May cause respiratory irritation.

Precautionary statement(s)

P261

Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove

contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard Statements none

According to European Directive 67/548/EEC as amended.

Hazard symbol(s)



R-phrase(s)

R36/37/38

Irritating to eyes, respiratory system and skin.

S-phrase(s)

S26

In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S36/37

Wear suitable protective clothing and gloves.

2.3 Other hazards - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : [84]PCBM
Methyl 3'-phenyl-3'H-cyclopropa[18,7][5,6]fullerene-C84-D2d-3'-butanoate

Formula : C₉₆H₁₄O₂

Molecular Weight : 1.199,14 g/mol

Component	Concentration
[6,6]-Phenyl C85 butyric acid methyl ester, mixture of isomers	
CAS-No. 905843-95-0	-

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.

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

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

4.3 Indication of immediate medical attention and special treatment needed

no data available

5. FIRE-FIGHTING 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 Precautions for fire-fighters**
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 dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.
- 6.2 Environmental precautions**
Do not let product enter drains.
- 6.3 Methods and materials for containment and cleaning up**
Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.
- 7.2 Conditions for safe storage, including any incompatibilities**
Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

Handle under inert gas. Protect from moisture.
- 7.3 Specific end uses**
no data available

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

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

Safety glasses with side-shields conforming to EN166 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 EU Directive 89/686/EEC and the standard EN 374 derived from it.

Body Protection

impervious 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

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

9. PHYSICAL AND CHEMICAL PROPERTIES**9.1 Information on basic physical and chemical properties**

- | | |
|---|-------------------|
| a) Appearance | Form: solid |
| b) Odour | no data available |
| c) Odour Threshold | no data available |
| d) pH | no data available |
| e) Melting/freezing point | no data available |
| f) Initial boiling point and boiling range | no data available |
| g) Flash point | no data available |
| 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 | no data available |
| l) Vapour density | no data available |
| m) Relative density | no data available |
| n) Water solubility | no data available |
| o) Partition coefficient: n-octanol/water | no data available |
| p) Autoignition temperature | no data available |
| 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

no data available

10. STABILITY AND REACTIVITY**10.1 Reactivity**

no data available

10.2 Chemical stability

no data available

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
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

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.

Reproductive toxicity
no data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes serious eye irritation.

Signs and Symptoms of Exposure

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

Additional Information
RTECS: Not available

12. ECOLOGICAL INFORMATION

12.1 Toxicity
no data available

12.2 Persistence and degradability
no data available

12.3 Bioaccumulative potential
no data available

