

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : 1,3-Dimethyl-8-phenylxanthine

Product Number : P2278

Brand : Sigma

CAS-No. : 961-45-5

#### 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 # : +1-703-527-3887 (CHEMTREC)

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

#### 2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

#### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Synonyms : 8-Phenyltheophylline

Formula :  $C_{13}H_{12}N_4O_2$

Molecular Weight : 256.26 g/mol

CAS-No. : 961-45-5

No ingredients are hazardous according to OSHA criteria.

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

### 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

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**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>)

**5.3 Advice for firefighters**

Wear self contained breathing apparatus for fire fighting if necessary.

**5.4 Further information**

no data available

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**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

Avoid dust formation. Avoid breathing vapours, mist or gas.

For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**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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**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

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.

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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**8. EXPOSURE CONTROLS/PERSONAL PROTECTION****8.1 Control parameters****Components 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.

### 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

Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

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|---|---|
| a) Appearance                                   | Form: crystalline<br>Colour: white              |
| b) Odour  | no data available                               |
| c) Odour Threshold                              | no data available                               |
| d) pH   | no data available                               |
| e) Melting point/freezing point                 | Melting point/range: > 300 °C (> 572 °F) - lit. |
| 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) Auto-ignition 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

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## 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

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

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

no data available

Inhalation: no data available

Dermal: no data available

no data available

#### Skin corrosion/irritation

no data available

#### Serious eye damage/eye irritation

no data available

#### Respiratory or skin sensitisation

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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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

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

**Additional Information**

RTECS: UO8445700

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

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**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 Other adverse effects**

no data available

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**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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**14. TRANSPORT INFORMATION****DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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**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**

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

No SARA Hazards

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

1,3-Dimethyl-8-phenylxanthine

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961-45-5

Revision Date

**New Jersey Right To Know Components**

1,3-Dimethyl-8-phenylxanthine

CAS-No.  
961-45-5

Revision Date

**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.

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**16. OTHER INFORMATION****HMIS Rating**

Health hazard: 0

Chronic Health Hazard:

Flammability: 0

Physical Hazard 0

**NFPA Rating**

Health hazard: 0

Fire Hazard: 0

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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