

**SAFETY DATA SHEET**

Version 5.5

Revision Date 08/23/2014

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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Meptyldinocap

Product Number : 32098

Brand : Sigma-Aldrich

CAS-No. : 131-72-6

**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****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 4), H332

Skin irritation (Category 2), H315

Skin sensitisation (Category 1), H317

Reproductive toxicity (Category 1B), H360

Specific target organ toxicity - repeated exposure, Oral (Category 2), H373

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

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)

H302 + H332

Harmful if swallowed or if inhaled

H315

Causes skin irritation.

H317

May cause an allergic skin reaction.

H360

May damage fertility or the unborn child.

H373

May cause damage to organs through prolonged or repeated exposure if swallowed.

H410

Very toxic to aquatic life with long lasting effects.

|                            |  |
|----------------------------|--|
| Precautionary statement(s) |  |
| P201                       | Obtain special instructions before use.  |
| P202                       | Do not handle until all safety precautions have been read and understood.                        |
| P260                       | Do not breathe 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.  |
| P272                       | Contaminated work clothing should not be allowed out of the workplace.                           |
| P273                       | Avoid release to the environment.  |
| P280                       | Wear protective gloves.  |
| P301 + P312                | IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.                      |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.  |
| P304 + P340                | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. |
| P308 + P313                | IF exposed or concerned: Get medical advice/ attention.  |
| P321                       | Specific treatment (see supplemental first aid instructions on this label).                      |
| P330                       | Rinse mouth.   |
| P333 + P313                | If skin irritation or rash occurs: Get medical advice/ attention.                                |
| P362                       | Take off contaminated clothing and wash before reuse.  |
| P391                       | Collect spillage.  |
| P405                       | Store locked up.   |
| 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

#### 3.1 Substances

|                  |   |  |
|------------------|---|--|
| Synonyms         | : | 2-(1-Methylheptyl)-4,6-dinitrophenyl (2E)-2-butenoate<br>(RS)-2-(1-Methylheptyl)-4,6-dinitrophenyl crotonate |
| Formula          | : | C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>  |
| Molecular weight | : | 364.39 g/mol   |
| CAS-No.          | : | 131-72-6   |

#### Hazardous components

| Component   | Classification  | Concentration |
|---|---|---------------|
| <b>Mixture of 2,4-dinitro-6-octylphenyl crotonate and 2,6-dinitro-4-octylphenyl crotonate</b> |   |               |
|   | Acute Tox. 4; Skin Irrit. 2; Skin Sens. 1; Repr. 1B; STOT RE 2; Aquatic Acute 1; Aquatic Chronic 1; H302 + H332, H315, H317, H360, H373, H410 | -             |

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**

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

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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 (NOx)

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting 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**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe 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. Discharge into the environment must be avoided.

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

Soak up with inert absorbent material and dispose of as hazardous waste. 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**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

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

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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**

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

Face shield and safety glasses 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, 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. Discharge into the environment must be avoided.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

|   |  |
|---|--|
| a) Appearance                                   | Form: liquid<br>Colour: yellow, brown                |
| b) Odour  | characteristic                                       |
| c) Odour Threshold                              | No data available                                    |
| d) pH   | No data available                                    |
| e) Melting point/freezing point                 | Melting point/range: -22.5 °C (-8.5 °F)              |
| f) Initial boiling point and boiling range      | 138 - 140 °C (280 - 284 °F) at 0.07 hPa (0.05 mmHg)  |
| 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                             | 1.10 g/cm3 at 20 °C (68 °F)                          |
| n) Water solubility                             | 0.00025 g/l at 20 °C (68 °F) - practically insoluble |
| o) Partition coefficient: n-octanol/water       | log Pow: 4.54 at 20 °C (68 °F)                       |
| 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

Exposure to light. Avoid heating above: 30°C

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - female - 1,212 mg/kg

LC50 Inhalation - Rat - 4 h - > 3 mg/l

LD50 Dermal - Rabbit - > 2,000 mg/kg

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: irritating

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Mild eye irritation

#### Respiratory or skin sensitisation

- Guinea pig

Result: May cause sensitisation by skin contact.

#### 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

Experiments have shown reproductive toxicity effects on laboratory animals. Presumed human reproductive toxicant May damage the unborn child.

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

Ingestion - May cause damage to organs through prolonged or repeated exposure.

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

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

Toxicity to fish LC50 - Lepomis macrochirus (Bluegill sunfish) - 0.062 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia (water flea) - 0.0041 mg/l - 48 h

Toxicity to algae EbC50 - Pseudokirchneriella subcapitata - 4.6 mg/l - 72 h

### 12.2 Persistence and degradability

Biodegradability Result: - rapidly biodegradable

### 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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting 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. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

**DOT (US)**

Not dangerous goods

**IMDG**

UN number: 3082

Class: 9

Packing group: III

EMS-No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Mixture of 2,4-dinitro-6-octylphenyl crotonate and 2,6-dinitro-4-octylphenyl crotonate)

Marine pollutant: Marine pollutant

**IATA**

UN number: 3082      Class: 9      Packing group: III  
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Mixture of 2,4-dinitro-6-octylphenyl crotonate and 2,6-dinitro-4-octylphenyl crotonate)

**Further information**

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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**15. REGULATORY INFORMATION****SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

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**

Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

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

**Pennsylvania Right To Know Components**

|  | CAS-No.  | Revision Date |
|--|----------|---------------|
| Mixture of 2,4-dinitro-6-octylphenyl crotonate and 2,6-dinitro-4-octylphenyl crotonate | 131-72-6 |               |

**New Jersey Right To Know Components**

|  | CAS-No.  | Revision Date |
|--|----------|---------------|
| Mixture of 2,4-dinitro-6-octylphenyl crotonate and 2,6-dinitro-4-octylphenyl crotonate | 131-72-6 |               |

**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****Full text of H-Statements referred to under sections 2 and 3.**

|                 |   |
|-----------------|---|
| Acute Tox.      | Acute toxicity  |
| Aquatic Acute   | Acute aquatic toxicity  |
| Aquatic Chronic | Chronic aquatic toxicity  |
| H302            | Harmful if swallowed.   |
| H302 + H332     | Harmful if swallowed or if inhaled  |
| H315            | Causes skin irritation.   |
| H317            | May cause an allergic skin reaction.  |
| H332            | Harmful if inhaled.   |
| H360            | May damage fertility or the unborn child.                                       |
| H373            | May cause damage to organs through prolonged or repeated exposure if swallowed. |
| H400            | Very toxic to aquatic life.   |

**HMIS Rating**

|                        |   |
|------------------------|---|
| Health hazard:         | 2 |
| Chronic Health Hazard: | * |
| Flammability:          | 0 |
| Physical Hazard        | 0 |

**NFPA Rating**

|                |   |
|----------------|---|
| Health hazard: | 2 |
|----------------|---|

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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