

## Chemical Safety Data Sheet MSDS / SDS

**2,6-Dimethyl-2,5-heptadien-4-one**Revision Date:2023-12-02 Revision Number:1

---

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 2,6-Dimethyl-2,5-heptadien-4-one  
CBnumber : CB9351608  
CAS : 504-20-1  
EINECS Number : 207-986-3  
Synonyms : PHORONE,2,6-Dimethyl-2,5-heptadien-4-one

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

---

**SECTION 2: Hazards identification****Classification of the substance or mixture**

Not classified.

**Label elements****Pictogram(s)**

Signal word : No signal word

**Hazard statement(s)**

none

**Precautionary statement(s)****Prevention**

none

**Response**

none

**Storage**

none

**Disposal**

none

#### Other hazards

no data available

---

## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 2,6-Dimethyl-2,5-heptadien-4-one
Synonyms	: PHORONE,2,6-Dimethyl-2,5-heptadien-4-one
CAS	: 504-20-1
EC number	: 207-986-3
MF	: C9H14O
MW	: 138.21

---

## SECTION 4: First aid measures

### Description of first aid measures

#### If inhaled

Fresh air, rest. Refer for medical attention.

#### Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

#### Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

#### Following ingestion

Rinse mouth. Refer for medical attention .

### Most important symptoms and effects, both acute and delayed

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: Inhalation or contact with material may irritate or burn skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

### Indication of any immediate medical attention and special treatment needed

no data available

---

## SECTION 5: Firefighting measures

### Extinguishing media

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: CAUTION: All these products have a very low flash point: Use of water spray when fighting fire may be inefficient. CAUTION: For mixtures containing alcohol or polar solvent, alcohol-resistant foam may be more effective. SMALL FIRE: Dry chemical, CO<sub>2</sub>, water spray or regular foam. LARGE FIRE: Water spray, fog or regular foam. Do not use straight

streams. Move containers from fire area if you can do it without risk. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

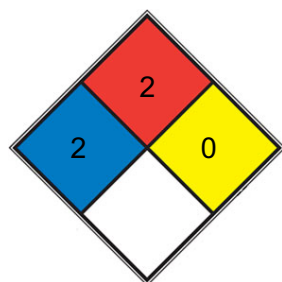
### Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. Substance may be transported hot. For hybrid vehicles, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. If molten aluminum is involved, refer to ERG Guide 169. (ERG, 2016)

### Advice for firefighters

Use powder, AFFF, foam, carbon dioxide.

### NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 2 Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

SPEC.

HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. If solid: sweep spilled substance into containers. Carefully collect remainder. Then store and dispose of according to local regulations.

### Environmental precautions

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. If solid: sweep spilled substance into containers. Carefully collect remainder. Then store and dispose of according to local regulations.

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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

---

## SECTION 7: Handling and storage

### **Precautions for safe handling**

NO open flames. Above 85°C use a closed system and ventilation. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

---

## SECTION 8: Exposure controls/personal protection

### **Control parameters**

#### **Occupational Exposure limit values**

no data available

#### **Biological limit values**

no data available

### **Exposure controls**

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### **Individual protection measures**

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

Wear safety spectacles.

#### **Skin protection**

Protective gloves.

#### **Respiratory protection**

Avoid inhalation of dust and mist. Use ventilation, local exhaust or breathing protection.

#### **Thermal hazards**

no data available

---

## SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Physical state	Solid
Colour	Light Yellow to Yellow Oil to Low-Melting
Odour	no data available
Melting point/freezing point	23-26°C(lit.)
Boiling point or initial boiling point and boiling range	198-199°C(lit.)
Flammability	Combustible.
Lower and upper explosion limit/flammability limit	no data available
Flash point	79°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Chloroform (Slightly), Methanol (Slightly)
Partition coefficient n-octanol/water	no data available
Vapour pressure	0.38 mm Hg ( 20 °C)
Density and/or relative density	0.885
Relative vapour density	4.8 (vs air)
Particle characteristics	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Slightly soluble in water.

### Chemical stability

no data available

### Possibility of hazardous reactions

Ketones, such as PHORONE, are reactive with many acids and bases liberating heat and flammable gases (e.g., H<sub>2</sub>). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H<sub>2</sub>) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO<sub>3</sub>, HNO<sub>3</sub> + H<sub>2</sub>O<sub>2</sub>, and HClO<sub>4</sub>.

### Conditions to avoid

no data available

### Incompatible materials

no data available

## Hazardous decomposition products

no data available

---

## SECTION 11: Toxicological information

### Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

### Skin corrosion/irritation

no data available

### Serious eye damage/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

### STOT-single exposure

See Notes.

### STOT-repeated exposure

See Notes.

### Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

---

## SECTION 12: Ecological information

### Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

### **Persistence and degradability**

no data available

### **Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

### **Other adverse effects**

no data available

---

## SECTION 13: Disposal considerations

### **Disposal methods**

#### **Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### **Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

---

## SECTION 14: Transport information

### **UN Number**

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### **UN Proper Shipping Name**

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### **Transport hazard class(es)**

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### **Packing group, if applicable**

ADR/RID: no data available

IMDG: no data available

IATA: no data available

### **Environmental hazards**

ADR/RID: No

IMDG: No

IATA: No

### **Special precautions for user**

no data available

### **Transport in bulk according to IMO instruments**

no data available

---

## SECTION 15: Regulatory information

### **Safety, health and environmental regulations specific for the product in question**

#### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

#### **EC Inventory**

Listed.

#### **United States Toxic Substances Control Act (TSCA) Inventory**

Listed.

#### **China Catalog of Hazardous chemicals 2015**

Not Listed.

#### **New Zealand Inventory of Chemicals (NZIoC)**

Listed.

#### **PICCS**

Listed.

#### **Vietnam National Chemical Inventory**

Not Listed.

#### **IECSC**

Listed.

#### **Korea Existing Chemicals List (KECL)**

Listed.

---

## SECTION 16: Other information

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road



RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

## References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pagelD=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

## Other Information

Insufficient data are available on the effect of this substance on human health, therefore utmost care must be taken. No primary references were found. The relation between odour and the occupational exposure limit cannot be indicated.

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.