Chemical Safety Data Sheet MSDS / SDS

2,6-dimethylhepta-2,5-dien-4-one SDS

Revision Date: 2024-04-25 Revision Number: 1

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

Product identifier

Product name: 2,6-dimethylhepta-2,5-dien-4-one

CAS: 504-20-1

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

Relevant identified For R&D use only. Not for medicinal, household or other use.

uses:

Uses advised none

against:

Company Identification

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification

Classification of the substance or mixture

Not classified.

GHS label elements, including precautionary statements Signal word No signal word Hazard statement(s) none Precautionary statement(s) Prevention none Response none Storage none Disposal none

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name: 2,6-dimethylhepta-2,5-dien-4-one

100%

Common names and

2,6-dimethylhepta-2,5-dien-4-one

synonyms:

CAS number: 504-20-1 EC number: 207-986-3

Concentration:

SECTION 4: First aid measures

Description of necessary 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/effects, 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 immediate medical attention and special treatment needed, if necessary

no data available

SECTION 5: Firefighting measures

Suitable 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, CO2, 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 FLAWWABLE: 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)

Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide.

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

Appropriate engineering 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, such as personal protective equipment (PPE)

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 and safety characteristics

Physical state: Phorone is a yellowish liquid with a solvent-like odor. Combustible but difficult to ignite.

Used as a solvent for lacquers and coatings.

Colour: no data available
Odour: no data available

 $\textit{Melting} \hspace{1cm} 23\text{-}26^{\circ}C(lit.)$

point/freezing

point:

Boiling point or 198-199°C(lit.)

initial boiling point and boiling range:

Flammability: Combustible.

Lower and upper

explosion

limit/flammability

limit:

Flash point: 79°C

Auto-ignition no data available

temperature:

Decomposition

no data available

no data available

temperature:

pH: no data available

Kinematic no data available

viscosity:

Solubility: in water: poor

Partition no data available

coefficient noctanol/water:

Vapour pressure: 0.38 mm Hg (20 °C)

Density and/or 0.885

relative density:

Relative vapour

4.8 (vs air)

density:

Particle no data available

characteristics:

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., H2). 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 (H2) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO3, HNO3 + H2O2, and HClO4.

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?pageID=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-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 above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any