Chemical Safety Data Sheet MSDS / SDS

P-XYLENE-ALPHA, ALPHA'-13C2

Revision Date:2025-02-01 Revision Number:1

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

Product identifier

| Product name | : P-XYLENE-ALPHA,ALPHA'-13C2 | |
|---|--|--|
| CBnumber | : CB9705814 | |
| CAS | : 116598-94-8 | |
| 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

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word

Warning

Precautionary statements

P280 Wear protective gloves/protective clothing/eye protection/face protection.

Hazard statements

H226 Flammable liquid and vapour

H312 Harmful in contact with skin

H315 Causes skin irritation

H332 Harmful if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name

: P-XYLENE-ALPHA,ALPHA'-13C2

| CAS | : 116598-94-8 |
|-----|---------------|
| MF | : C8H10 |
| MW | : 108.18 |

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material 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

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

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.

Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet- brushing and place in container for disposal according to local regulations (see section 13).

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

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

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Store in cool place. 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.

Store under inert gas. hygroscopic

Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it. Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective 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

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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| Appearance | liquid |
|---|---|
| Odour | No data available |
| Odour Threshold | No data available |
| рН | No data available |
| Melting point/freezing point | Melting point/range: 12 - 13 °C - lit. |
| Initial boiling point and boiling range | 138 °C - lit. |
| Flash point | 25,00 °C - closed cup |
| Evaporation rate | No data available |
| Flammability (solid, gas) | No data available |
| Upper/lower flammability or explosive | Upper explosion limit: 7,00 %(V) Lower explosion limit: 1,10 %(V) |
| limits | |
| Vapour pressure | 21 hPa at 37,70 °C 12 hPa at 20,00 °C |
| Vapour density | No data available |
| Relative density | 0,882 g/mL at 25 °C0,882 g/cm3 at 25 °C |
| Water solubility | No data available |
| Partition coefficient: n-octanol/water | log Pow: 3,150 |
| Autoignition temperature | No data available |
| Decomposition temperature | No data available |
| Viscosity | No data available |
| Explosive properties | No data available |
| Oxidizing properties | No data available |

Other safety information

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 5.000 mg/kg

LC50 Inhalation - Rat - 4,00 h - 19,758 mg/l

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 ingredient 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

May cause reproductive disorders.

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: Not available

narcosis, Lung irritation, chest pain, pulmonary edema, Central nervous system depression, Dermatitis, Gastrointestinal disturbance, Liver injury may occur., Kidney injury may occur., Blood disorders

SECTION 12: Ecological information

Toxicity

Toxicity to fish

LC50 - Oncorhynchus mykiss (rainbow trout) - 2,6 mg/l - 96,0 h LC50 - Carassius auratus (goldfish) - 18 mg/l - 24,0 h

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

Other adverse effects

Toxic to aquatic life. No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

UN number

ADR/RID: 1307 IMDG: 1307

UN proper shipping name

ADR/RID: XYLENES IMDG: XYLENES IATA: Xylenes

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Not Listed. website: https://chemicaldata.gov.vn/

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: https://www.epa.gov/

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: https://echa.europa.eu/

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: https://www.epa.govt.nz/

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/ EC Inventory:Not Listed.

Korea Existing Chemicals List (KECL):Not Listed. website: http://ncis.nier.go.kr

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: https://emb.gov.ph/

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

- [1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- [2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- [3] ECHA European Chemicals Agency, website: https://echa.europa.eu/
- [4] eChemPortal The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

- [5] ERG Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- [6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- [7] HSDB Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- [8] IARC International Agency for Research on Cancer, website: http://www.iarc.fr/
- [9] IPCS The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

[10] Sigma-Aldrich, website: https://www.sigmaaldrich.com/

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.