

Chemical Safety Data Sheet MSDS / SDS

m-Xylene-alpha,alpha'-13C2

Revision Date:2026-09-13 Revision Number:1

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

Product name : m-Xylene-alpha,alpha'-13C2
CBnumber : CB6482167
CAS : 117713-57-2
Synonyms : m-Xylene-(dimethyl-13C?);1,3-dimethyl-13c2-benzene

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 : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P370+P378 In case of fire: Use ... for extinction.

Hazard statements

H226 Flammable liquid and vapour
H315 Causes skin irritation
H411 Toxic to aquatic life with long lasting effects

SECTION 3: Composition/information on ingredients

Substance

Product name	: m-Xylene-alpha,alpha'-13C2
Synonyms	: m-Xylene-(dimethyl-13C?); 1,3-dimethyl-13c2-benzene
CAS	: 117713-57-2
MF	: C8H10
MW	: 108.18

SECTION 4: First aid measures

4.1 Description of first-aid measures

No data available

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) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO2) Foam Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

5.3 Advice for firefighters

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.

6.2 Environmental precautions

No data available

6.3 Methods and materials for containment and cleaning up

No data available

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

No data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['m-Xylene- dimethyl-13C2', '117713- 57-2', 'PC-TWA', '50 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.']	['', 'PC-STEL', '100 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.']
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Biological occupational exposure limits

['Component', 'CAS-No.', 'Parameters', 'Value', 'Biological specimen', 'Basis']	['', '117713- 57-2', 'methylhipp uric acids', '0.3g/g creatinin e', 'Urine', 'China. Biological Occupational Exposure Indices']	['', 'Remarks', 'End of shift', 'None, None, None']	['', 'methylhipp uric acids', '0.4 g/l', 'Urine', 'China. Biological Occupational Exposure Indices']	['', 'End of shift', 'None, None, None']
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8.2 Exposure controls

Personal protective equipment

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de.

Full contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Respiratory protection

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Prevent product from entering drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	Melting point/ range: -48 °C - lit.
e) Initial boiling point and boiling range	138 - 139 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 7 %(V) Lower explosion limit: 1.1 %(V)
h) Flash point	25 °C - closed cup
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: < 0.001 Pas
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	8 hPa at 20.0 °C 21.3 hPa at 37.7 °C
p) Density	0.884 g/mL at 25 °C 0.884 g/cm3 at 25 °C
Relative density	0.884 g/mL at 25 °C
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

No data available

10.2 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents conc. sulfuric acid

Nitric acid uranium hexafluoride sulfur

10.3 Conditions to avoid

No data available

10.4 Incompatible materials

No data available

10.5 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 3,523 mg/kg (EC Directive 92/69/EEC B.1 Acute Toxicity (Oral))

Remarks: The value is given in analogy to the following substances: m-xylene

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

LC50 Inhalation - Rat - male and female - 4 h - 27.12 mg/l - vapor (US-EPA)

Remarks: The value is given in analogy to the following substances: m-xylene

Symptoms: Inhalation may lead to the formation of oedemas in the respiratory tract.

LD50 Dermal - Rabbit - male - 12,126 mg/kg

Remarks: (ECHA)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: m-xylene

Skin corrosion/irritation

Skin - Rabbit

Result: Moderate skin irritation - 4 h (Regulation (EC) No. 440/2008, Annex, B.4)

Remarks: The value is given in analogy to the following substances: m-xylene

Remarks: Drying-out effect resulting in rough and chapped skin.

After long-term exposure to the chemical:

Dermatitis

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Severe eye irritation - 24 h

Remarks: (RTECS)

The value is given in analogy to the following substances: m-xylene

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative (OECD Test Guideline 429)

Remarks: The value is given in analogy to the following substances: m-xylene

Germ cell mutagenicity

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: Regulation (EC) No. 440/2008, Annex, B.19

Result: negative

Remarks: The value is given in analogy to the following substances: m-xyleneTest Type:

Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: (National Toxicology Program)

The value is given in analogy to the following substances: m-xyleneTest Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: Mutagenicity (in vitro mammalian cytogenetic test)

Result: negative

Remarks: The value is given in analogy to the following substances: m-xylene

Test Type: dominant lethal test

Species: Mouse

Application Route: Subcutaneous

Method: OECD Test Guideline 478

Result: negative

Remarks: The value is given in analogy to the following substances: m-xylene

Test Type: Mutagenicity (mammal cell test): micronucleus.

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Intraperitoneal

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: m-xylene

Carcinogenicity

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

Reproductive toxicity

Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory Tract

Remarks: The value is given in analogy to the following substances: m-xylene

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

May be fatal if swallowed and enters airways.

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 90 Days - NOAEL (No observed adverse effect level) - 200 mg/kg

Remarks: The value is given in analogy to the following substances: m-xylene

Liver injury may occur., Kidney injury may occur., Blood disorders, burning sensation,

Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, narcosis,

Lung irritation, chest pain, pulmonary edema, Central nervous system depression,

Dermatitis, Gastrointestinal disturbance

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

After absorption of toxic quantities:

Headache somnolence

Dizziness agitation, spasms narcosis

Effect potentiated by: ethanol

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Kidney -

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish static test LC50 - *Oncorhynchus mykiss* (rainbow trout) - 2.60 mg/l - 96 h (OECD Test Guideline 203)

Remarks: The value is given in analogy to the following substances: m-xylene

Toxicity to algae static test EC50 - *Pseudokirchneriella subcapitata* - 4.36 mg/l - 73 h (OECD Test Guideline 201)

Remarks: The value is given in analogy to the following substances: m-xylene (m-Xylene-dimethyl-13C2)

Toxicity to bacteria Remarks: (ECHA)

The value is given in analogy to the following substances: m-xylene (m-Xylene-dimethyl-13C2)

Toxicity to flow-through test NOEC - *Danio rerio* (zebra fish) - 0.71 mg/l - 35 d fish(Chronic toxicity) (OECD Test Guideline 210)

Remarks: The value is given in analogy to the following substances: m-xylene

Toxicity to daphnia NOEC - *Daphnia magna* (Water flea) - 1.57 mg/l - 21 d and other aquatic (OECD Test Guideline 211)

invertebrates(Chronic Remarks: The value is given in analogy to the following substances: toxicity) m-xylene

EC50 - *Daphnia magna* (Water flea) - 2.9 mg/l - 21 d (OECD Test Guideline 211)

Remarks: The value is given in analogy to the following substances: m-xylene

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 98 % - Readily biodegradable.

(OECD Test Guideline 301F)

Remarks: The value is given in analogy to the following substances: m-xylene

12.3 Bioaccumulative potential

Bioaccumulation Oncorhynchus mykiss (rainbow trout) - 56 d at 10 °C - 1.3 mg/l(m-Xylene-dimethyl-13C2)

Bioconcentration factor (BCF): 7.4 - 18.5

Remarks: The value is given in analogy to the following substances: m-xylene

Due to the distribution coefficient n-octanol/water, accumulation in organisms is not expected.

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1307

IMDG: 1307

IATA-DGR: 1307

14.2 UN proper shipping name

ADR/RID: XYLENES

IMDG: XYLENES

IATA-DGR: Xylenes

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA-DGR: 3

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA-DGR: III

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

SECTION 15: Regulatory information

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

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222232086

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

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

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.