Safety Data Sheet

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product identifiers

Product Name: JP-2-196 alkyne
Catalog Number: 8047
CAS Number: 2901113-25-3
IUPAC Name: 1-(4-Methoxyphenyl)-4-[4-(2-propyn-1-yl)-1-piperazinyl]-2-butene-1,4-dione

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: Tocris Bioscience
The Watkins Building,
Atlantic Road,
Bristol, BS11 9QD, UK

Telephone: + 44 (0)117 916-3333
Fax: + 44 (0)117 916-3344
Internet: www.tocris.com
E-mail address: info@bio-techne.com

1.4 Emergency Telephone number

Emergency Tel: + 44 (0)117 916-3333 (09.00 - 17.00 GMT)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

This substance does not meet the classification criteria of the EC Directives 67/548/EEC, 1999/45/EC or 1272/2008.

2.2 Label elements

The product does not need to be labelled in accordance with EC directives or respective national laws.

2.3 Other hazards - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product Name: JP-2-196 alkyne
Formula: $C_{18}H_{20}N_2O_3$ Molecular Weight: 312.37
CAS Number: 2901113-25-3

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a doctor and show this safety data sheet.

If inhaled
Remove to fresh air and monitor breathing. If breathing becomes difficult, give oxygen. If breathing stops, give artificial respiration. Consult a doctor.

In case of skin contact
Immediately wash skin with copious amounts of soap and water for at least 15 minutes. Remove contaminated clothing and shoes and wash before reuse. Consult a doctor.

In case of eye contact
Flush with copious amounts of water for at least 15 minutes. Consult a doctor.

If swallowed
Rinse mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Consult a doctor.

4.2 Most important symptoms and effects, both acute and delayed

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

4.3 Indication of immediate medical attention and special treatment needed

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

5. FIRE-FIGHTING 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

In combustion, may emit toxic fumes.

5.3 Precautions for fire-fighters

Wear suitable protective clothing to prevent contact with skin and eyes and self-contained breathing apparatus.

6. ACCIDENTIAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Do not take action without suitable protective clothing - see section 8 of SDS. Evacuate personnel to safe areas. Ensure adequate ventilation. Avoid breathing vapors, mist, dust or gas.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover spillage with suitable absorbent material. Sweep up material and place in an appropriate container. Hold all material for appropriate disposal as described under section 13 of SDS.

6.4 Reference to other sections

For required PPE see section 8. For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Use in a chemical fume hood, with air supplied by an independent system. Avoid inhalation, contact with eyes, skin and clothing. Avoid the formation of dust and aerosols. Use in a well-ventilated area. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

7.2 Conditions for safe storage, including any incompatibilities.

Store in cool, well-ventilated area. Keep away from direct sunlight. Keep container tightly sealed until ready for use. Recommended storage temperature: Store at -20°C

7.3 Specific end uses

Use in a laboratory fume hood where possible. Refer to employer's COSHH risk assessment.

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
Use in a fume hood where applicable. Ensure all engineering measures described under section 7 of SDS are in place. Ensure laboratory is equipped with a safety shower and eye wash station.

Personal protective equipment

Eye/face protection
Use appropriate safety glasses.

Skin protection
Use appropriate chemical resistant gloves (minimum requirement use standard BS EN 374:2003). Gloves should be inspected before use. Wash and dry hands thoroughly after handling.

Body protection
Wear appropriate protective clothing.

Respiratory protection
If risk assessment indicates necessary, use a suitable respirator.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Appearance	Cream solid	Vapor pressure	No data available
Odor	No data available	Vapor density	No data available
Odor threshold	No data available	Relative density	No data available
pH	No data available	Solubility(ies)	Soluble to 100 mM in DMSO
Melting / freezing point	No data available	Partition coefficient	No data available
Boiling point / range	No data available	Auto-ignition temperature	No data available
Flash point	No data available	Decomposition temperature	No data available
Evaporation rate	No data available	Viscosity	No data available
Flammability (solid, gas)	No data available	Explosive properties	No data available
Upper / lower flammability or explosive limits	No data available	Oxidising properties	No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

Stable under recommended transport or storage conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Hazardous reactions will not occur under normal transport or storage conditions. Decomposition may occur on exposure to conditions or materials listed below.

10.4 Conditions to avoid

Heat, moisture.

10.5 Incompatible materials

Strong acids/alkalis, strong oxidising/reducing agents.

10.6 Hazardous decomposition products

In combustion may emit toxic fumes. No known decomposition information.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute Toxicity
No data available

Skin corrosion/irritation
Classification criteria are not met based on available data

Serious eye damage/irritation
Classification criteria are not met based on available data

Respiratory or skin sensitization
Classification criteria are not met based on available data

Germ cell mutagenicity
Classification criteria are not met based on available data

Carcinogenicity
Classification criteria are not met based on available data

Reproductive toxicity
Classification criteria are not met based on available data

Specific target organ toxicity - single exposure
Classification criteria are not met based on available data

Specific target organ toxicity - repeated exposure
Classification criteria are not met based on available data

Aspiration hazard
Classification criteria are not met based on available data

Symptoms / Routes of exposure

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

Ingestion: There may be irritation of the throat.

Skin: There may be mild irritation at the site of contact.

Eyes: There may be irritation and redness.

Delayed / Immediate Effects: No known symptoms.

Additional Information
RTECS No: Not available
Exposure may cause irritaiton of eyes, mucous membranes, upper respiratory tract and skin.
To the best of our knowledge, the chemical, physical and toxicological properties have not been fully investigated

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumlative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

No data available

12.6 Other adverse effects

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Transfer to a suitable container and arrange for collection by specialized disposal company in accordance with National legislation.

Contaminated packaging
Dispose of in a regulated landfill site or other method for hazardous or toxic wastes in accordance with National legislation.

14. TRANSPORT INFORMATION

Classified according to the criteria of the UN Model Regulations as reflected in the IMDG Code, ADR, RID and IATA.

14.1 UN-Number

Does not meet the criteria for classification as hazardous for transport.

14.2 UN proper shipping name

Does not meet the criteria for classification as hazardous for transport.

14.3 Transport hazard class(es)

Does not meet the criteria for classification as hazardous for transport.

14.4 Packaging group

Does not meet the criteria for classification as hazardous for transport.

14.5 Environmental hazards

This product is not classified as environmentally hazardous according to the UN Model Regulations, nor a marine pollutant according to the IMDG Code.

14.6 Special precautions for users

No data available

15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulation (EC) No. 453/2010.

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

No data available

California Proposition 65
Not applicable

15.2 Chemical safety assessment

A Chemical Safety Assessment has not been made for this product.

16. OTHER INFORMATION

Further Information
Copyright © 2025 Tocris Bioscience. This company shall not be held liable for any damage resulting from handling or from contact with the above product. This material must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The above information is believed to be correct but does not purport to be all inclusive and should be used as a guide only for experienced personnel. Always consult your safety advisor and follow appropriate local and national safety legislature. The absence of warning must not, under any circumstance, be taken to mean that no hazard exists.

End of safety data sheet