

SAFETY DATA SHEET

Version 5.4
Revision Date 10/11/2017
Print Date 10/26/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacos-5-ene solution

Product Number : 308579

Brand : Aldrich

CAS-No. : 31250-18-7

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Reproductive toxicity (Category 2), H361

Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336

Specific target organ toxicity - repeated exposure (Category 2), H373

Acute aquatic toxicity (Category 2), H401

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Warning

Hazard statement(s)

H315

Causes skin irritation.

H319

Causes serious eye irritation.

H335

May cause respiratory irritation.

H336

May cause drowsiness or dizziness.

H361

Suspected of damaging fertility or the unborn child.

H373

May cause damage to organs through prolonged or repeated exposure.

H401

Toxic to aquatic life.

Precautionary statement(s)	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.2 Mixtures

Synonyms : Kryptand 222B
Kryptofix® 222B

Formula : $C_{22}H_{36}N_2O_6$

Molecular weight : 424.53 g/mol

Hazardous components

Component		Classification	Concentration
Toluene			
CAS-No.	108-88-3	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; H225, H304, H315, H336, H361, H373, H401	50 - 70 %
EC-No.	203-625-9		
Index-No.	601-021-00-3		
Registration number	01-2119471310-51-XXXX		
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacos-5-ene			
CAS-No.	31250-18-7	Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H315, H319, H335	50 - 70 %
EC-No.	250-532-4		

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

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

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING 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

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

6.2 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.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Toluene	108-88-3	TWA	100 ppm 375 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	150 ppm 560 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	200 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
	Remarks	Z37.12-1967		
		CEIL	300 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		Peak	500 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Visual impairment Female reproductive Pregnancy loss 2016 Adoption Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen		
		TWA	100 ppm 375 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	150 ppm 560 mg/m3	USA. NIOSH Recommended Exposure Limits

Hazardous components without workplace control parameters

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Toluene	108-88-3	Toluene	0.0200 mg/l	In blood	ACGIH - Biological Exposure Indices (BEI)
	Remarks	Prior to last shift of workweek			
		Toluene	0.0300 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			
		o-Cresol	0.3000 mg/g	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			
		Toluene	0.02 mg/l	In blood	ACGIH - Biological Exposure Indices (BEI)
		Prior to last shift of workweek			
		Toluene	0.03 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

		o-Cresol	0.3mg/g Creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

8.2 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

Safety glasses with side-shields conforming to EN166 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.

Body Protection

Complete suit protecting against chemicals, 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 particle respirator type N100 (US) or type P3 (EN 143) 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|--|
| a) Appearance | Form: solid |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | 8 °C (46 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapour pressure | No data available |
| l) Vapour density | No data available |
| m) Relative density | 0.995 g/cm ³ at 25 °C (77 °F) |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | No data available |

- | | |
|------------------------------|-------------------|
| p) Auto-ignition temperature | No data available |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

No data available

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

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence (Toluene)

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION**DOT (US)**

UN number: 1993 Class: 3 Packing group: II

Proper shipping name: Flammable liquids, n.o.s. (Toluene)

Reportable Quantity (RQ): 2000 lbs

Poison Inhalation Hazard: No

IMDG

UN number: 1993 Class: 3 Packing group: II

EMS-No: F-E, S-E

Proper shipping name: FLAMMABLE LIQUID, N.O.S. (Toluene)

IATA

UN number: 1993 Class: 3 Packing group: II

Proper shipping name: Flammable liquid, n.o.s. (Toluene)

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacos-5-ene	31250-18-7	

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacos-5-ene	31250-18-7	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01
5,6-Benzo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacos-5-ene	31250-18-7	

California Prop. 65 Components

	CAS-No.	Revision Date
WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.	108-88-3	2009-02-01
Toluene		

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Asp. Tox.	Aspiration hazard
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H361	Suspected of damaging fertility or the unborn child.
H373	May cause damage to organs through prolonged or repeated exposure.
H401	Toxic to aquatic life.
Repr.	Reproductive toxicity
Skin Irrit.	Skin irritation
STOT RE	Specific target organ toxicity - repeated exposure
STOT SE	Specific target organ toxicity - single exposure

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.4

Revision Date: 10/11/2017

Print Date: 10/26/2018