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### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : Toluene- $\alpha$ ,  $\alpha$ ,  $\alpha$ -d<sub>3</sub>

Product Number : 487074

Brand : Aldrich

CAS-No. : 1124-18-1

#### 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 Inc.  
3050 Spruce Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887

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### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

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

Flammable liquids (Category 2), H225

Acute toxicity, Inhalation (Category 4), H332

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Reproductive toxicity (Category 2), H361

Specific target organ toxicity - single exposure (Category 2), H371

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

Aspiration hazard (Category 1), H304

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 2), H411

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

Danger

Hazard statement(s)

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H336	May cause drowsiness or dizziness.
H361	Suspected of damaging fertility or the unborn child.
H371	May cause damage to organs.
H411	Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
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.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
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 + P311	IF exposed or concerned: Call a POISON CENTER/doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P331	Do NOT induce vomiting.
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.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
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

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### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Synonyms : Methyl-d<sub>3</sub>-benzene

Formula : C<sub>7</sub>D<sub>3</sub>H<sub>5</sub>

Molecular weight : 95.13 g/mol

CAS-No. : 1124-18-1

#### Hazardous components

Component	Classification	Concentration
<b>Toluene-<math>\alpha,\alpha,\alpha</math>-d<sub>3</sub></b>		
	Flam. Liq. 2; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Repr. 2; STOT SE 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H304, H315, H319, H332, H336, H361, H371, H411	<= 100 %

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

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### 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

Do NOT induce vomiting. 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

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### 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

Carbon oxides

#### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

Use water spray to cool unopened containers.

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

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

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

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).

### 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 inhalation of vapour or mist.

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

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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

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- $\alpha,\alpha,\alpha$ -d3	1124-18-1	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Visual impairment Female reproductive Pregnancy loss 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/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		ST	150 ppm 560 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		See Table Z-2		
		TWA	200 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		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		
		PEL	10 ppm 37 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		C	500 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	150 ppm 560 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

**Biological occupational exposure limits**

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Toluene- $\alpha,\alpha,\alpha$ -d3	1124-18-1	Toluene	0.02 mg/l	In blood	ACGIH - Biological Exposure Indices (BEI)
	Remarks	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**

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.

**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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -93 °C (-135 °F) - lit.
f) Initial boiling point and boiling range	110 °C (230 °F) - lit.
g) Flash point	4 °C (39 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 7 %(V) Lower explosion limit: 1.2 %(V)
k) Vapour pressure	29.1 hPa at 20.0 °C (68.0 °F)
l) Vapour density	No data available
m) Relative density	0.895 g/mL at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition temperature	535.0 °C (995.0 °F)
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

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## 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

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available  
In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - > 5,580 mg/kg  
LC50 Inhalation - Rat - 4 h - 12,500 - 28,800 mg/m<sup>3</sup>  
LD50 Dermal - Rabbit - 12,196 mg/kg  
No data available

#### Skin corrosion/irritation

Skin - Rabbit  
Result: Skin irritation - 24 h

#### Serious eye damage/eye irritation

Eyes - Rabbit  
Result: Severe eye irritation - 24 h

#### 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 on OSHA's list of regulated carcinogens.

#### Reproductive toxicity

Damage to fetus possible  
Suspected human reproductive toxicant  
Experiments have shown reproductive toxicity effects in male and female laboratory animals.

#### Specific target organ toxicity - single exposure

May cause damage to organs.  
May cause drowsiness or dizziness.

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

#### Additional Information

RTECS: Not available

Lung irritation, chest pain, pulmonary edema, Inhalation studies on toluene have demonstrated the development of inflammatory and ulcerous lesions of the penis, prepuce, and scrotum in animals.

Stomach - Irregularities - Based on Human Evidence  
Stomach - Irregularities - Based on Human Evidence

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

Toxicity to fish                      LC50 - Lepomis macrochirus (Bluegill) - 74.00 - 340.00 mg/l - 96 h(Toluene-

α,α,α-d3)  
 LC50 - Oncorhynchus mykiss (rainbow trout) - 7.63 mg/l - 96 h(Toluene-α,α,α-d3)  
 NOEC - Pimephales promelas (fathead minnow) - 5.44 mg/l - 7 d(Toluene-α,α,α-d3)  
 LOEC - Pimephales promelas (fathead minnow) - 8.04 mg/l - 7 d(Toluene-α,α,α-d3)  
 Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 8.00 mg/l - 24 h(Toluene-α,α,α-d3)  
 Immobilization EC50 - Daphnia magna (Water flea) - 6 mg/l - 48 h(Toluene-α,α,α-d3)  
 Toxicity to algae EC50 - Chlorella vulgaris (Fresh water algae) - 245.00 mg/l - 24 h(Toluene-α,α,α-d3)  
 EC50 - Pseudokirchneriella subcapitata (green algae) - 10.00 mg/l - 24 h(Toluene-α,α,α-d3)

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

Bioaccumulation Leuciscus idus (Golden orfe) - 3 d - 0.05 mg/l(Toluene-α,α,α-d3)

Bioconcentration factor (BCF): 94

**12.4 Mobility in soil**

No data available(Toluene-α,α,α-d3)

**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**

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. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

**14. TRANSPORT INFORMATION**

**DOT (US)**

UN number: 1294 Class: 3 Packing group: II  
 Proper shipping name: Toluene  
 Reportable Quantity (RQ) : 1000 lbs

Poison Inhalation Hazard: No

**IMDG**

UN number: 1294 Class: 3 Packing group: II EMS-No: F-E, S-D



Proper shipping name: TOLUENE

**IATA**

UN number: 1294      Class: 3  
Proper shipping name: Toluene

Packing group: II

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**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- $\alpha,\alpha,\alpha$ -d3	1124-18-1	2007-07-01

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

	CAS-No.	Revision Date
Toluene- $\alpha,\alpha,\alpha$ -d3	1124-18-1	2007-07-01

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Toluene- $\alpha,\alpha,\alpha$ -d3	1124-18-1	2007-07-01

**New Jersey Right To Know Components**

	CAS-No.	Revision Date
Toluene- $\alpha,\alpha,\alpha$ -d3	1124-18-1	2007-07-01

**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.	1124-18-1	2009-02-01

Toluene- $\alpha,\alpha,\alpha$ -d3

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**16. OTHER INFORMATION**

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

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H336	May cause drowsiness or dizziness.
H361	Suspected of damaging fertility or the unborn child.
H371	May cause damage to organs.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

**Further information**

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**Preparation Information**

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Product Safety – Americas Region  
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