

SAFETY DATA SHEET

Version 5.8
Revision Date 08/06/2018
Print Date 10/18/2019

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Carbonate ionophore IV solution

Product Number : 21856

Brand : Sigma-Aldrich

CAS-No. : 40739-44-4

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)

Flammable liquids (Category 2), H225

Acute toxicity, Oral (Category 4), H302

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Carcinogenicity (Category 2), H351

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

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.

H302 Harmful if swallowed.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

H351 Suspected of causing cancer.

Precautionary statement(s)

P201 Obtain special instructions before use.

P202 Do not handle until all safety precautions have been read and

P210	understood.
P233	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P240	Keep container tightly closed.
P241	Ground/bond container and receiving equipment.
P242	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P243	Use only non-sparking tools.
P261	Take precautionary measures against static discharge.
P264	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P270	Wash skin thoroughly after handling.
P271	Do not eat, drink or smoke when using this product.
P280	Use only outdoors or in a well-ventilated area.
P301 + P312 + P330	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P304 + P340 + P312	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P305 + P351 + P338	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
P308 + P313	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313	IF exposed or concerned: Get medical advice/ attention.
P337 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	If eye irritation persists: Get medical advice/ attention.
P370 + P378	Take off contaminated clothing and wash before reuse.
P403 + P233	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep container tightly closed.
P405	Store in a well-ventilated place. Keep cool.
P501	Store locked up.
	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	:	4-Butyl- α,α,α -trifluoroacetophenone
Formula	:	C ₁₂ H ₁₃ F ₃ O
Molecular weight	:	230.23 g/mol

Hazardous components

Component	Classification	Concentration
Tetrahydrofuran		
CAS-No. 109-99-9	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; Carc. 2; STOT SE 3; H225, H302, H319, H335, H351	70 - 90 %
EC-No. 203-726-8		
Index-No. 603-025-00-0		
Registration number 01-2119444314-46-XXXX		
4-Butyl-α,α,α-trifluoroacetophenone		
CAS-No. 40739-44-4	Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H315, H319, H335	10 - 20 %

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

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

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

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.

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.

Dry residue is explosive. Store under inert gas. Test for peroxide formation periodically and before distillation.
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
Tetrahydrofuran	109-99-9	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment Upper Respiratory Tract irritation Kidney damage Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		STEL	100 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation Kidney damage Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		ST	250 ppm 735 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	200 ppm 590 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	200 ppm 590 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		PEL	200 ppm 590 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	250 ppm 735 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Hazardous components without workplace control parameters

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
	-	Tetrahydrofuran	2 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	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.

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 10 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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.

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 | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | -17 °C (1 °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 | No data available |
| n) Water solubility | No data available |

- | | |
|---|--------------------|
| o) Partition coefficient: n-octanol/water | No data available |
| p) Auto-ignition temperature | ca.215 °C (419 °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

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.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

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

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 1,650 mg/kg (Tetrahydrofuran)

LC50 Inhalation - Rat - 6 h - 14.7 mg/l (Tetrahydrofuran)

Remarks: Material may be irritating to mucous membranes and upper respiratory tract.

LD50 Dermal - Rat - > 2,000 mg/kg (Tetrahydrofuran)

No data available (Tetrahydrofuran)

Skin corrosion/irritation

Skin - Rabbit (Tetrahydrofuran)

Result: No skin irritation

(Draize Test)

Serious eye damage/eye irritation

Eyes - Rabbit (Tetrahydrofuran)

Result: Risk of serious damage to eyes.

(Draize Test)

Respiratory or skin sensitisation

Local lymph node assay (LLNA) - Mouse (Tetrahydrofuran)

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

In vivo tests did not show mutagenic effects (Tetrahydrofuran)

Ames test (Tetrahydrofuran)

Salmonella typhimurium

Result: negative

In vitro mammalian cell gene mutation test (Tetrahydrofuran)

Chinese hamster ovary cells

Result: negative

sister chromatid exchange assay (Tetrahydrofuran)

Chinese hamster ovary cells

Result: negative

Carcinogenicity

Suspected human carcinogens (Tetrahydrofuran)

(Tetrahydrofuran)

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

No data available (Tetrahydrofuran)

No toxicity to reproduction (Tetrahydrofuran)

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Nervous system (Tetrahydrofuran)

May cause respiratory irritation. (Tetrahydrofuran)

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification (Tetrahydrofuran)

Additional Information

RTECS: Not available

Central nervous system depression, Cough, chest pain, Difficulty in breathing, Exposure to high airborne concentrations can cause anesthetic effects. (Tetrahydrofuran)

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence (Tetrahydrofuran)

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish flow-through test LC50 - Pimephales promelas (fathead minnow) - 2,160 mg/l - 96 h (Tetrahydrofuran)
(OECD Test Guideline 203)

Toxicity to algae Growth inhibition IC50 - Algae - 3,700 mg/l - 192 h (Tetrahydrofuran)

Toxicity to bacteria

12.2 Persistence and degradability

Biodegradability

(OECD Test Guideline 301)

Remarks: According to the results of tests of biodegradability this product is not readily biodegradable.

12.3 Bioaccumulative potential

No bioaccumulation is to be expected (log Pow <= 4).

12.4 Mobility in soil

No data available (Tetrahydrofuran)

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

No data available

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: 2056 Class: 3 Packing group: II
Proper shipping name: Tetrahydrofuran, solution
Reportable Quantity (RQ): 1112 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 2056 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: TETRAHYDROFURAN, SOLUTION

IATA

UN number: 2056 Class: 3 Packing group: II
Proper shipping name: Tetrahydrofuran, solution

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

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

Tetrahydrofuran

CAS-No.
109-99-9

Revision Date

Pennsylvania Right To Know Components

Tetrahydrofuran

4-Butyl- α , α , α -trifluoroacetophenone

CAS-No.
109-99-9
40739-44-4

Revision Date

New Jersey Right To Know Components

Tetrahydrofuran

4-Butyl- α , α , α -trifluoroacetophenone

CAS-No.
109-99-9
40739-44-4

Revision Date

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

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

Acute Tox.	Acute toxicity
Carc.	Carcinogenicity
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H351	Suspected of causing cancer.
Skin Irrit.	Skin irritation
STOT SE	Specific target organ toxicity - single exposure

Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

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

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