

SECTION 1: Identification

1.1. Identification

Product form	: Mixture
Product name	: 3-(Trifluoromethyl)butyraldehyde, 50% in toluene
Product code	: 2115-3-08
Synonyms	: 4,4,4-Trifluoro-3-methylbutanal, 50% in toluene

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

Use of the substance/mixture	: Laboratory chemicals Manufacture of substances Scientific research and development
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1.3. Details of the supplier of the safety data sheet

SynQuest Laboratories, Inc.
P.O. Box 309
Alachua, FL 32615 - United States of America
T (386) 462-0788 - F (386) 462-7097
info@synquestlabs.com - www.synquestlabs.com

1.4. Emergency telephone number

Emergency number : (844) 523-4086 (3E Company - Account 10069)

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Liq. 2	H225 - Highly flammable liquid and vapour
Skin Irrit. 2	H315 - Causes skin irritation
Eye Irrit. 2A	H319 - Causes serious eye irritation
Repr. 2	H361 - Suspected of damaging fertility or the unborn child
STOT SE 3	H336 - May cause drowsiness or dizziness
STOT SE 3	H335 - May cause respiratory irritation
STOT RE 2	H373 - May cause damage to organs through prolonged or repeated exposure
Asp. Tox. 1	H304 - May be fatal if swallowed and enters airways
Aquatic Acute 2	H401 - Toxic to aquatic life

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H225 - Highly flammable liquid and vapor
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

Precautionary statements (GHS-US) :

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

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P260 - Do not breathe dust/fume/gas/mist/vapors/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
P301+P310 - If swallowed: Immediately call a poison center/doctor/...
P302+P352 - If on skin: Wash with plenty of soap and water
P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing
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
P312 - Call a POISON CENTER or doctor/physician if you feel unwell
P314 - Get medical advice/attention if you feel unwell
P321 - Specific treatment (see supplemental first aid instructions on this label)
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+P364 - Take off contaminated clothing and wash it before reuse
P370+P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
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. Other hazards

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/information on ingredients

3.1. Substance

Not applicable

3.2. Mixture

Name	Product identifier	%	Classification (GHS-US)
3-(Trifluoromethyl)butyraldehyde	(CAS No) 95853-69-3	45 - 55	Flam. Liq. 3, H226 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335
Toluene	(CAS No) 108-88-3	45 - 55	Flam. Liq. 2, H225 Acute Tox. 4 (Inhalation:vapour), H332 Skin Irrit. 2, H315 Repr. 2, H361 STOT SE 3, H336 STOT RE 2, H373 Asp. Tox. 1, H304 Aquatic Acute 2, H401

Full text of H-phrases: see section 16

SECTION 4: First aid measures

4.1. Description of first aid measures

- First-aid measures general : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.
- First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get immediate medical advice/attention.
- First-aid measures after skin contact : Wash with plenty of soap and water. Get immediate medical advice/attention.
- First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get immediate medical advice/attention.
- First-aid measures after ingestion : Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get immediate medical advice/attention.

4.2. Most important symptoms and effects, both acute and delayed

- Symptoms/injuries : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

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4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Thermal decomposition generates: Carbon oxides. Hydrogen fluoride.
Explosion hazard : Risk of explosion if heated under confinement. Use water spray or fog for cooling exposed containers. May form flammable/explosive vapor-air mixture.

5.3. Advice for firefighters

Firefighting instructions : In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.
Protection during firefighting : Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection".

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe gas, fumes, vapor or spray.

6.1.1. For non-emergency personnel

Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
Emergency procedures : Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level. Consider the risk of potentially explosive atmospheres. Eliminate every possible source of ignition.

6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

For containment : Stop leak if safe to do so. Dike for recovery or absorb with appropriate material.
Methods for cleaning up : Take up large spills with pump or vacuum and finish with dry chemical absorbent. Use explosion-proof equipment. Take up small spills with dry chemical absorbent. Sweep or shovel spills into appropriate container for disposal. Ventilate area.
Other information : For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable.
Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe fumes, mist, spray, vapors. Wear personal protective equipment. Avoid contact with skin and eyes. Keep away from ignition sources (including static discharges). Proper grounding procedures to avoid static electricity should be followed. Use only non-sparking tools.
Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Comply with applicable regulations.
Storage conditions : Keep container closed when not in use. Keep away from ignition sources. Air sensitive. Keep contents under inert gas.
Incompatible materials : Refer to Section 10 on Incompatible Materials.
Storage area : Store in dry, cool, well-ventilated area.

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SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Toluene (108-88-3)		
ACGIH	ACGIH TWA (ppm)	20 ppm
ACGIH	Remark (ACGIH)	Visual impair; female repro;
OSHA	OSHA PEL (TWA) (ppm)	200 ppm
OSHA	OSHA PEL (Ceiling) (ppm)	300 ppm
OSHA	Remark (OSHA)	(2) See Table Z-2.

8.2. Exposure controls

Appropriate engineering controls	: Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.
Hand protection	: Protective gloves. 29 CFR 1910.138: Hand Protection.
Eye protection	: Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection.
Skin and body protection	: Wear suitable protective clothing.
Respiratory protection	: In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection.
Other information	: Safety shoes. 29 CFR 1910.136: Foot Protection.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Color	: Mixture contains one or more component(s) which have the following colour(s): Clear Colorless
Odor	: There may be no odour warning properties, odour is subjective and inadequate to warn of overexposure. Mixture contains one or more component(s) which have the following odour(s): model airplane glue
Odor threshold	: No data available
pH	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: No data available
Flash point	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Vapor pressure	: No data available
Relative density	: No data available
Relative vapor density at 20 °C	: No data available
Solubility	: Water: Solubility in water of component(s) of the mixture : • Toluene: 515 mg/l (at 20 °C)
Log Pow	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available

9.2. Other information

No additional information available

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SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

The product is stable at normal handling and storage conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Keep away from heat, sparks and flame.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Toluene (108-88-3)	
LD50 oral rat	2600 mg/kg
LD50 dermal rabbit	12000 mg/kg
LC50 inhalation rat (mg/l)	12.5 mg/l/4h

Skin corrosion/irritation : Causes skin irritation.
Serious eye damage/irritation : Causes serious eye irritation.
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified

Toluene (108-88-3)	
IARC group	3 - Not classifiable

Reproductive toxicity : Suspected of damaging fertility or the unborn child.
Specific target organ toxicity (single exposure) : May cause drowsiness or dizziness. May cause respiratory irritation.
Specific target organ toxicity (repeated exposure) : May cause damage to organs through prolonged or repeated exposure.
Aspiration hazard : May be fatal if swallowed and enters airways.

SECTION 12: Ecological information

12.1. Toxicity

Toluene (108-88-3)	
LC50 fish 1	15.22 - 19.05 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
EC50 Daphnia 1	5.46 - 9.83 mg/l (Exposure time: 48 h - Species: Daphnia magna [Static])
LC50 fish 2	12.6 mg/l (Exposure time: 96 h - Species: Pimephales promelas [static])
EC50 Daphnia 2	11.5 mg/l (Exposure time: 48 h - Species: Daphnia magna)

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

Toluene (108-88-3)	
Log Pow	2.65

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12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Effect on the global warming : No known ecological damage caused by this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste treatment methods : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
Waste disposal recommendations : Dispose of contents/container in accordance with licensed collector's sorting instructions.
Additional information : Recycle the material as far as possible.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

Transport document description : UN1993 Flammable liquids, n.o.s., 3, II
UN-No.(DOT) : UN1993
Proper Shipping Name (DOT) : Flammable liquids, n.o.s.
Transport hazard class(es) (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120
Hazard labels (DOT) : 3 - Flammable liquid



Packing group (DOT) : II - Medium Danger
DOT Packaging Non Bulk (49 CFR 173.xxx) : 202
DOT Packaging Bulk (49 CFR 173.xxx) : 242
DOT Symbols : G - Identifies PSN requiring a technical name
DOT Special Provisions (49 CFR 172.102) : IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized.
T7 - 4 178.274(d)(2) Normal..... 178.275(d)(3)
TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = $97 / 1 + a (tr - tf)$ Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.
TP8 - A portable tank having a minimum test pressure of 1.5 bar (150 kPa) may be used when the flash point of the hazardous material transported is greater than 0 C (32 F).
TP28 - A portable tank having a minimum test pressure of 2.65 bar (265 kPa) may be used provided the calculated test pressure is 2.65 bar or less based on the MAWP of the hazardous material, as defined in 178.275 of this subchapter, where the test pressure is 1.5 times the MAWP.
DOT Packaging Exceptions (49 CFR 173.xxx) : 150
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 60 L
DOT Vessel Stowage Location : B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.
Other information : No supplementary information available.

TDG

No additional information available

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Transport by sea

UN-No. (IMDG)	: 1993
Proper Shipping Name (IMDG)	: FLAMMABLE LIQUID, N.O.S.
Class (IMDG)	: 3 - Flammable liquids
Packing group (IMDG)	: II - substances presenting medium danger

Air transport

UN-No. (IATA)	: 1993
Proper Shipping Name (IATA)	: Flammable liquid, n.o.s.
Class (IATA)	: 3 - Flammable Liquids
Packing group (IATA)	: II - Medium Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory except for:

3-(Trifluoromethyl)butyraldehyde	CAS No 95853-69-3	45 - 55%
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Chemical(s) subject to the reporting requirements of Section 313 or Title III of the Superfund Amendments and Reauthorization Act (SARA) of 1986 and 40 CFR Part 372.

Toluene	CAS No 108-88-3	45 - 55%
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Toluene (108-88-3)

Subject to reporting requirements of United States SARA Section 313

SARA Section 313 - Emission Reporting	1.0 %
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15.2. International regulations

CANADA

No additional information available

Toluene (108-88-3)

Listed on the Canadian DSL (Domestic Substances List)

WHMIS Classification	Class B Division 2 - Flammable Liquid Class D Division 2 Subdivision A - Very toxic material causing other toxic effects Class D Division 2 Subdivision B - Toxic material causing other toxic effects
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EU-Regulations

No additional information available

National regulations

Toluene (108-88-3)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory
Listed on the Korean ECL (Existing Chemicals List)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)
Japanese Poisonous and Deleterious Substances Control Law
Japanese Pollutant Release and Transfer Register Law (PRTR Law)
Listed on the Canadian IDL (Ingredient Disclosure List)
Listed on INSQ (Mexican national Inventory of Chemical Substances)
Listed on Turkish inventory of chemical

15.3. US State regulations

California Proposition 65 - This product contains, or may contain, trace quantities of a substance(s) known to the state of California to cause cancer and/or reproductive toxicity

Toluene (108-88-3)				
U.S. - California - Proposition 65 - Carcinogens List	U.S. - California - Proposition 65 - Developmental Toxicity	U.S. - California - Proposition 65 - Reproductive Toxicity - Female	U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No significance risk level (NSRL)
No	Yes	No	No	

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Toluene (108-88-3)

U.S. - Massachusetts - Right To Know List
U.S. - New Jersey - Right to Know Hazardous Substance List
U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List
U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

Full text of H-phrases:

Acute Tox. 4 (Inhalation:vapour)	Acute toxicity (inhalation:vapour) Category 4
Aquatic Acute 2	Hazardous to the aquatic environment - Acute Hazard Category 2
Asp. Tox. 1	Aspiration hazard Category 1
Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A
Flam. Liq. 2	Flammable liquids Category 2
Flam. Liq. 3	Flammable liquids Category 3
Repr. 2	Reproductive toxicity Category 2
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT RE 2	Specific target organ toxicity (repeated exposure) Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H225	Highly flammable liquid and vapor
H226	Flammable liquid and vapor
H304	May be fatal if swallowed and enters airways
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
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

NFPA health hazard

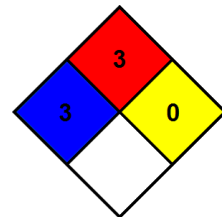
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

NFPA fire hazard

: 3 - Liquids and solids that can be ignited under almost all ambient conditions.

NFPA reactivity

: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given

* - Chronic (long-term) health effects may result from repeated overexposure

Flammability

: 3 Serious Hazard - Materials capable of ignition under almost all normal temperature conditions. Includes flammable liquids with flash points below 73 F and boiling points above 100 F. as well as liquids with flash points between 73 F and 100 F. (Classes IB & IC)

Physical

: 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

SDS US (GHS HazCom 2012)

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 offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable or any damage resulting from handling or from contact with the above product.