

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations SDS ID: 17009Y0 Issue date: 3/14/2023

SECTION 1: Identification

1.1. Identification

Product form : Substance

Substance name : 4-Methylbenzyl bromide

CAS-No. : 104-81-4
Product code : 1700-9-Y0
Formula : C8H9Br

1.2. Recommended use and restrictions on use

Use of the substance/mixture : Laboratory chemicals

Manufacture of substances

Scientific research and development

1.3. Supplier

SynQuest Laboratories, Inc. Inc.

P.O. Box 309

Alachua, FL, Alachua, 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

GHS US classification

Corrosive to metals Category 1 H290 May be corrosive to metals Acute toxicity (oral) Category 3 H301 Toxic if swallowed Acute toxicity (dermal) Category 3 H311 Toxic in contact with skin

Skin corrosion/irritation Category 1 H314 Causes severe skin burns and eye damage

Serious eye damage/eye irritation Category 1 H318 Causes serious eye damage
Specific target organ toxicity – Single exposure, Category 3, H335 May cause respiratory irritation

Respiratory tract irritation

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US)







Signal word (GHS US) : Danger

Hazard statements (GHS US) : H290 - May be corrosive to metals

H301+H311 - Toxic if swallowed or in contact with skin H314 - Causes severe skin burns and eye damage

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Precautionary statements (GHS US)

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H318 - Causes serious eye damage

H335 - May cause respiratory irritation

: P234 - Keep only in original container.

P260 - Do not breathe dust/fume/gas/mist/vapors/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.

P280 - Wear protective gloves/protective clothing/eye protection/face protection.

P301+P310 - If swallowed: Immediately call a poison center or doctor. P301+P330+P331 - If swallowed: rinse mouth. Do NOT induce vomiting.

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.

P310 - Immediately call a POISON CENTER or doctor/ physician

P321 - Specific treatment (see supplemental first aid instructions on this label)

P322 - Specific treatment (see supplemental first aid instruction on this label)

P330 - Rinse mouth.

P361+P364 - Take off immediately all contaminated clothing and wash it before reuse.

P363 - Wash contaminated clothing before reuse.

P390 - Absorb spillage to prevent material-damage.

P403+P233 - Store in a well-ventilated place. Keep container tightly closed.

P405 - Store locked up.

P406 - Store in corrosive resistant container with a resistant inner liner

P501 - Dispose of contents/container to an approved waste disposal plant

2.3. Other hazards which do not result in classification

Other hazards which do not result in classification : Lachrymator.

2.4. Unknown acute toxicity (GHS US)

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	GHS US classification
4-Methylbenzyl bromide (Main constituent)	CAS-No.: 104-81-4	≤ 100	Met. Corr. 1, H290 Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Skin Corr. 1, H314 Eye Dam. 1, H318 STOT SE 3, H335

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

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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. Remove contaminated clothing and shoes. 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 (acute and delayed)

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

and/or in section 11.

Symptoms/effects after inhalation : Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough,

shortness of breath, headache, nausea.

4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media

appropriate for surrounding fire.

5.2. Specific hazards arising from the chemical

Fire hazard : Thermal decomposition generates: Carbon oxides. Hydrogen bromide.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions : In case of fire: Evacuate area.

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 dust. 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".

6.2. Environmental precautions

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

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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 : Minimize generation of dust. 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

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 dust, fumes, mist, spray, vapors. Wear personal

protective equipment. Avoid contact with skin and eyes.

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. Moisture sensitive. Keep contents under inert gas.

Protect from sunlight.

Incompatible materials : Refer to Section 10 on Incompatible Materials.

Storage area : Store in dry, cool, well-ventilated area.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

4-Methylbenzyl bromide (104-81-4)

No additional information available

8.2. Appropriate engineering 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.

8.3. Individual protection measures/Personal protective equipment

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

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Personal protective equipment symbol(s):









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 : Solid

Appearance : Low melting solid.

Color : No data available

Odor : No data available

Odor threshold : No data available

pH : No data available

Melting point : 34 - 36 °C

Freezing point : No data available

Boiling point : 218 – 220 °C (@ 760 mm Hg)

Flash point : No data available Relative evaporation rate (butyl acetate=1) : No data available Flammability (solid, gas) : No data available Vapor pressure : No data available Relative vapor density at 20 °C : No data available : No data available Relative density : 1.32 g/ml Density Molecular mass : 185.061 g/mol : No data available Solubility Partition coefficient n-octanol/water (Log Pow) : No data available : No data available Auto-ignition temperature No data available Decomposition temperature Viscosity, kinematic No data available Viscosity, dynamic No data available **Explosion limits** No data available Explosive properties : No data available

9.2. Other information

Oxidizing properties

No additional information available

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

: No data available

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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 (oral) : Toxic if swallowed.

Acute toxicity (dermal) : Toxic in contact with skin.

Acute toxicity (inhalation) : Not classified

ATE US (oral)	100 mg/kg body weight
ATE US (dermal)	300 mg/kg body weight

Skin corrosion/irritation : Causes severe skin burns.
Serious eye damage/irritation : Causes serious eye damage.
Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified Carcinogenicity : Not classified Reproductive toxicity : Not classified

STOT-single exposure : May cause respiratory irritation.

STOT-repeated exposure : Not classified
Aspiration hazard : Not classified
Viscosity, kinematic : No data available

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

and/or in section 11.

Symptoms/effects after inhalation : Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough,

shortness of breath, headache, nausea.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

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12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

Waste treatment methods

Product/Packaging disposal recommendations

Additional information

: Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.

: Dispose of contents/container in accordance with licensed collector's sorting instructions.

: Recycle the material as far as possible.

SECTION 14: Transport information

14.1. UN number

DOT NA NO : UN3417 UN-No. (TDG) : UN3417 UN-No. (IMDG) : 3417 UN-No. (IATA) : 3417

14.2. UN proper shipping name

Proper Shipping Name (DOT) : Xylyl bromide, solid
Proper Shipping Name (TDG) : XYLYL BROMIDE, SOLID
Proper Shipping Name (IMDG) : XYLYL BROMIDE, SOLID
Proper Shipping Name (IATA) : Xylyl bromide, solid

14.3. Transport hazard class(es)

DOT

Transport hazard class(es) (DOT) : 6.1 Hazard labels (DOT) : 6.1



TDG

Transport hazard class(es) (TDG) : 6.1 Hazard labels (TDG) : 6.1



IMDG

Transport hazard class(es) (IMDG) : 6.1 Hazard labels (IMDG) : 6.1



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IATA

Transport hazard class(es) (IATA) : 6.1 Hazard labels (IATA) : 6.1



14.4. Packing group

Packing group (DOT) : 11 : II Packing group (TDG) Packing group (IMDG) : II Packing group (IATA) : 11

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

DOT

UN-No.(DOT) : UN3417

DOT Special Provisions (49 CFR 172.102)

: A3 - For combination packaging, if glass inner packaging (including ampoules) are used, they must be packed with absorbent material in tightly closed metal receptacles before packing in outer packaging.

A6 - For combination packaging, if plastic inner packaging are used, they must be packed in tightly closed metal receptacles before packing in outer packaging.

A7 - Steel packaging must be corrosion-resistant or have protection against corrosion.

IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2).

IP2 - When IBCs other than metal or rigid plastics IBCs are used, they must be offered for transportation in a closed freight container or a closed transport vehicle.

IP4 - Flexible, fiberboard or wooden IBCs must be sift-proof and water-resistant or be fitted with a sift-proof and water-resistant liner.

N33 - Aluminum drums are not authorized.

T3 - 2.65 178.274(d)(2) Normal..... 178.275(d)(2)

TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.

DOT Packaging Exceptions (49 CFR 173.xxx) None 340 DOT Packaging Non Bulk (49 CFR 173.xxx) DOT Packaging Bulk (49 CFR 173.xxx) None DOT Quantity Limitations Passenger aircraft/rail (49 25 kg

CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 100 kg

CFR 175.75)

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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.

DOT Vessel Stowage Other : 40 - Stow "clear of living quarters"

TDG

UN-No. (TDG) : UN3417

TDG Special Provisions : 38 - A person must not handle, offer for transport or transport these dangerous goods in a large

means of containment if they are in direct contact with the large means of containment.

Explosive Limit and Limited Quantity Index : 0

Excepted quantities (TDG) : E4

Passenger Carrying Road Vehicle or Passenger : Forbidden

Carrying Railway Vehicle Index

Emergency Response Guide (ERG) Number : 152

IMDG

Limited quantities (IMDG) : 0

Excepted quantities (IMDG) : E4

Packing instructions (IMDG) : P002

IBC packing instructions (IMDG) : IBC08

IBC special provisions (IMDG) : B21, B4

Tank instructions (IMDG) : T3

Tank special provisions (IMDG) : TP33

EmS-No. (Fire) : F-A - FIRE SCHEDULE Alfa - GENERAL FIRE SCHEDULE

EmS-No. (Spillage) : S-G - SPILLAGE SCHEDULE Golf - FLAMMABLE SOLIDS AND SELF-REACTIVE

SUBSTANCES

Stowage category (IMDG) : D Stowage and handling (IMDG) : SW2

Properties and observations (IMDG) : Crystals or powder, evolving irritating vapour ("Tear Gas"). Toxic if swallowed, by skin contact or

by inhalation.

IATA

PCA Excepted quantities (IATA) : E4 PCA Limited quantities (IATA) : Forbidden PCA limited quantity max net quantity (IATA) : Forbidden PCA packing instructions (IATA) 669 PCA max net quantity (IATA) 25kg CAO packing instructions (IATA) 676 CAO max net quantity (IATA) : 100kg ERG code (IATA) 6L

14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

All components of this product are present and listed as Active on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory, except for:

4-Methylbenzyl bromide	CAS-No. 104-81-4	100%
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15.2. International regulations

CANADA

4-Methylbenzyl bromide (104-81-4)

Listed on the Canadian NDSL (Non-Domestic Substances List)

EU-Regulations

4-Methylbenzyl bromide (104-81-4)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

National regulations

4-Methylbenzyl bromide (104-81-4)

Listed on the Japanese ENCS (Existing New Chemical Substances) inventory

Listed on the Japanese ISHL (Industrial Safety and Health Law)

Listed on the TCSI (Taiwan Chemical Substance Inventory)

Listed on the NCI (Vietnam - National Chemical Inventory)

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

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Full text of H-phrases	
H290	May be corrosive to metals
H301	Toxic if swallowed
H311	Toxic in contact with skin
H314	Causes severe skin burns and eye damage
H318	Causes serious eye damage
H335	May cause respiratory irritation

NFPA health hazard

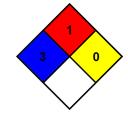
: 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA fire hazard NFPA reactivity

: 1 - Materials that must be preheated before ignition can occur.

: $\,$ 0 - Material that in themselves are normally stable, even under fire

conditions.



Hazard Rating

Health

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

Flammability

: 1 Slight Hazard - Materials that must be preheated before ignition will occur. Includes liquids, solids and semi solids having a flash point above 200 F. (Class IIIB)

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.

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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 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.