

MATERIAL SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

National Institute of Standards and Technology
Standard Reference Materials Program
100 Bureau Drive, Stop 2300
Gaithersburg, Maryland 20899-2300

SRM Number: 3016
MSDS Number: 3016
SRM Name: sec-Butylbenzene in
Methanol (Nominal Mass Fraction 0.01 g/g)

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Description: This Standard Reference Material (SRM) is intended primarily for the calibration of instrumentation and validation of methods for volatile organic compound (VOC) determinations. A unit of SRM 3016 consists of two 5 mL sealed borosilicate glass ampoules of a gravimetrically prepared solution of sec-Butylbenzene in methanol. Approximately 2.5 mL of this mixture is supplied in each 5 mL glass ampoule.

Substance: sec-Butylbenzene in Methanol.

Other Designations:

Methanol (methyl alcohol; methyl hydroxide; wood alcohol; wood spirit).
sec-Butylbenzene (benzene (1-methylpropyl); 2-phenylbutane; secondary-butyl benzene; C₁₀H₁₄).

2. HAZARDS IDENTIFICATION

NFPA Ratings (Scale 0–4): Health = 2 Fire = 3 Reactivity = 0

NOTE: This sec-butylbenzene in methanol solution has not been tested as a whole. The health and physical hazard information are for sec-butylbenzene and methanol. The actual effects of the solution may differ from the individual components.

Major Health Hazards: Skin, eye, and/or respiratory tract irritation, central nervous system depression, blood disorder, liver damage, nerve damage, and aspiration hazard.

Physical Hazards: Flammable liquid and vapor. Vapor may cause flash fire. Electrostatic charges may be generated by flow or agitation.

Potential Health Effects (Acute and Chronic):

Inhalation: Methanol may cause irritation, cough, ringing in the ears, constipation, headache, drowsiness, dizziness, tingling sensation, pain in extremities, tremors, loss of coordination, blood disorders, and nerve damage. No data available for exposure to sec-butylbenzene.

Skin Contact: Methanol can cause irritation, absorption may occur, headache, drowsiness, dizziness, loss of coordination, and blood disorders. Acute exposure to sec-butylbenzene may cause irritation. Repeated or prolonged contact may cause dermatitis.

Eye Contact: Methanol vapors may cause irritation and eye damage. Repeated or prolonged contact may cause conjunctivitis. Exposure to sec-butylbenzene may cause irritation.

Ingestion: Ingestion of methanol may result in mild and transient inebriation, and subsequent drowsiness. Liver, kidney, heart, stomach, intestine and pancreatic damage may also occur. Death may occur due to respiratory failure. As little as 15 mL has caused blindness; the usual fatal dose is 60 mL to 240 mL. No data listed for chronic exposure to sec-butylbenzene.

Listed as a Carcinogen/Potential Carcinogen

In the National Toxicology Program (NTP) Report on Carcinogens
In the International Agency for Research on Cancer (IARC) Monographs
By the Occupational Safety and Health Administration (OSHA)

Yes	No
_____	<u>X</u>
_____	<u>X</u>
_____	<u>X</u>

3. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Component	CAS Number	EC Number (EINECS)	Nominal Mass Concentration ^(a) (%)
Methanol	67-56-1	200-659-6	99
sec-Butylbenzene	135-98-8	205-227-0	1

^(a) Hazardous components 1 % or greater; carcinogens 0.1 % or greater are listed in compliance with OSHA 29 CFR 1910.1200.

Component: Methanol

EC Classification: T, F
EC Risk (R No.): 11, 23/24/25, 39/23/24/25
EC Safety (S No.): 7, 16, 36/37, 45

Component: sec-Butylbenzene

EC Classification: Xi
EC Risk (R No.): 10, 38
EC Safety (S No.): 24, 46

EC Risk/Safety Phrases: See Section 15, "Regulatory Information".

4. FIRST AID MEASURES

Inhalation: If adverse effects occur, remove to uncontaminated area. If not breathing, give artificial respiration or oxygen by qualified personnel. Seek medical attention if needed.

Eye Contact: Immediately flush eyes with copious amounts of water for at least 15 minutes.

Skin Contact: Wash exposed skin with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Thoroughly clean and dry contaminated clothing and shoes before reuse.

Ingestion: Ingestion of this material is not likely under normal conditions of use. Potential aspiration hazard if ingested. If swallowed, seek medical attention.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards: Severe fire hazard. Vapor/air mixtures are explosive. The vapor is heavier than air. Vapors or gases may ignite at distant ignition sources and flash back. Electrostatic discharges may be generated by flow or agitation resulting in ignition or explosion.

Extinguishing Media: Alcohol-resistant foam, carbon dioxide, regular dry chemical, water.

Fire Fighting: Avoid inhalation of material or combustion by-products. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus (SCBA).

Note: The data listed below is for methanol.

Flash Point (°C): 11 (52 °F)

Method Used: Closed Cup

Autoignition Temp. (°C): 385 (725 °F)

Flammability Limits in Air
UPPER (Volume %): 36
LOWER (Volume %): 6

6. ACCIDENTAL RELEASE MEASURES

Occupational Release: Remove sources of ignition. Do not touch spilled material. Absorb small spills with sand or other non-combustible material. Collect spilled material in appropriate container for proper disposal.

Disposal: Refer to Section 13, "Disposal Considerations".

7. HANDLING AND STORAGE

Storage: Store and handle in accordance with all current regulations and standards. Sealed ampoules should be stored in the dark at temperatures between 10 °C and 30 °C. Grounding and bonding required. Keep separated from incompatible substances. Subject to storage regulations: U.S. OSHA 29 CFR 1910.106.

Safe Handling Precautions: See Section 8, "Exposure Controls and Personal Protection".

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Exposure Limits

Component: Methanol

OSHA (PEL): 200 ppm, 260 mg/m³ (TWA)

ACGIH (TLV): 200 ppm (TWA); 250 ppm (STEL);

Skin – potential significant contribution to overall exposure by the cutaneous route.

NIOSH (REL): 200 ppm, 260 mg/m³ (TWA); 250 ppm, 325 mg/m³ (STEL); 6000 ppm (IDLH);

Potential for dermal absorption.

Component: sec-Butylbenzene

No established occupational exposure limits.

Ventilation: Provide local exhaust or process enclosure ventilation system. Ensure compliance with applicable exposure limits.

Respirator: If workplace conditions warrant a respirator, a respiratory protection program that meets OSHA 29 CFR 1910.134 must be followed. Refer to NIOSH 42 CFR 84 for applicable certified respirators.

Eye Protection: Wear safety goggles. An eyewash station and drench shower should be readily available near the handling and use areas.

Personal Protection: In accordance with OSHA 29 CFR 1910.132, subpart I, wear appropriate Personal Protective Equipment (PPE) to minimize exposure to this material.

9. PHYSICAL AND CHEMICAL PROPERTIES

Component	Methanol	sec-Butylbenzene
Appearance and Odor	clear and colorless liquid, alcohol odor (threshold 100 ppm)	clear and colorless liquid, pungent odor
Molecular Formula	CH ₃ OH	C ₁₀ H ₁₄
Molar Mass (g/mol)	32.04	134.22
Density (g/cm ³)	0.79	Not available
Vapor Density (air = 1)	1.11	4.6
Specific Gravity (water = 1)	0.79	0.868
Kinematic Viscosity	0.59 cP 20 °C	Not available
Boiling Point (°C)	65 (149 °F)	173 (343.4 °F)
Melting Point (°C)	-94 (-137 °F)	-83 (-117.4 °F)
Water Solubility	soluble	insoluble
Solvent Solubility	acetone, alcohol, benzene, chloroform, ethanol, ether, ketones, organic solvents	Alcohol, acetone, acids, benzene, ether

NOTE: The physical and chemical data provided are for the pure components. No physical or chemical data are available for the solution of sec-butylbenzene in methanol. The actual behavior of the solution may differ from the individual components.

10. STABILITY AND REACTIVITY

Stability: Stable Unstable

Conditions to Avoid: Avoid heat, flames, sparks, and other sources of ignition. Ampoules may rupture or explode if exposed to heat. Keep out of water supplies and sewers. Avoid inhalation of material or combustion by-products. Avoid contact with incompatible materials.

Incompatible Materials: Halo carbons, combustible materials, metals, oxidizing materials, halogens, metal carbide, bases, acids, amines, and metal salts.

Fire/Explosion Information: See Section 5, "Fire Fighting Measures".

Hazardous Decomposition: Oxides of carbon, various organic fragments.

Hazardous Polymerization: Will Occur Will Not Occur

11. TOXICOLOGICAL INFORMATION

Route of Entry: Inhalation Skin Ingestion

Toxicity Data: End points listed by Registry of Toxic Effects of Chemical Substances (RTECS).

Component: Methanol

Rat, Oral LD50: 5628 mg/kg

Rabbit, Skin LD50: 15 800 mg/kg

Rat, Inhalation LC50: 83.2 mg/L (4 h); 64 000 ppm (4 h)

Component: sec-Butylbenzene

Rat, Oral LD50: 2240 mg/kg.

Rat, Inhalation LC50: No information listed.

Rabbit, Skin LD50: >16 mL/kg

Irritation Data:

Component: Methanol

Rabbit, eyes: 100 mg (24 h), moderate

Rabbit, skin: 20 mg (24 h), moderate

Component: sec-Butylbenzene

Rabbit, eyes: 500 mg (24 h), mild.

Rabbit, skin: 100 mg (24 h), moderate.

Health Effects: See Section 2, "Hazards Identification" for potential health effects.

Target Organs: Liver, kidneys, central, central nervous system.

Medical Conditions Aggravated by Exposure: Allergies and disorders of the blood system, immune system, eye, skin, and kidney.

Mutagen/Teratogen: The components of this material have been reviewed and the Registry of Toxic Effects of Chemical Substances (RTECS) publishes the following endpoints.

Component: Methanol

Tumorigenic: Rat, Inhalation TCLo: 1000 ppm (2 years)

Mutagenic: Human: 300 mmol/L

Reproductive: Mouse, Inhalation TCLo: 2000 ppm (7 h, pregnant 6–15 d)

Component: sec-Butylbenzene

Tumorigenic: No data listed.

Mutagenic: No data listed.

Reproductive: No data listed.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data:

Component: Methanol

Fish Toxicity: Rainbow trout (*Oncorhynchus mykiss*) LC50 (static): 18 mL/L to 20 mL/L (96 h).

Component: sec-Butylbenzene

Fish Toxicity: No data listed.

Invertebrate: No data listed.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose in accordance with all applicable federal, state, and local requirements. Subject to disposal regulations: U.S. EPA 40 CFR 262; Hazardous Waste Number(s): U154 (methanol).

14. TRANSPORTATION INFORMATION

U.S. DOT and IATA: UN1230, Methanol solution, Hazard Class 3 (6.1), Packing Group II, Excepted Qty: Yes, E2.

15. REGULATORY INFORMATION

U.S. REGULATIONS

CERCLA Sections 102a/103 (40 CFR 302.4): 5000 lb (2270 kg) final RQ for methanol and isopropylbenzene.

SARA Title III Section 302 (40 CFR 355.30): Not regulated.

SARA Title III Section 304 (40 CFR 355.40): Not regulated.

SARA Title III Section 313 (40 CFR 372.65): Methanol de minimis concentration 1.0 %.

OSHA Process Safety (29 CFR 1910.119): Not regulated.

SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21)

ACUTE HEALTH: Yes

CHRONIC HEALTH: Yes

FIRE: Yes

REACTIVE: No

PRESSURE: No

STATE REGULATIONS

California Proposition 65: WARNING! This product contains chemicals known to the state of California to cause reproductive/developmental effects (methanol). Keep out of water supplies and sewers.

CANADIAN REGULATIONS

WHMIS Information: Not provided for this material.

EUROPEAN REGULATIONS

Component: Methanol

EC Classification: F – Highly Flammable, T – Toxic (Concentration ≥ 20 %)

EC Risk Phrases:

R11 – Highly flammable.

R23/24/25 – Toxic by inhalation, in contact with skin and if swallowed.

R39/23/24/25 – Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed.

EC Safety Phrases:

S7 – Keep container tightly closed.

S16 – Keep away from sources of ignition – No smoking.

S36/37 – Wear suitable protective clothing and gloves.

S45 – In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

Component: sec-Butylbenzene.

EC Classification: Xi – Irritant

EC Risk Phrases:

10 – Flammable.

R38 – Irritating to skin.

EC Safety Phrases:

S24 – Avoid contact with skin.

S46 – If swallowed, seek medical advice immediately and show this container or label.

NATIONAL INVENTORY STATUS

U.S. Inventory (TSCA): Methanol is listed.

TSCA 12(b), Export Notification: Not listed.

16. OTHER INFORMATION

Sources: ChemADVISOR, Inc., MSDS *Methyl Alcohol*, 03 December 2012.

ChemADVISOR, Inc., MSDS, *sec-Butylbenzene*, 13 March 2013.

EC; European Chemical Substance Information System (ESIS), *sec-Butylbenzene*, CAS No. 135-98-8; available at <http://esis.jrc.ec.europa.eu/> (accessed Apr 2013).

EC; ESIS, *Methanol*, CAS No. 67-56-1; available at <http://esis.jrc.ec.europa.eu/> (accessed Apr 2013).

Disclaimer: Physical and chemical data contained in this MSDS are provided only for use in assessing the hazardous nature of the material. The MSDS was prepared carefully, using current references; however, NIST does not certify the data in the MSDS. The certified values for this material are given in the NIST Certificate of Analysis.