

SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

Product Identifier

SRM Number: 1816a
SRM Name: Reference Fuel Isooctane (2,2,4-Trimethylpentane)
Other Means of Identification: Not applicable.

Recommended Use of This Material and Restrictions of Use

This Standard Reference Material (SRM) is intended for use as a primary standard in the octane rating of motor aviation fuels as specified in ASTM test methods and evaluating ASTM methods for chemical analysis of fuels by gas chromatography. A unit of SRM 1816a consists of one ampoule, containing approximately 100 mL of isooctane.

Company Information

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2. HAZARDS IDENTIFICATION

Classification

Physical Hazard:	Flammable liquid	Category 2
Health Hazard:	Skin Corrosion/Irritation	Category 2
	Eye Irritation	Category 2B
	STOT, Single Exposure	Category 3
	Aspiration Hazard	Category 1

Label Elements
Symbol

Signal Word

DANGER

Hazard Statement(s)

H225 Highly flammable liquid and vapor.
 H304 May be fatal if swallowed and enters airways.
 H315+H320 Causes skin and eye irritation.
 H336 May cause drowsiness or dizziness.

Precautionary Statement(s)

P210 Keep away from heat, sparks, open flames, hot surfaces. — No smoking.
 P241 Use explosion-proof electrical, ventilating, and lighting equipment.
 P242 Use only non-sparking tools.
 P243 Take precautionary measures against static discharge.
 P261 Avoid breathing mist, vapors, or spray.
 P264 Wash hands thoroughly after handling.
 P271 Use only outdoors or in a well-ventilated area.
 P280 Wear protective gloves, eye protection, and protective clothing.
 P301+P310 If swallowed: Immediately call a doctor.

P331	Do NOT induce vomiting.
P303+P361+P353	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P305+P351+P338	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332+P337+P313	If skin or eye irritation occurs: Get medical attention.
P304+P340 P312	If inhaled: Remove person to fresh air and keep comfortable for breathing. Call a doctor if you feel unwell.
P362+P364	Take off contaminated clothing and wash it before reuse.
P403+P235+P233 P405	Store in a well-ventilated place. Keep cool. Keep container tightly closed. Store locked up.
P501	Dispose of contents and container according to local regulations.

Hazards Not Otherwise Classified: None.

Ingredients(s) with Unknown Acute Toxicity: None.

3. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Substance: 2,2,4-Trimethylpentane

Other Designations: Isooctane; isobutyltrimethylmethane

Hazardous Component(s)	CAS Number	EC Number (EINECS)	Nominal Mass Concentration (%)
2,2,4-Trimethylpentane	540-84-1	208-759-1	>99.9

4. FIRST AID MEASURES

Description of First Aid Measures

Inhalation: If adverse effects occur, remove to well-ventilated (uncontaminated) area. Give artificial respiration if not breathing. Get immediate medical attention.

Skin Contact: Wash skin with soap and water for at least 15 minutes while removing contaminated clothing and shoes. Thoroughly clean and dry before reuse. Get medical attention, if needed.

Eye Contact: Flush eyes with plenty of water for at least 15 minutes. Then get immediate medical attention.

Ingestion: Aspiration hazard. Do not induce vomiting. If vomiting occurs, keep head lower than hips to help prevent aspiration. Get immediate medical attention. Give artificial respiration if not breathing.

Most Important Symptoms/Effects, Acute and Delayed: Respiratory tract irritation, aspiration hazard, central nervous system depression.

Indication of any immediate medical attention and special treatment needed, if necessary: If any of the above symptoms are present, seek immediate medical attention.

5. Fire Fighting Measures

Fire and Explosion Hazards: Severe fire hazard. The vapor is heavier than air. Vapor/air mixtures are explosive above the flash point. Vapors or gases may ignite at distant ignition sources and flash back. See Section 9, "Physical and Chemical Properties" for flammability properties.

Extinguishing Media

Suitable: Regular dry chemical, carbon dioxide, water, or alcohol-resistant foam.

Unsuitable: None listed.

Specific Hazards Arising from the Chemical: Not applicable.

Special Protective Equipment and Precautions for Fire-Fighters: Move container from fire area if it can be done without personal risk. Avoid inhalation of material or combustion by-products. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus (SCBA).

NFPA Ratings (0 = Minimal; 1 = Slight; 2 = Moderate; 3 = Serious; 4 = Severe)

Health = 2

Fire = 3

Reactivity = 0

6. ACCIDENTAL RELEASE MEASURES

Personal Precautions, Protective Equipment and Emergency Procedures: Use suitable protective equipment; see Section 8, “Exposure Controls and Personal Protection”. Keep out of waters supplies and sewers.

Methods and Materials for Containment and Clean up: Avoid heat, flames, sparks and other sources of ignition. Stop leak if possible without personal risk, with water spray to reduce vapors. Absorb spilled material with sand or non-combustible material and collect in appropriate container for disposal.

7. HANDLING AND STORAGE

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

Storage and Incompatible Materials: Store in a well-ventilated area. Keep separated from incompatible substances (see Section 10, “Stability and Reactivity”).

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Exposure Limits: No occupational exposure limits established.

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

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

Respiratory Protection: 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: Splash resistant safety goggles and emergency eyewash are recommended.

Skin and Body Protection: Chemical resistant clothing and gloves are recommended.

9. PHYSICAL AND CHEMICAL PROPERTIES

Descriptive Properties	2,2,4-Trimethylpentane
Molar Mass (g/mol)	114.23
Molecular Formula	C ₈ H ₁₈
Appearance (physical state, color, etc.)	clear, colorless, free-flowing liquid
Odor	gasoline odor
Odor threshold	not available
pH	not available
Evaporation rate	<1 (ether = 1)
Melting point/freezing point	−107 °C (−161 °F)
Relative Density (water = 1)	0.6919
Density	not available
Vapor Pressure	41 mmHg at 21 °C
Vapor Density (air = 1)	3.9
Viscosity	not available
Solubilities	immiscible with water; soluble in ether, alcohol, acetone, benzene, toluene, chloroform, xylene, carbon disulfide, carbon tetrachloride, dimethylformamide, oils
Partition coefficient (n-octanol/water)	not available

Thermal Stability Properties	2,2,4-Trimethylpentane
Autoignition Temperature	415 °C (779 °F)
Thermal Decomposition	not available
Initial boiling point and boiling range	99 °C (210 °F)
Explosive Limits, LEL (Volume %)	1.1
Explosive Limits, UEL (Volume %)	6
Flash Point (Closed Cup)	-12 °C (10 °F)
Flammability (solid, gas)	not available

10. STABILITY AND REACTIVITY

Reactivity: Stable at normal temperatures and pressure.

Stability: X Stable Unstable

Possible Hazardous Reactions: Not applicable.

Conditions to Avoid: Avoid heat, flames, sparks, and other sources of ignition. Minimize contact with material. Avoid inhalation of material or combustion by-products. Keep out of water supplies and sewers.

Incompatible Materials: Oxidizing materials, reducing agents.

Hazardous Decomposition: Oxides of carbon.

Hazardous Polymerization: Will Occur X Will Not Occur

11. TOXICOLOGICAL INFORMATION

Route of Exposure: X Inhalation X Skin X Ingestion

Symptoms Related to the Physical, Chemical and Toxicological Characteristics: Skin irritation, eye irritation, central nervous system depression, and nerve damage.

Potential Health Effects (Acute, Chronic, and Delayed)

Inhalation: Acute exposure may cause irritation of the mucous membranes, rapid breathing, dizziness, fatigue, and headache. Extreme exposure may cause unconsciousness and respiratory arrest. Repeated and prolonged exposure may cause polyneuropathy.

Skin Contact: Short term exposure may cause irritation with redness. If sufficient amounts are absorbed, systemic toxicity may occur. Long term exposure may cause dermatitis due to defatting action.

Eye Contact: May cause irritation with redness.

Ingestion: Aspiration hazard. Lung damage may occur if aspirated into the lungs and may be fatal. Symptoms may include coughing, difficulty breathing, cyanosis and pulmonary edema. May cause diarrhea, fatigue and slight central nervous system depression.

Numerical Measures of Toxicity

Acute Toxicity: Not classified.

Rat, Oral, LD50: >2500 mg/kg

Rat, Inhalation, LC50: 34.7 mg/L (4 h); 47.4 mg/L (1 h)

Skin Corrosion/Irritation: Category 2; may cause irritation, redness, and defatting of the skin.

Serious Eye Damage/Eye Irritation: Category 2B; may cause irritation with redness.

Respiratory Sensitization: Not classified; no data available.

Skin Sensitization: Not classified; no data available.

Germ Cell Mutagenicity: Not classified.

Rat: 500 mg/kg

Carcinogenicity: Not classified.

Listed as a Carcinogen/Potential Carcinogen Yes X No

2,2,4-Trimethylpentane is not listed by IARC, NTP, or OSHA as a carcinogen/potential carcinogen.

Reproductive Toxicity: Not classified; no data available.

STOT, Single Exposure: Category 3, has shown to cause central nervous system depressant.

STOT, Repeated Exposure: Not classified; no data available.

Aspiration Hazard: Category 1; aspiration hazard.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data: No data available.

Persistence and Degradability: No data available.

Bioaccumulative Potential: No data available.

Mobility in Soil: No data available.

Other Adverse effects: No data available.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose in accordance with all applicable federal, state, and local regulations. Subject to hazardous waste regulations US EPA 40 CFR 262: Hazardous waste number D001.

14. TRANSPORTATION INFORMATION

U.S. DOT and IATA: UN1262; Octanes; Hazard Class 3; Packing Group II; Excepted Quantity: E2.

15. REGULATORY INFORMATION

U.S. Regulations

CERCLA Sections 102a/103 (40 CFR 302.4): 1000 lbs (454 kg) final RQ.

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): Not regulated.

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: No

FIRE: Yes

REACTIVE: No

PRESSURE: No

State Regulations

California Proposition 65: Not listed.

U.S. TSCA Inventory: 2,2,4-trimethylpentane is listed.

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

Canadian Regulations: WHMIS Information is not provided for this material.

16. OTHER INFORMATION

Issue Date: 30 April 2015

Sources: ChemADVISOR, Inc., SDS 2,2,4-Trimethylpentane, 20 March 2015.

Key of Acronyms:

ACGIH	American Conference of Governmental Industrial Hygienists	NTP	National Toxicology Program
CAS	Chemical Abstracts Service	OSHA	Occupational Safety and Health Administration
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act	PEL	Permissible Exposure Limit
CFR	Code of Federal Regulations	RCRA	Resource Conservation and Recovery Act
DOT	Department of Transportation	REL	Recommended Exposure Limit
EINECS	European Inventory of Existing Commercial Chemical Substances	RQ	Reportable Quantity
EPCRA	Emergency Planning and Community Right-to-Know Act	RTECS	Registry of Toxic Effects of Chemical Substances
IARC	International Agency for Research on Cancer	SARA	Superfund Amendments and Reauthorization Act
IATA	International Air Transportation Agency	SCBA	Self-Contained Breathing Apparatus
IDLH	Immediately Dangerous to Life and Health	SRM	Standard Reference Material
LC50	Lethal Concentration	STEL	Short Term Exposure Limit
LD50	Median Lethal Dose or Lethal Dose, 50 %	STOT	Specific Target Organ Toxicity
LEL	Lower Explosive Limit	TLV	Threshold Limit Value
MSDS	Material Safety Data Sheet	TPQ	Threshold Planning Quantity
NFPA	National Fire Protection Association	TSCA	Toxic Substances Control Act
NIOSH	National Institute for Occupational Safety and Health	TWA	Time Weighted Average
NIST	National Institute of Standards and Technology	UEL	Upper Explosive Limit
n.o.s.	Not Otherwise Specified	WHMIS	Workplace Hazardous Materials Information System

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

Users of this SRM should ensure that the SDS in their possession is current. This can be accomplished by contacting the SRM Program: telephone (301) 975-2200; fax (301) 948-3730; e-mail srmmsds@nist.gov; or via the Internet at <http://www.nist.gov/srm>.