



# SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 04/16/2014

Version 1.2

## SECTION 1. Identification

### Product identifier

Product number	104718
Product name	Isooctane for spectroscopy Uvasol®
CAS-No.	540-84-1

### Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Reagent for analysis
-----------------	----------------------

### Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation   290 Concord Road, Billerica, MA 01821, United States of America   General Inquiries: +1-978-715-4321   Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
---------	--

Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
---------------------	--

## SECTION 2. Hazards identification

### GHS Classification

Flammable liquid, Category 2, H225  
Aspiration hazard, Category 1, H304  
Skin irritation, Category 2, H315  
Specific target organ systemic toxicity - single exposure, Category 3, H336  
Acute aquatic toxicity, Category 1, H400  
Chronic aquatic toxicity, Category 1, H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

### GHS-Labeling

*Hazard pictograms*



*Signal Word*  
Danger

# SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number 104718  
Product name Isooctane for spectroscopy Uvasol®

---

Version 1.2

## *Hazard Statements*

H225 Highly flammable liquid and vapor.  
H304 May be fatal if swallowed and enters airways.  
H315 Causes skin irritation.  
H336 May cause drowsiness or dizziness.  
H410 Very toxic to aquatic life with long lasting effects.

## *Precautionary Statements*

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.  
P233 Keep container tightly closed.  
P240 Ground/bond container and receiving equipment.  
P273 Avoid release to the environment.  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.  
P331 Do NOT induce vomiting.  
P403 + P235 Store in a well-ventilated place. Keep cool.

## **OSHA Hazards**

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200). This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS and may deviate from the GHS information.

## **Other hazards**

None known.

---

## **SECTION 3. Composition/information on ingredients**

Formula	$\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$	$\text{C}_8\text{H}_{18}$ (Hill)
Molar mass	114.23 g/mol	

## **Hazardous ingredients**

*Chemical Name (Concentration)*  
CAS-No.  
*isooctane (>= 90 % - <= 100 % )*  
540-84-1

Exact percentages are being withheld as a trade secret.

---

## **SECTION 4. First aid measures**

### **Description of first-aid measures**

#### *Inhalation*

After inhalation: fresh air. Consult doctor if feeling unwell.

#### *Skin contact*

After skin contact: wash off with plenty of water. Remove contaminated clothing.

#### *Eye contact*

After eye contact: rinse out with plenty of water with the eyelid held wide open. Call in ophthalmologist if necessary.

---

## SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number

104718

Version 1.2

Product name

Isooctane for spectroscopy Uvasol®

---

### *Ingestion*

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

Never give anything by mouth to an unconscious person.

### **Most important symptoms and effects, both acute and delayed**

irritant effects, Drowsiness, drowsiness

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

### **Indication of any immediate medical attention and special treatment needed**

No information available.

---

## **SECTION 5. Fire-fighting measures**

### **Extinguishing media**

#### *Suitable extinguishing media*

Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

#### *Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

### **Special hazards arising from the substance or mixture**

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

Pay attention to flashback.

Development of hazardous combustion gases or vapors possible in the event of fire.

### **Advice for firefighters**

#### *Special protective equipment for fire-fighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

#### *Further information*

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

## **SECTION 6. Accidental release measures**

### **Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact.

Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

### **Environmental precautions**

Do not empty into drains. Risk of explosion.

### **Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills.

---

# SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number

104718

Version 1.2

Product name

Isooctane for spectroscopy Uvasol®

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

## SECTION 7. Handling and storage

### Precautions for safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapors/aerosols.

Observe label precautions.

### *Advice on protection against fire and explosion*

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

### Conditions for safe storage, including any incompatibilities

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place.

Storage temperature: no restrictions.

## SECTION 8. Exposure controls/personal protection

### Exposure limit(s)

#### *Ingredients*

Basis	Value	Threshold limits	Remarks
<i>isooctane 540-84-1</i>			
ACGIH	Time Weighted Average (TWA):	300 ppm	
NIOSH/GUIDE	Recommended exposure limit (REL):	75 ppm	
		350 mg/m <sup>3</sup>	
OSHA_TRANS	Ceiling Limit Value and Time Period (if specified):	385 ppm	Ceiling Limit Value 15-min
	PEL:	1,800 mg/m <sup>3</sup>	
Z1A	Time Weighted Average (TWA):	500 ppm	
		2,350 mg/m <sup>3</sup>	
Z1A	Time Weighted Average (TWA):	300 ppm	
		1,450 mg/m <sup>3</sup>	
Z1A	Short Term Exposure Limit (STEL):	375 ppm	
		1,800 mg/m <sup>3</sup>	
ACGIH	Time Weighted Average (TWA):	300 ppm	

### Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

### Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

# SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number

104718

Version 1.2

Product name

Isooctane for spectroscopy Uvasol®

---

### *Hygiene measures*

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

### *Eye/face protection*

Safety glasses

### *Hand protection*

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

### *Other protective equipment:*

Flame retardant antistatic protective clothing

### *Respiratory protection*

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

---

## SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	benzine-like
Odor Threshold	No information available.
pH	neutral
Melting point	-107 °C
Boiling point/boiling range	210 °F (99 °C) at 1,013 hPa
Flash point	10 °F (-12 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1 %(V)
Upper explosion limit	6 %(V)
Vapor pressure	51 hPa at 68 °F (20 °C)
Relative vapor density	3.9

---

## SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number	104718	Version 1.2
Product name	Isooctane for spectroscopy Uvasol®	

---

Density	0.69 g/cm <sup>3</sup> at 68 °F (20 °C)
Relative density	No information available.
Water solubility	0.56 mg/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: 4.09 (calculated) Potential bioaccumulation
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0.50 mPa.s at 68 °F (20 °C)
Explosive properties	Not classified as explosive.
Oxidizing properties	none
Ignition temperature	770 °F (410 °C)
Saturated vapor concentration	239 g/m <sup>3</sup> at 68 °F (20 °C)

---

### SECTION 10. Stability and reactivity

#### Reactivity

Vapors may form explosive mixture with air.

#### Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

#### Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

#### Conditions to avoid

Warming.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

#### Incompatible materials

various plastics

#### Hazardous decomposition products

no information available

SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number

104718

Version 1.2

Product name

Isooctane for spectroscopy Uvasol®

---

**SECTION 11. Toxicological information**

**Information on toxicological effects**

*Likely route of exposure*

Inhalation, Eye contact, Skin contact

*Acute oral toxicity*

LD50 rat: > 2,500 mg/kg (IUCLID)

absorption

*Acute inhalation toxicity*

LC50 rat: 37.5 mg/l; 4 h (IUCLID)

Symptoms: mucosal irritations

*Skin irritation*

Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Causes skin irritation.

*Eye irritation*

slight irritation

*Genotoxicity in vitro*

Mutagenicity (mammal cell test):

Result: negative

(IUCLID)

*Specific target organ systemic toxicity - single exposure*

May cause drowsiness or dizziness.

*Specific target organ systemic toxicity - repeated exposure*

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

*Aspiration hazard*

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

**Carcinogenicity**

IARC

No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

OSHA

No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

NTP

No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

ACGIH

No ingredient of this product present at levels greater than or

## SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number 104718  
Product name Isooctane for spectroscopy Uvasol®

---

Version 1.2

equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

### Further information

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

Handle in accordance with good industrial hygiene and safety practice.

---

## SECTION 12. Ecological information

### Ecotoxicity

#### *Toxicity to fish*

LC0 Leuciscus idus (Golden orfe): 500 mg/l; 48 h (External MSDS)

#### *Toxicity to bacteria*

EC0 Pseudomonas putida: 10,000 mg/l(IUCLID)

### Persistence and degradability

No information available.

### Bioaccumulative potential

#### *Partition coefficient: n-octanol/water*

log Pow: 4.09

(calculated)

Potential bioaccumulation

### Mobility in soil

#### *Distribution among environmental compartments*

log Koc: 4.35

(HSDB) High mobility of the substance in soil is not expected (log koc  $\geq$ 3).

### Other adverse effects

#### *Henry constant*

305000 Pa\*m<sup>3</sup>/mol

(HSDB) Distribution preferentially in air.

#### *Additional ecological information*

Biological effects:

Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.

Further information on ecology

Discharge into the environment must be avoided.

---

## SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

---



# SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number 104718  
Product name Isooctane for spectroscopy Uvasol®

Version 1.2

---

## SECTION 14. Transport information

### Land transport (DOT)

UN number	UN 1262
Proper shipping name	OCTANES
Class	3
Packing group	II
Environmentally hazardous	--

### Air transport (IATA)

UN number	UN 1262
Proper shipping name	OCTANES
Class	3
Packing group	II
Environmentally hazardous	--
Special precautions for user	no

### Sea transport (IMDG)

UN number	UN 1262
Proper shipping name	OCTANES
Class	3
Packing group	II
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-E S-E

---

## SECTION 15. Regulatory information

### United States of America

#### OSHA Hazards

Flammable Liquid  
Skin irritant

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

#### SARA 311/312 Hazards

Fire Hazard  
Acute Health Hazard

#### SARA 313

SARA 313: 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 302

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

# SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number

104718

Version 1.2

Product name

Isooctane for spectroscopy Uvasol®

---

## Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

## DEA List I

Not listed

## DEA List II

Not listed

## US State Regulations

### Massachusetts Right To Know

#### *Ingredients*

isooctane

### Pennsylvania Right To Know

#### *Ingredients*

isooctane

### New Jersey Right To Know

#### *Ingredients*

isooctane

### California Prop 65 Components

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

## Notification status

TSCA: All components of the product are listed in the TSCA-inventory.

DSL: All components of this product are on the Canadian DSL.

---

## SECTION 16. Other information

### Training advice

Provide adequate information, instruction and training for operators.

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

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

### Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

## SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Product number

104718

Version 1.2

Product name

Isooctane for spectroscopy Uvasol®

---

Revision Date 04/16/2014

---

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

*All rights reserved. Millipore and the "M" Mark are registered trademarks of Merck KGaA, Darmstadt, Germany.*