



2,2,4-TRIMETHYLPENTANE (D18, 98%)

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 06/01/2011

Revision date: 28/09/2016

Supersedes: 17/12/2012

Version: 3.0

DLM-1353

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form : Substance
Substance name : 2,2,4-TRIMETHYLPENTANE (D18, 98%)
EC index no : 601-009-00-8 (Unlabeled)
EC no : 208-759-1(Unlabeled)
CAS No : 51685-57-5
REACH registration No : 01-2119457965-22
Product code : DLM-1353
Formula : (CD3)2CD2C(CD3)3
Synonyms : Isooctane

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

1.2.1. Relevant identified uses

Main use category : Professional use
Industrial/Professional use spec : For professional use only.

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810
USA

USA: 1-800-322-1174 Int: 1-978-749-8000
cilsales@isotope.com www.isotope.com

Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)
International: 1-703-741-5970 (24 hours)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Flam. Liq. 2 H225
Skin Irrit. 2 H315
STOT SE 3 H336
Asp. Tox. 1 H304
Aquatic Acute 1 H400
Aquatic Chronic 1 H410

Full text of H-phrases: see section 16

Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

F; R11
Xi; R38
R67
Xn; R65
N; R50/53

Full text of R-phrases: see section 16

Classification (GHS-US)

Flam. Liq. 2 H225
Skin Irrit. 2 H315
STOT SE 3 H336
Asp. Tox. 1 H304
Aquatic Chronic 1 H410

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Adverse physicochemical, human health and environmental effects

Liver, Kidney.

2.2. Label elements

Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



Signal word (CLP) :

Danger

Hazard statements (CLP) :

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 (CLP) :

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P233 - Keep container tightly closed
P240 - Ground/bond container and receiving equipment
P241 - Use explosion-proof electrical, ventilating, lighting equipment
P261 - Avoid breathing dust, gas, fume, mist, spray, vapors
P264 - Wash hands, forearms and face thoroughly after handling
P271 - Use only outdoors or in a well-ventilated area
P273 - Avoid release to the environment

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
H336 - May cause drowsiness or dizziness
H410 - Very toxic to aquatic life with long lasting effects

Precautionary statements (GHS-US) :

P210 - Keep away from heat, hot surfaces, open flames, sparks. - No smoking
P233 - Keep container tightly closed
P240 - Ground/bond container and receiving equipment
P241 - Use explosion-proof electrical, lighting, ventilating equipment
P242 - Use only non-sparking tools
P243 - Take precautionary measures against static discharge
P261 - Avoid breathing dust, fume, gas, mist, spray, vapors
P264 - Wash Both hands thoroughly after handling
P271 - Use only outdoors or in a well-ventilated area
P273 - Avoid release to the environment
P280 - Wear protective clothing, protective gloves
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P302+P352 - IF ON SKIN: Wash with plenty of soap and water
P303+P361+P353 - IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower
P304+P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
P312 - Call a POISON CENTER or doctor/physician if you feel unwell
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)
P331 - Do NOT induce vomiting
P332+P313 - If skin irritation occurs: Get medical advice/attention
P362 - Take off contaminated clothing and wash it before reuse
P370+P378 - In case of fire: Use Alcohol resistant foam., Carbon dioxide., Dry chemical. to extinguish
P391 - Collect spillage
P403+P233 - Store in a well-ventilated place. Keep container tightly closed
P403+P235 - Store in a well-ventilated place. Keep cool

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

P405 - Store locked up
P501 - Dispose of contents/container to Comply with applicable regulations.

2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substance

Name	Product identifier	%	Classification according to Directive 67/548/EEC
2,2,4-TRIMETHYLPENTANE (D18, 98%) (Main constituent)	(CAS No) 51685-57-5 (EC no) 208-759-1 (Unlabeled) (EC index no) 601-009-00-8 (Unlabeled) (REACH-no) 01-2119457965-22	100	F; R11 Xi; R38 R67 Xn; R65 N; R50/53
Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
2,2,4-TRIMETHYLPENTANE (D18, 98%) (Main constituent)	(CAS No) 51685-57-5 (EC no) 208-759-1 (Unlabeled) (EC index no) 601-009-00-8 (Unlabeled) (REACH-no) 01-2119457965-22	100	Flam. Liq. 2, H225 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

Full text of R- and H- phrases: see section 16

Name	Product identifier	%	Classification (GHS-US)
2,2,4-TRIMETHYLPENTANE (D18, 98%) (Main constituent)	(CAS No) 51685-57-5	100	Flam. Liq. 2, H225 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Chronic 1, H410

Full text of H-phrases: see section 16

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
First-aid measures after inhalation	: If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
First-aid measures after skin contact	: Wash off with soap and plenty of water. Consult a physician.
First-aid measures after eye contact	: Flush eyes with water as a precaution.
First-aid measures after ingestion	: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

Symptoms/injuries after inhalation	: Harmful if inhaled. Causes respiratory tract irritation. Vapors may cause drowsiness and dizziness.
Symptoms/injuries after skin contact	: Harmful if absorbed through skin. Causes skin irritation.
Symptoms/injuries after eye contact	: May cause eye irritation.
Symptoms/injuries after ingestion	: May be fatal if swallowed and enters airways.

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

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	: For small fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.
------------------------------	--

5.2. Special hazards arising from the substance or mixture

Explosion hazard	: Flash back possible over considerable distance. Container explosion may occur under fire conditions.
------------------	--

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Reactivity : Vapors may form explosive mixture with air.

5.3. Advice for firefighters

Firefighting instructions : Wear self contained breathing apparatus for fire fighting if necessary.
Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.
Other information : Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment, and ensure adequate ventilation. Avoid breathing vapors, mist, gas. Remove ignition sources, and move personnel to safe area. Vapors accumulate especially in low areas to form explosive concentrations.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3. Methods and material for containment and cleaning up

For containment : Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations.

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 : Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage conditions : Store at room temperature away from light and moisture.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

2,2,4-TRIMETHYLPENTANE (D18, 98%) (51685-57-5)		
Italy - Portugal - USA ACGIH	ACGIH TWA (ppm)	300 ppm USA. ACGIH Threshold Limit Values (TLV)
Italy - Portugal - USA ACGIH	Remark (ACGIH)	Upper Respiratory Tract irritation.

8.2. Exposure controls

Appropriate engineering controls : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment : Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.



Materials for protective clothing : Wear suitable protective clothing and gloves.

Hand protection : Wear suitable protective clothing and gloves.

Eye protection : Safety glasses with side-shields conforming to EN166. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH or EN 166.

Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place. Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

Environmental exposure controls : Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Liquid.
Molecular mass	: 132.34 g/mol (Labeled)
Color	: Colorless.
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Melting point	: -107 °C (- 161 °F)
Freezing point	: No data available
Boiling point	: 98 - 99 °C (208 - 210 °F)
Flash point	: -12 °C (10 °F) - closed cup
Auto-ignition temperature	: 396 °C (745 °F)
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: 55 hPa (41 mmHg) at 21 °C (70 °F); 117 hPa (88 mmHg) at 37.80 °C (100.04 °F)
Relative vapor density at 20 °C	: 3.94 - (Air = 1.0)
Relative density	: No data available
Specific gravity / density	: 0.692 g/ml at 25 °C (77 °F)
Solubility	: Insoluble in water. Water: Insoluble
Log Pow	: 4.6
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosive limits	: 1 - 6 % (V)

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

Vapors may form explosive mixture with air.

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Carbon oxides (CO, CO₂).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

2,2,4-TRIMETHYLPENTANE (D18, 98%) (51685-57-5)	
LD50 oral rat	> 5000 mg/kg (OECD Test Guideline 401)
LD50 dermal rabbit	> 2000 mg/kg (OECD Test Guideline 402)
LC50 inhalation rat (mg/l)	> 33.52 mg/l (OECD Test Guideline 403) - 4 h

Skin corrosion/irritation : Skin - Rabbit Result: Irritating to skin. (OECD Test Guideline 404)

Serious eye damage/irritation : Eyes - Rabbit Result: No eye irritation (OECD TEST Guideline 405)

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Respiratory or skin sensitization	: Not available No data available
Germ cell mutagenicity	: Rat - Unscheduled DNA synthesis
Carcinogenicity	: Not classified
Reproductive toxicity	: Not available
Specific target organ toxicity (single exposure)	: May cause drowsiness or dizziness.
Specific target organ toxicity (repeated exposure)	: Not classified No data available
Aspiration hazard	: The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.
Potential Adverse human health effects and symptoms	: To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Liver - Irregularities - Based on Human Evidence.
Symptoms/injuries after inhalation	: Harmful if inhaled. Causes respiratory tract irritation. Vapors may cause drowsiness and dizziness.
Symptoms/injuries after skin contact	: Harmful if absorbed through skin. Causes skin irritation.
Symptoms/injuries after eye contact	: May cause eye irritation.
Symptoms/injuries after ingestion	: May be fatal if swallowed and enters airways.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

2,2,4-TRIMETHYLPENTANE (D18, 98%) (51685-57-5)

Persistence and degradability	Not available.
-------------------------------	----------------

12.3. Bioaccumulative potential

2,2,4-TRIMETHYLPENTANE (D18, 98%) (51685-57-5)

Log Pow	4.6
Bioaccumulative potential	Not available.

12.4. Mobility in soil

2,2,4-TRIMETHYLPENTANE (D18, 98%) (51685-57-5)

Ecology - soil	Not available.
----------------	----------------

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Other adverse effects : An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Very toxic to aquatic organisms.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste)	: Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.
Waste disposal recommendations	: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
Ecology - waste materials	: Dispose of as unused product.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

14.1. UN number

UN-No.(DOT)	: 1262
DOT NA no.	UN1262

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Octanes
Transport hazard class(es) (DOT)	: 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Hazard labels (DOT) : 3 - Flammable liquid



Packing group (DOT) : II - Medium Danger

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.
T4 - 2.65 178.274(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.

DOT Packaging Exceptions (49 CFR 173.xxx) : 150

DOT Packaging Non Bulk (49 CFR 173.xxx) : 202

DOT Packaging Bulk (49 CFR 173.xxx) : 242

DOT RQ : 1000 lbs

Marine pollutant : No



14.3. Additional information

Other information : No supplementary information available.

Overland transport

Packing group (ADR) : II

Class (ADR) : 3 - Flammable liquid

Hazard identification number (Kemler No.) : 33

Classification code (ADR) : F1

Hazard labels (ADR) : 3 - Flammable liquids



Orange plates : 

Tunnel restriction code : D/E

Limited quantities (ADR) : 11

EAC : 3YE

Excepted quantities (ADR) : E2

Transport by sea

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.

MFAG-No : 128

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 5 L

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 60 L

Civil Aeronautics Law : Flammable liquids

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

14.4. Environmental hazards

Dangerous for the environment :



Other information : No supplementary information available.

14.5. Special precautions for user

14.6. 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

2,2,4-TRIMETHYLPENTANE (D18, 98%) (51685-57-5)

SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard Delayed (chronic) health hazard
-------------------------------------	---

15.2. International regulations

CANADA

2,2,4-TRIMETHYLPENTANE (D18, 98%) (51685-57-5)

Listed on the Canadian DSL (Domestic Substances List) inventory.

15.2.1. National regulations

No additional information available

15.3. US State regulations

2,2,4-TRIMETHYLPENTANE (D18, 98%)(51685-57-5)

State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.
----------------------------	---

SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of R-, H- and EUH-phrases:

Aquatic Acute 1	Hazardous to the aquatic environment - Acute Hazard Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment - Chronic Hazard Category 1
Asp. Tox. 1	Aspiration hazard Category 1
Flam. Liq. 2	Flammable liquids Category 2
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 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
R11	Highly flammable
R38	Irritating to skin

2,2,4-TRIMETHYLPENTANE (D18, 98%) DLM-1353

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

R50/53	Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment
R65	Harmful: may cause lung damage if swallowed
R67	Vapors may cause drowsiness and dizziness
F	Highly flammable
N	Dangerous for the environment
Xi	Irritant
Xn	Harmful

NFPA health hazard

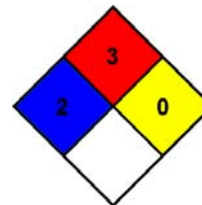
: 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.

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

: 2 Moderate Hazard - Temporary or minor injury may occur

Flammability

: 3 Serious Hazard

Physical

: 0 Minimal Hazard

CIL Multi-Solvent Mixture SDS

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product