



TERT-BUTYL-D9 ACETATE (D, 99%)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 30/11/2017
DLM-10515

Revision date: 04/03/2019

Supersedes: 30/04/2018

Version: 3.0

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

1.1. Product identifier

Product form : Substance
Substance name : TERT-BUTYL-D9 ACETATE (D, 99%)
EC Index-No. : 607-026-00-7 (Unlabeled)
EC-No. : 208-760-7 (Unlabeled)
CAS-No. : 358731-03-0
Product code : DLM-10515
Formula : CH₃COOC(CD₃)₃

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
Acute Tox. 4 (Inhalation) H332
Skin Irrit. 2 H315
Eye Irrit. 2 H319

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

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

F; R11
Xi; R36/38
Xn; R20

Full text of R-phrases: see section 16

GHS-US classification

Flam. Liq. 2 H225
Acute Tox. 4 (Inhalation) H332
Skin Irrit. 2 H315
Eye Irrit. 2 H319

Full text of H statements : see section 16

Adverse physicochemical, human health and environmental effects

No additional information available

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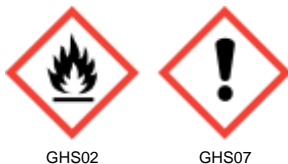
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2.2. Label elements

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

Hazard pictograms (CLP) :



Signal word (CLP) :

Danger

Hazard statements (CLP) :

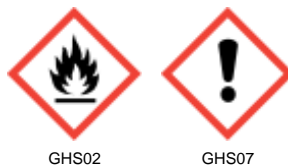
H225 - Highly flammable liquid and vapor
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H332 - Harmful if inhaled

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 equipment
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray.
P264 - Wash hands, forearms and face thoroughly after handling.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear protective clothing, protective gloves.

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H225 - Highly flammable liquid and vapor
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H332 - Harmful if inhaled

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 equipment
P242 - Use only non-sparking tools.
P243 - Take precautionary measures against static discharge.
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray.
P264 - Wash hands, forearms and face thoroughly after handling.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear protective clothing, protective gloves.
P302+P352 - If on skin: Wash with plenty of 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
P312 - Call a doctor, a POISON CENTER if you feel unwell
P321 - Specific treatment (see Hazardous component(s) for labeling on this label)
P332+P313 - If skin irritation occurs: Get medical advice/attention.
P337+P313 - If eye irritation persists: Get medical advice/attention.
P362+P364 - Take off contaminated clothing and wash it before reuse.
P370+P378 - In case of fire: Use alcohol resistant foam, carbon dioxide (CO₂), D-powder to extinguish.
P403+P235 - Store in a well-ventilated place. Keep cool.
P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

TERT-BUTYL-D9 ACETATE (D, 99%)

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according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Name	Product identifier	%	Classification according to Directive 67/548/EEC
TERT-BUTYL-D9 ACETATE (D, 99%)	(CAS-No.) 358731-03-0 (EC-No.) 208-760-7 (Unlabeled) (EC Index-No.) 607-026-00-7 (Unlabeled)	100	F; R11 Xi; R36/38 Xn; R20
Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
TERT-BUTYL-D9 ACETATE (D, 99%)	(CAS-No.) 358731-03-0 (EC-No.) 208-760-7 (Unlabeled) (EC Index-No.) 607-026-00-7 (Unlabeled)	100	Flam. Liq. 2, H225 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2, H319

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

Name	Product identifier	%	GHS-US classification
TERT-BUTYL-D9 ACETATE (D, 99%) (Main constituent)	(CAS-No.) 358731-03-0	100	Flam. Liq. 2, H225 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2, H319

Full text of H-phrases: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: If you feel unwell, seek medical advice (show the label where possible). Evacuate danger area.
First-aid measures after inhalation	: When symptoms occur: go into open air and ventilate suspected area. If not breathing, give artificial respiration. Get medical advice/attention.
First-aid measures after skin contact	: Wash with plenty of soap and water. Get immediate medical advice/attention. Rinse skin with water/shower. Remove/Take off immediately all contaminated clothing.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.

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

Symptoms/effects after inhalation	: Harmful if inhaled.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: May be harmful if swallowed.

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 : Water spray. Dry chemical powder, alcohol-resistant foam, carbon dioxide (CO₂).

5.2. Special hazards arising from the substance or mixture

Fire hazard	: Highly flammable liquid and vapor.
Explosion hazard	: May form flammable/explosive vapor-air mixture.

5.3. Advice for firefighters

Firefighting instructions	: Fight fire with normal precautions from a reasonable distance. Wear a self contained breathing apparatus. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection. Wear recommended personal protective equipment.
Other information	: Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Remove ignition sources. Use special care to avoid static electric charges. No open flames. No smoking.

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6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment as required. Avoid breathing vapors, mist, gas. Avoid dust formation. Ensure adequate air ventilation. Evacuate unnecessary personnel. Evacuate danger area.

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

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

For containment : Small quantities of liquid spill: take up in non-combustible absorbent material and shovel into container for disposal. For large spills, confine the spill in a dike and charge it with wet sand or earth for subsequent safe disposal.

Methods for cleaning up : This material and its container must be disposed of in a safe way, and as per local legislation.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable.

Precautions for safe handling : Provide adequate ventilation to minimize dust and/or vapor concentrations. No open flames. No smoking. Use only non-sparking tools. Take measures to prevent the build up of electrostatic charge.

Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Store in a well-ventilated place. Keep container tightly closed. Proper grounding procedures to avoid static electricity should be followed. Ground/bond container and receiving equipment. Use explosion-proof ventilating equipment.

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

Incompatible materials : Heat sources.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)		
Italy - Portugal - USA ACGIH	ACGIH TWA (ppm)	200.00000000 ppm USA. ACGIH Threshold Limit Values (TLV)
Italy - Portugal - USA ACGIH	ACGIH STEL (ppm)	150 ppm USA. ACGIH Threshold Limit Values (TLV)
Italy - Portugal - USA ACGIH	ACGIH Ceiling (ppm)	50 ppm USA. ACGIH Threshold Limit Values (TLV)
Italy - Portugal - USA ACGIH	Remark (ACGIH)	Upper Respiratory Tract irritation; Eye irritation; Adopted values or notations enclosed are those for which changes ; are proposed in the NIC; See Notice of Intended Changes (NIC)
USA NIOSH	NIOSH REL (TWA) (mg/m ³)	950 mg/m ³ USA. NIOSH Recommended Exposure Limits
USA NIOSH	NIOSH REL (TWA) (ppm)	200 ppm USA. NIOSH Recommended Exposure Limits
USA OSHA	OSHA PEL (TWA) (mg/m ³)	950 mg/m ³ USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
USA OSHA	OSHA PEL (TWA) (ppm)	200 ppm USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants. California permissible exposure limits for chemical contaminants (Title 8, Article 107)
USA OSHA	Remark (OSHA)	The value in mg/m ³ is approximate.

8.2. Exposure controls

Appropriate engineering controls : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

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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 : Wear eye protection. Chemical goggles or face shield with safety glasses.
Skin and body protection : Wear suitable protective clothing, gloves and eye/face protection.
Respiratory protection : In case of inadequate ventilation wear respiratory protection. Approved supplied air respirator.
Environmental exposure controls : Avoid release to the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Liquid
Appearance : Liquid
Molecular mass : 125.21 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 : < -57.99 °C (< -72.38 °F)
Freezing point : No data available
Boiling point : 97 - 98 °C (207 - 208 °F) - lit.
Flash point : 4 °C (39 °F) - closed cup
Auto-ignition temperature : 589 °C (1,092 °F) at 1,015 hPa (761 mmHg)
Decomposition temperature : No data available
Flammability (solid, gas) : Highly flammable liquid and vapor
Vapor pressure : 63 hPa (47 mmHg) at 25 °C (77 °F)
Relative vapor density at 20 °C : 4.65 at 20 °C (68 °F)
Relative density : No data available
Specific gravity / density : 0.866 g/cm³
Solubility : Water: 6.7 g/l at 23 °C (73 °F) - OECD Test Guideline 105 - soluble
Log Pow : 1.64 at 21.7 °C (71.1 °F)
Log Kow : No data available
Viscosity, kinematic : < 1 mm²/s at 25 °C (77 °F)
Viscosity, dynamic : No data available
Explosive properties : No data available
Oxidizing properties : No data available
Explosion limits : 1.5 - 1.7 vol % (Lower)

9.2. Other information

Additional information : Surface tension 64 mN/m at 20 °C (68 °F)

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

Vapors may form explosive mixture with air.

10.4. Conditions to avoid

Open flame. Direct sunlight. Heat. Sparks. Extremes of temperature and direct sunlight.

10.5. Incompatible materials

Strong oxidizing agents.

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10.6. Hazardous decomposition products

Carbon oxides (CO, CO₂).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Inhalation: Harmful if inhaled.

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)	
LD50 oral rat	4100 - male - 4,100 mg/kg
LD50 dermal rabbit	> 2000 mg/kg - male and female
LC50 inhalation rat (mg/l)	> 2230 mg/m ³ - 4 h
ATE CLP (oral)	4100.000 mg/kg body weight
ATE CLP (gases)	4500.000 ppmV/4h
ATE CLP (vapors)	11.000 mg/l/4h
ATE CLP (dust, mist)	1.500 mg/l/4h

Skin corrosion/irritation : Skin - Rabbit Result: Mild skin irritation
Serious eye damage/irritation : Eyes - Rabbit Result: Mild eye irritation
Respiratory or skin sensitization : Buehler Test. Guinea pig Result: Did not cause sensitisation on laboratory animals.
Germ cell mutagenicity : Reverse Mutation Assays *S. typhimurium* Result: negative.
Mutagenicity (micronucleus test) - Mouse - male and female - Result: negative
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
Specific target organ toxicity – single exposure : Not classified
Specific target organ toxicity – repeated exposure : Not classified

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)	
NOAEC (inhalation, rat, vapour, 90 days)	0.48 mg/l/6h/day - Mouse - male and female

Aspiration hazard : Not classified
Potential Adverse human health effects and symptoms : 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.
Symptoms/effects after inhalation : Harmful if inhaled.
Symptoms/effects after skin contact : Causes skin irritation.
Symptoms/effects after eye contact : Causes serious eye irritation.
Symptoms/effects after ingestion : May be harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)	
LC50 fish 1	240 mg/l - <i>Oncorhynchus mykiss</i> (rainbow trout) - 96 h (OECD Test Guideline 203)
EC50 Daphnia 1	350 mg/l - <i>Daphnia magna</i> (Water flea)- 48 h (OECD Test Guideline 202)
LC50 fish 2	296 - 362 mg/l - <i>Pimephales promelas</i> (fathead minnow) - 96 h

12.2. Persistence and degradability

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)	
Biodegradation	50 % - Inherently biodegradable. (OECD Test Guideline 301D) aerobic - Exposure time 28 d

12.3. Bioaccumulative potential

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)	
Log Pow	1.64 at 21.7 °C (71.1 °F)

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

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12.6. Other adverse effects

No additional information available

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.
- Product/Packaging 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) : 1123
- DOT NA no. : UN1123

14.2. UN proper shipping name

- Proper Shipping Name (DOT) : Butyl acetates
- Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120
- 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

14.3. Additional information

- Emergency Response Guide (ERG) Number : 129
- Other information : No supplementary information available.
- Special transport precautions : Not classified as dangerous in the meaning of transport regulations.

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 : An orange rectangular label with a black border. The number "33" is in the top half and "1123" is in the bottom half, both in black text.

- Tunnel restriction code (ADR) : D/E
- Limited quantities (ADR) : 1l

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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 : 129

Air transport

DOT Quantity Limitations Passenger aircraft/rail : 5 L
(49 CFR 173.27)
DOT Quantity Limitations Cargo aircraft only (49 : 60 L
CFR 175.75)
Civil Aeronautics Law : Flammable liquids

14.4. Environmental hazards

Other information : No supplementary information available.

14.5. Special precautions for user

Special transport precautions : Not classified as dangerous in the meaning of transport regulations.

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

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313.

15.2. International regulations

CANADA

TERT-BUTYL-D9 ACETATE (D, 99%) (358731-03-0)
Listed on the Canadian DSL (Domestic Substances List)

15.2.1. National regulations

No additional information available

15.3. US State regulations

TERT-BUTYL-D9 ACETATE (D, 99%)(358731-03-0)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List

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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.

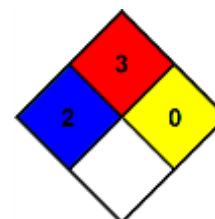
Full text of R-, H- and EUH-phrases:

Acute Tox. 4 (Inhalation)	Acute toxicity (inhalation) Category 4
Eye Irrit. 2	Serious eye damage/eye irritation Category 2
Flam. Liq. 2	Flammable liquids Category 2
Skin Irrit. 2	Skin corrosion/irritation Category 2
H225	Highly flammable liquid and vapor
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
R11	Highly flammable
R20	Harmful by inhalation
R36/38	Irritating to eyes and skin
F	Highly flammable
Xi	Irritant
Xn	Harmful

NFPA health hazard : 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard : 3 - Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions.

NFPA reactivity : 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 : 3 Serious Hazard

Physical : 0 Minimal Hazard

CIL Substance 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