



# 2,2',3,3',4,5,5'-HEPTACB UNLABELED 35 UG/ML IN ISOCTANE

## 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: 29/09/2014

Revision date:

Version: 1.0

## PCB-172

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

#### 1.1. Product identifier

Product form : Mixture  
Product name. : 2,2',3,3',4,5,5'-HEPTACB UNLABELED 35 UG/ML IN ISOCTANE  
Product code : PCB-172

#### 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.  
Industrial.

##### 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](mailto:cilsales@isotope.com) [www.isotope.com](http://www.isotope.com)

#### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)  
International: 1-202-483-7616 (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. 1	H224
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 or 1999/45/EC

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

Full text of R-phrases: see section 16

##### GHS-US classification

Flam. Liq. 1	H224
Skin Irrit. 2	H315
STOT SE 3	H336
Asp. Tox. 1	H304
Aquatic Acute 1	H400
Aquatic Chronic 1	H410

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### Adverse physicochemical, human health and environmental effects

Liver, Kidney.

## 2.2. Label elements

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

Hazard pictograms (CLP) :



Signal word (CLP) :

Danger

Hazard statements (CLP) :

H224 - Extremely flammable liquid and vapour  
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, lighting, ventilating equipment  
P261 - Avoid breathing dust, fume, gas, mist, spray, vapours  
P264 - Wash Both hands thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P273 - Avoid release to the environment

### GHS-US labelling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H224 - Extremely flammable liquid and vapour  
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

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, vapours  
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/doctor/physician if you feel unwell  
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)  
P331 - If swallowed, do NOT induce vomiting  
P332+P313 - If skin irritation occurs: Get medical advice/attention  
P362 - Take off contaminated clothing and wash before reuse  
P370+P378 - In case of fire: Use Alcohol resistant foam, Carbon dioxide., Dry chemical, Water spray for extinction

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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  
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. Substances

Not applicable

### 3.2. Mixture

Name	Product identifier	%	Classification according to Directive 67/548/EEC
ISOOCTANE UNLABELED	(CAS No)540-84-1 (EC no)208-759-1 (EC index no)601-009-00-8	99.9949	F; R11 Xn; R65 Xi; R38 N; R50/53 R67
2,2',3,3',4,5,5'-HEPTACB UNLABELED	(CAS No)52663-74-8 (Unlabeled) (EC index no)602-039-00-4	0.0051	N; R50/53 R33 R48

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
ISOOCTANE UNLABELED	(CAS No)540-84-1 (EC no)208-759-1 (EC index no)601-009-00-8	99.9949	Flam. Liq. 1, H224 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Acute 1, H400 Aquatic Chronic 1, H410
2,2',3,3',4,5,5'-HEPTACB UNLABELED	(CAS No)52663-74-8 (Unlabeled) (EC index no)602-039-00-4	0.0051	STOT RE 2, H373 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

Name	Product identifier	%	GHS-US classification
ISOOCTANE UNLABELED	(CAS No)540-84-1	99.9949	Flam. Liq. 1, H224 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

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

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general	: Never give anything by mouth to an unconscious person. If you feel unwell, seek medical advice (show the label where possible).
First-aid measures after inhalation	: Remove to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER/doctor/physician if you feel unwell.
First-aid measures after skin contact	: Rinse skin with water/shower. Remove/Take off immediately all contaminated clothing. Wash with plenty of soap and water. Wash contaminated clothing before reuse. Get medical advice/attention.
First-aid measures after eye contact	: Rinse immediately with plenty of water. Obtain medical attention if pain, blinking or redness persist.
First-aid measures after ingestion	: Rinse mouth. Do NOT induce vomiting. Immediately call a POISON CENTER or doctor/physician.

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

Symptoms/injuries after inhalation	: May cause drowsiness or dizziness.
Symptoms/injuries after skin contact	: Causes skin 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

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### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media

Suitable extinguishing media : Foam. Dry powder. Carbon dioxide. Water spray. Sand.  
Unsuitable extinguishing media : Do not use a heavy water stream.

#### 5.2. Special hazards arising from the substance or mixture

Fire hazard : Extremely flammable liquid and vapour.  
Explosion hazard : May form flammable/explosive vapour-air mixture.  
Reactivity : Vapour is explosive with air above.

#### 5.3. Advice for firefighters

Firefighting instructions : Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire. Avoid (reject) fire-fighting water to enter environment.  
Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

### 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 naked lights. No smoking.

##### 6.1.1. For non-emergency personnel

Emergency procedures : Evacuate unnecessary personnel.

##### 6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection. Avoid breathing dust, mist or spray.  
Emergency procedures : Ventilate area.

#### 6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters. Avoid release to the environment.

#### 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.  
Methods for cleaning up : Soak up spills with inert solids, such as clay or diatomaceous earth as soon as possible. Collect spillage. Store away from other materials.

#### 6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapours are flammable.  
Precautions for safe handling : Wash hands and other exposed areas with mild soap and water before eat, drink or smoke and when leaving work. Provide good ventilation in process area to prevent formation of vapour. No naked lights. No smoking. Take precautionary measures against static discharge. Use only non-sparking tools. Use only outdoors or in a well-ventilated area. Avoid breathing dust, mist or spray.  
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 : Ground/bond container and receiving equipment. Use explosion-proof electrical equipment.  
Storage conditions : Store at room temperature away from light and moisture.  
Incompatible products : Strong bases. strong acids.  
Incompatible materials : Sources of ignition. Direct sunlight. Heat sources.

#### 7.3. Specific end use(s)

No additional information available

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

No additional information available

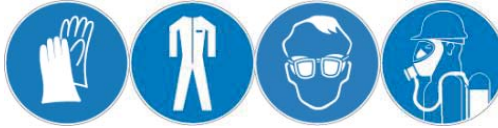
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### 8.2. Exposure controls

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



Hand protection : Wear protective gloves.  
Eye protection : Chemical goggles or safety glasses.  
Skin and body protection : Wear suitable protective clothing.  
Respiratory protection : Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. Wear respiratory protection.  
Other information : When using, do not eat, drink or smoke.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

*The properties listed below are for the solvent, the main component of this mixture.*

Physical state : Liquid  
Appearance : Liquid.  
Molecular mass : 114.23  
Colour : Colourless.  
Odour : characteristic.  
Odour threshold : No data available  
pH : No data available  
Relative evaporation rate (butylacetate=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  
Self ignition temperature : 396 °C (745 °F)  
Decomposition temperature : No data available  
Flammability (solid, gas) : Extremely flammable liquid and vapour  
Vapour pressure : 55 hPa (41 mmHg) at 21 °C (70 °F)  
Relative vapour density at 20 °C : 3.94 - (Air = 1.0)  
Relative density : No data available  
Solubility : Water: 0 %  
Log Pow : No data available  
Log Kow : No data available  
Viscosity, kinematic : No data available  
Viscosity, dynamic : No data available  
Explosive properties : No data available  
Oxidising 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

Vapour is explosive with air above.

### 10.2. Chemical stability

See storage and expiration date on CoA.

### 10.3. Possibility of hazardous reactions

Not established.

### 10.4. Conditions to avoid

Direct sunlight. Extremely high or low temperatures. Sparks. Heat. Overheating. Open flame.

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### 10.5. Incompatible materials

strong acids. Strong bases.

### 10.6. Hazardous decomposition products

fume. Carbon monoxide. Carbon dioxide. May release flammable gases.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity	: Not classified
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Not classified Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: Not classified Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified Based on available data, the classification criteria are not met
Specific target organ toxicity (single exposure)	: May cause drowsiness or dizziness.
Specific target organ toxicity (repeated exposure)	: Not classified Based on available data, the classification criteria are not met
Aspiration hazard	: May be fatal if swallowed and enters airways.
Potential Adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.
Symptoms/injuries after inhalation	: May cause drowsiness or dizziness.
Symptoms/injuries after skin contact	: Causes skin irritation.
Symptoms/injuries after ingestion	: May be fatal if swallowed and enters airways.

## SECTION 12: Ecological information

### 12.1. Toxicity

Ecology - water : Very toxic to aquatic life with long lasting effects.

### 12.2. Persistence and degradability

#### 2,2',3,3',4,5,5'-HEPTACB UNLABELED 35 UG/ML IN ISOOCTANE

Persistence and degradability	May cause long-term adverse effects in the environment.
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#### ISOOCTANE UNLABELED (540-84-1)

Persistence and degradability	Not available.
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#### 2,2',3,3',4,5,5'-HEPTACB UNLABELED (52663-74-8 (Unlabeled))

Persistence and degradability	Not available.
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### 12.3. Bioaccumulative potential

#### 2,2',3,3',4,5,5'-HEPTACB UNLABELED 35 UG/ML IN ISOOCTANE

Bioaccumulative potential	Not established.
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#### ISOOCTANE UNLABELED (540-84-1)

Bioaccumulative potential	Not available.
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#### 2,2',3,3',4,5,5'-HEPTACB UNLABELED (52663-74-8 (Unlabeled))

Bioaccumulative potential	Not available.
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### 12.4. Mobility in soil

#### ISOOCTANE UNLABELED (540-84-1)

Ecology - soil	Not available.
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#### 2,2',3,3',4,5,5'-HEPTACB UNLABELED (52663-74-8 (Unlabeled))

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Ecology - soil	Not available.
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### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Other adverse effects

Other information : Avoid release to the environment.

## 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 : Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to Comply with applicable regulations.

Additional information : Handle empty containers with care because residual vapours are flammable.

Ecology - waste materials : Avoid release to the environment. Hazardous waste due to toxicity.

## SECTION 14: Transport information

In accordance with ADR / RID / ADNR / IMDG / ICAO / IATA

### 14.1. UN number

UN-No.(DOT) : 1262

DOT NA no. UN1262

### 14.2. UN proper shipping name

DOT Proper Shipping Name : Octanes

Department of Transportation (DOT) Hazard Classes : 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

Marine pollutant : No



### 14.3. Additional information

Other information : No supplementary information available.

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### Overland transport

Packing group (ADR) : II  
Class (ADR) : 3 - Flammable liquids  
Hazard identification number (Kemler No.) : 33  
Classification code (ADR) : F1  
Danger labels (ADR) : 3 - Flammable liquids



Orange plates :



Tunnel restriction code : D/E  
Limited quantities (ADR) : 1L  
EAC code : 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

### 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',3,3',4,5,5'-HEPTACB UNLABELED 35 UG/ML IN ISOOCTANE

SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard Delayed (chronic) health hazard
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#### ISOOCTANE UNLABELED (540-84-1)

SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard Delayed (chronic) health hazard
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### 15.2. International regulations

#### CANADA

##### 2,2',3,3',4,5,5'-HEPTACB UNLABELED 35 UG/ML IN ISOOCTANE

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',3,3',4,5,5'-HEPTACB UNLABELED 35 UG/ML IN ISOOCTANE()

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.

#### ISOOCTANE UNLABELED (540-84-1)

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

- Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.
- 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.

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

Aquatic Acute 1	Hazardous to the aquatic environment — AcuteHazard, Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment — Chronic Hazard, Category 1
Asp. Tox. 1	Aspiration hazard, Category 1
Flam. Liq. 1	Flammable liquids, Category 1
Skin Irrit. 2	Skin corrosion/irritation, Category 2
STOT RE 2	Specific target organ toxicity — Repeated exposure, Category 2
STOT SE 3	Specific target organ toxicity — Single exposure, Category 3, Narcosis
H224	Extremely flammable liquid and vapour
H304	May be fatal if swallowed and enters airways
H315	Causes skin irritation
H336	May cause drowsiness or dizziness
H373	May cause damage to organs through prolonged or repeated exposure
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects
R11	Highly flammable
R33	Danger of cumulative effects
R38	Irritating to skin
R48	Danger of serious damage to health by prolonged exposure
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	Vapours 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 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*