



# 1-PHENYLETHANOL (2-13C, 90%) (95% PURE)

## 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: 13/01/2011

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Version: 3.0

CLM-3055

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

### 1.1. Product identifier

Product form	: Substance
Substance name	: 1-PHENYLETHANOL (2-13C, 90%) (95% PURE)
EC-No.	: 202-707-1 (Unlabeled)
CAS-No.	: 98-85-1 (Unlabeled)
Product code	: CLM-3055
Formula	: C6H5CH(OH)*CH3
Synonyms	: Methyl phenyl carbinol / Styrallyl alcohol / (±)-α-Methylbenzyl alcohol / Styrene alcohol / (±)-1-Phenylethanol

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

### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)

International: 1-703-741-5970 (24 hours)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

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

Acute Tox. 4 (Oral)	H302
Skin Irrit. 2	H315
Eye Dam. 1	H318
STOT SE 3	H335

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

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

Xn; R22

Xi; R41

Xi; R37/38

Full text of R-phrases: see section 16

#### GHS-US classification

Flam. Liq. 4	H227
Acute Tox. 4 (Oral)	H302
Skin Irrit. 2	H315
Eye Dam. 1	H318
STOT SE 3	H335

Full text of H statements : see section 16

#### Adverse physicochemical, human health and environmental effects

Harmful if swallowed. May cause respiratory irritation. Causes skin irritation. Causes serious eye irritation.

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### 2.2. Label elements

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

Hazard pictograms (CLP) :



GHS05

GHS07

Signal word (CLP) :

Danger

Hazard statements (CLP) :

H302 - Harmful if swallowed  
H315 - Causes skin irritation  
H318 - Causes serious eye damage  
H335 - May cause respiratory irritation

Precautionary statements (CLP) :

P261 - Avoid breathing dust, fume, gas, mist, spray, vapors.  
P264 - Wash hands, forearms and face thoroughly after handling.  
P270 - Do not eat, drink or smoke when using this product.  
P271 - Use only outdoors or in a well-ventilated area.  
P280 - Wear protective clothing, protective gloves.  
P301+P312 - IF SWALLOWED: Call a doctor, a POISON CENTER if you feel unwell.  
P302+P352 - IF ON SKIN: Wash with plenty of water.  
P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.

#### GHS-US labeling

Hazard pictograms (GHS-US) :



GHS05

GHS07

Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H227 - Combustible liquid  
H302 - Harmful if swallowed  
H315 - Causes skin irritation  
H318 - Causes serious eye damage  
H335 - May cause respiratory irritation

Precautionary statements (GHS-US) :

P210 - Keep away from heat, hot surfaces, open flames, sparks. - No smoking.  
P261 - Avoid breathing dust, fume, gas, mist, spray, vapors.  
P264 - Wash hands, forearms and face thoroughly after handling.  
P270 - Do not eat, drink or smoke when using this product.  
P271 - Use only outdoors or in a well-ventilated area.  
P280 - Wear protective clothing, protective gloves.  
P301+P312 - If swallowed: Call a doctor, a POISON CENTER if you feel unwell  
P302+P352 - If on skin: Wash with plenty of water  
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  
P310 - Immediately call a doctor, a POISON CENTER  
P312 - Call a doctor, a POISON CENTER if you feel unwell  
P321 - Specific treatment (see Hazardous component(s) for labeling on this label)  
P330 - Rinse mouth.  
P332+P313 - If skin irritation occurs: 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, dry extinguishing powder, dry sand to extinguish.  
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 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

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Name	Product identifier	%	Classification according to Directive 67/548/EEC
1-PHENYLETHANOL (2-13C, 90%) (95% PURE)	(CAS-No.) 98-85-1 (Unlabeled) (EC-No.) 202-707-1 (Unlabeled) (EC Index-No.)	100	Xn; R22 Xi; R41 Xi; R37/38

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
1-PHENYLETHANOL (2-13C, 90%) (95% PURE)	(CAS-No.) 98-85-1 (Unlabeled) (EC-No.) 202-707-1 (Unlabeled) (EC Index-No.)	100	Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Dam. 1, H318 STOT SE 3, H335

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

Name	Product identifier	%	GHS-US classification
1-PHENYLETHANOL (2-13C, 90%) (95% PURE) (Main constituent)	(CAS-No.) 98-85-1 (Unlabeled)	100	Flam. Liq. 4, H227 Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Dam. 1, H318 STOT SE 3, H335

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	: Call a poison center/doctor/physician if you feel unwell.
First-aid measures after inhalation	: Remove person to fresh air and keep comfortable for breathing. Call a poison center/doctor/physician if you feel unwell.
First-aid measures after skin contact	: Wash skin with plenty of water. Take off contaminated clothing. If skin irritation occurs: Get medical advice/attention.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Rinse mouth. Call a poison center/doctor/physician if you feel unwell.

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

Symptoms/effects after inhalation	: May cause respiratory irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: Harmful if swallowed.

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

Treat symptomatically.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : Water spray. Alcohol resistant foam. Dry powder. Dry chemical. Carbon dioxide.

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

No additional information available

### 5.3. Advice for firefighters

Firefighting instructions	: Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Wear respiratory protection. Self-contained breathing apparatus. Do not attempt to take action without suitable protective equipment. Complete protective clothing.
Other information	: Use water spray to cool exposed surfaces.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

#### 6.1.1. For non-emergency personnel

Protective equipment	: Wear recommended personal protective equipment. Avoid breathing dust, mist or spray. Avoid dust formation. Ensure there is adequate ventilation. Evacuate the danger area. Special attention should be given to low areas/pits where flammable vapors can accumulate.
Emergency procedures	: Ventilate spillage area. Avoid breathing vapors, mist, dust. Avoid contact with skin and eyes.

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### 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. Stop leak, if possible without risk. Do not discharge the product into the environment. Avoid release to the environment.

### 6.3. Methods and material for containment and cleaning up

For containment : Vacuum with an equipment that avoids ignition risk.  
Methods for cleaning up : Take up liquid spill into absorbent material. Vacuum with an equipment that avoids ignition risk. This material and its container must be disposed of in a safe way, and as per local legislation.  
Other information : Dispose of materials or solid residues at an authorized site.

### 6.4. Reference to other sections

For further information refer to section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Precautions for safe handling : Avoid contact with skin and eyes. Avoid dust formation. Provide good ventilation in process area to prevent formation of vapor. Use only outdoors or in a well-ventilated area. Avoid breathing dust, mist, vapors. Wear personal protective equipment. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Prevent the build-up of electrostatic charge. Store away from acids and oxidizing agents.  
Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Store locked up. Store in a well-ventilated place. Keep container tightly closed.  
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

No additional information available

### 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. Ensure good ventilation of the work station.  
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. 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. clear.  
Molecular mass : 123.16 g/mol (Labeled)  
Color : Colorless.  
Odor : No data available  
Odor threshold : No data available  
pH : 7.01 at 28 °C (82 °F) - neutral  
Relative evaporation rate (butyl acetate=1) : No data available

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Melting point	: 19 - 20 °C (66 - 68 °F) - lit.
Freezing point	: No data available
Boiling point	: 204 °C (399 °F) at 993 hPa (745 mmHg) - lit.
Flash point	: 86 °C (187 °F) - closed cup
Auto-ignition temperature	: not auto flammable
Decomposition temperature	: No data available
Flammability (solid, gas)	: Not applicable
Vapor pressure	: 0.1 hPa (0.1 mmHg) at 20 °C (68 °F)
Relative vapor density at 20 °C	: 4.22 - (Air = 1.0)
Relative density	: No data available
Specific gravity / density	: 1.012 g/ml at 25 °C (77 °F)
Solubility	: Water: 0.04 g/l at 28 °C (82 °F) - slightly soluble; Solubility in methanol: 5 g/l at 28 °C (82 °F)
Log Pow	: 0.5
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
Explosion limits	: No data available

### 9.2. Other information

No additional information available

## 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

No additional information available

### 10.4. Conditions to avoid

Heat. Open flame. Sparks.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong acids.

### 10.6. Hazardous decomposition products

Carbon oxides (CO, CO<sub>2</sub>).

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed.

1-PHENYLETHANOL (2-13C, 90%) (95% PURE) (98-85-1 (Unlabeled))	
LD50 oral rat	400 mg/kg
LD50 dermal rabbit	2500 mg/kg
ATE CLP (oral)	400.000 mg/kg body weight
ATE CLP (dermal)	2500.000 mg/kg body weight

Skin corrosion/irritation	: mild skin irritation pH: 7.01 at 28 °C (82 °F) - neutral
Serious eye damage/irritation	: Eyes. rabbit. Result: Irritating to eyes pH: 7.01 at 28 °C (82 °F) - neutral
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: S. typhimurium result: negative
Carcinogenicity	: Carcinogenicity. rat. oral. Tumorigenic: Neoplastic by RTECS criteria. Kidney, Ureter, Bladder: Tumors.
Reproductive toxicity	: Not classified
Specific target organ toxicity – single exposure	: May cause respiratory irritation.

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Specific target organ toxicity – repeated exposure	: Not classified
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: Coughing. Shortness of breath. Headache. Nausea. Vomiting. Effects on humans. stomach. 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	: May cause respiratory irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: 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.

#### 1-PHENYLETHANOL (2-13C, 90%) (95% PURE) (98-85-1 (Unlabeled))

LC50 fish 1	345 mg/l <i>Leuciscus idus</i> (Golden orfe) - 48 h
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### 12.2. Persistence and degradability

No additional information available

### 12.3. Bioaccumulative potential

#### 1-PHENYLETHANOL (2-13C, 90%) (95% PURE) (98-85-1 (Unlabeled))

Log Pow	0.5
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### 12.4. Mobility in soil

No additional information available

### 12.5. Results of PBT and vPvB assessment

No additional information available

### 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)	: 2937
DOT NA no.	UN2937

### 14.2. UN proper shipping name

Proper Shipping Name (DOT)	: alpha-Methylbenzyl alcohol, liquid
Class (DOT)	: 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132
Hazard labels (DOT)	: 6.1 - Poison



Packing group (DOT)	: III - Minor Danger
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DOT Special Provisions (49 CFR 172.102)	:	IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). 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, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672). 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)	:	153
DOT Packaging Non Bulk (49 CFR 173.xxx)	:	203
DOT Packaging Bulk (49 CFR 173.xxx)	:	241

### 14.3. Additional information

Emergency Response Guide (ERG) Number	:	153
Other information	:	No supplementary information available.
Special transport precautions	:	Not classified as dangerous in the meaning of transport regulations.

### Overland transport

Packing group (ADR)	:	III
Class (ADR)	:	6.1 - Toxic substances
Hazard identification number (Kemler No.)	:	60
Classification code (ADR)	:	T1
Hazard labels (ADR)	:	6.1 - Toxic substances



Orange plates	:	
Tunnel restriction code (ADR)	:	E
Limited quantities (ADR)	:	5I
EAC	:	2Z
Excepted quantities (ADR)	:	E1

### Transport by sea

DOT Vessel Stowage Location	:	A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
MFAG-No	:	153

### Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	:	60 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	:	220 L
Civil Aeronautics Law	:	Toxic and infectious substances/Toxic substances

### 14.4. Environmental hazards

Other information	:	No supplementary information available.
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### 14.5. Special precautions for user

Special transport precautions	:	Not classified as dangerous in the meaning of transport regulations.
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### 14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

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### SECTION 15: Regulatory information

#### 15.1. US Federal regulations

1-PHENYLETHANOL (2-13C, 90%) (95% PURE) (98-85-1 (Unlabeled))	
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 Delayed (chronic) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313.

#### 15.2. International regulations

##### CANADA

1-PHENYLETHANOL (2-13C, 90%) (95% PURE) (98-85-1 (Unlabeled))
Listed on the Canadian DSL (Domestic Substances List)

##### 15.2.1. National regulations

No additional information available

#### 15.3. US State regulations

1-PHENYLETHANOL (2-13C, 90%) (95% PURE)(98-85-1 (Unlabeled))	
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	RTK - U.S. - Pennsylvania - RTK (Right to Know) List RTK - U.S. - New Jersey - Right to Know Hazardous Substance List

### 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 (Oral)	Acute toxicity (oral) Category 4
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H302	Harmful if swallowed
H315	Causes skin irritation
H318	Causes serious eye damage
H335	May cause respiratory irritation
R22	Harmful if swallowed
R37/38	Irritating to respiratory system and skin
R41	Risk of serious damage to eyes
Xi	Irritant
Xn	Harmful

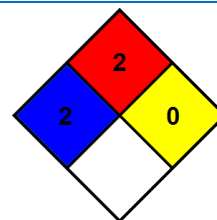


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NFPA health hazard	: 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.
NFPA fire hazard	: 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.
NFPA reactivity	: 0 - Material that in themselves are normally stable, even under fire conditions.



### Hazard Rating

Health	: 2 Moderate Hazard - Temporary or minor injury may occur
Flammability	: 2 Moderate 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*