



## **Characterization of Liquid “Smoke Juice” for Electronic Cigarettes**

prepared for

**Johnson Creek Enterprises**  
Johnson Creek, WI

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15 July 2009

**Client:** Johnson Creek Enterprises  
320 N Watertown St. Suite F  
Johnson Creek, WI 53038

**Requestor:** Robert Kieckbush

**Study:** Characterization of Liquid “Smoke Juice” for Electronic Cigarettes

**LIMS #:** 20090187

## SUMMARY

A liquid “smoke juice” formulation used in electronic cigarettes was tested by gas chromatography mass spectrometry (GC-MS) to identify the ingredients in the mixture and their relative concentrations. In addition, vapor produced from an electronic cigarette containing this smoke juice was assayed to compare the relative smoke composition to that of the liquid.

## EXPERIMENTAL

One sample of smoke juice and some blank cartridges were submitted for these experiments. The smoke juice and vapors generated from the cartridges infused with this smoke juice were characterized by gas chromatography mass spectrometry. The samples were designated as follows:

Table I: Sample Designations

| LIMS #      | Client ID                           | Description               |
|-------------|-------------------------------------|---------------------------|
| 20090187-01 | Blank Mini “103” Premium Cartridges | Johnson Creek Cartridges  |
| 20090187-02 | Original smoke juice 15 ml          | Johnson Creek Smoke Juice |

A Liberty Stix brand “smokeless nicotine mist cigarette” (Figure 1) was used as per the product instructions to produce the nicotine mist or vapor while 2 dilutions of the smoke juice were prepared in order to estimate the ingredients of the juice or collected vapors.

To capture the vapor emitted from an assembled Liberty Stix cigarette containing the Johnson Creek smoke juice, a 40ml evacuated gastight vial was used to draw

air through the Liberty Stix device and into the vial. The white vapor produced was captured and diluted with a solvent prior to GC-MS analysis.

Each of the prepared samples was characterized on a Shimadzu 2010S GC-MS instrument equipped with a ZB-5HT (Phenomenex) high temperature capillary column. Observed peaks were identified based on spectral matches with commercial MS libraries. Relative concentrations were estimated from the peak areas.

## RESULTS & DISCUSSION

A Total Ion Chromatogram (TIC) of a 1:100 diluted sample of the smoke juice (20090187-01) is shown in Figure 2. Since the concentration of propylene glycol (the first large peak) was significantly higher than the other ingredients, a second dilution was prepared to quantify the propylene glycol. Figure 3 shows the 1:1000 diluted sample overlaid with a 0.1% propylene glycol standard. Spectral library matches identified 3 ingredients - propylene glycol, glycerin, and nicotine - with retention times of about 3 minutes, 7 minutes and 11 minutes respectively.

The captured vapor dissolved in solvent resulted in the chromatogram shown in (Figure 4). Since the concentrations of glycerin and nicotine were much smaller than the propylene glycol and even more dilute in the vapors compared to the liquid smoke juice, single ion monitoring (SIM) was used to enhance the signal of each ingredient and estimate their relative concentrations (Figure 5).

Table II summarizes the estimated relative % of each ingredient in the smoke liquid and the extracted vapors. This analysis assumed that all of the volatile components were observed in the GC-MS analysis and that the sensitivity of the detector to each compound was similar.

General hazard and toxicity data were taken from published literature and a report titled "Analysis of Components from Gamucci Electronic Cigarette Cartridges, Tobacco Flavour Regular Smoking Liquid" provided by the client. MSDS information for each material is provided at the end of this report. Online resources for additional safety or toxicity information can be found for the 3 ingredients here:

<http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=24898528#safety>  
<http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=24895092>  
<http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=24862741>

or on Toxnet (<http://toxnet.nlm.nih.gov/index.html>).

Figure 1: Smoke Juice Sample & Cartridge with Electronic Cigarette



Figure 2: TIC of Smoke Juice (1:100 dilution)

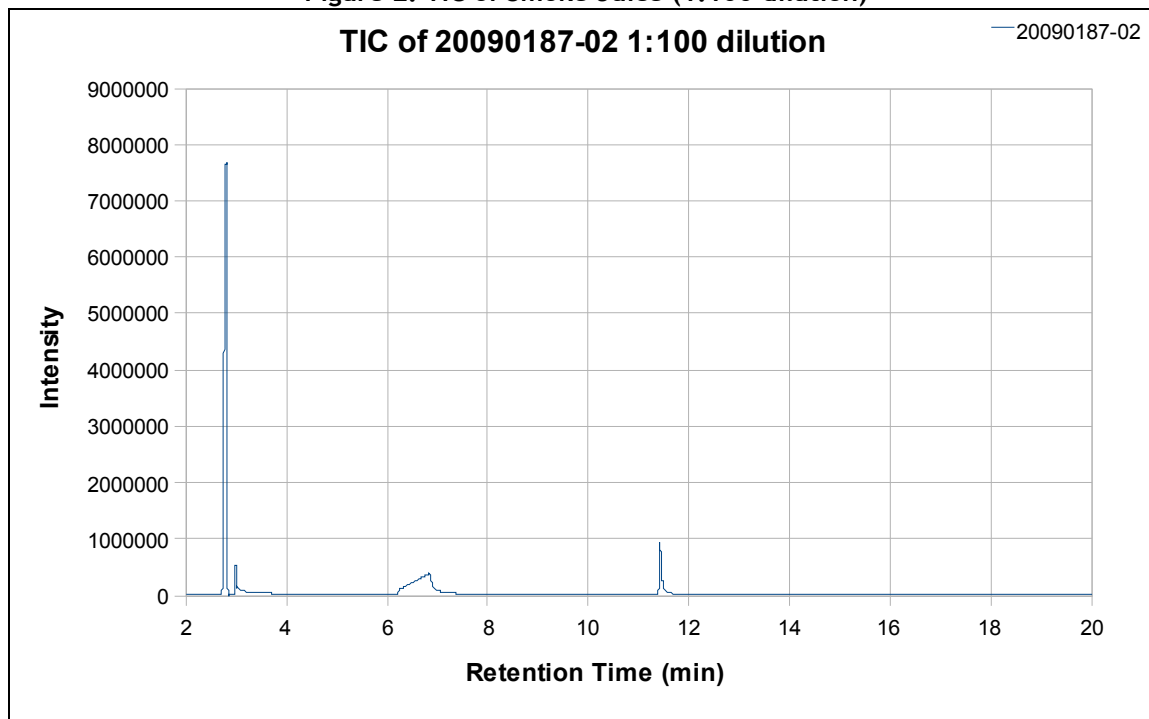


Figure 3: TIC of Smoke Juice (1:1000 dilution) vs. 0.1% Propylene Glycol Standard

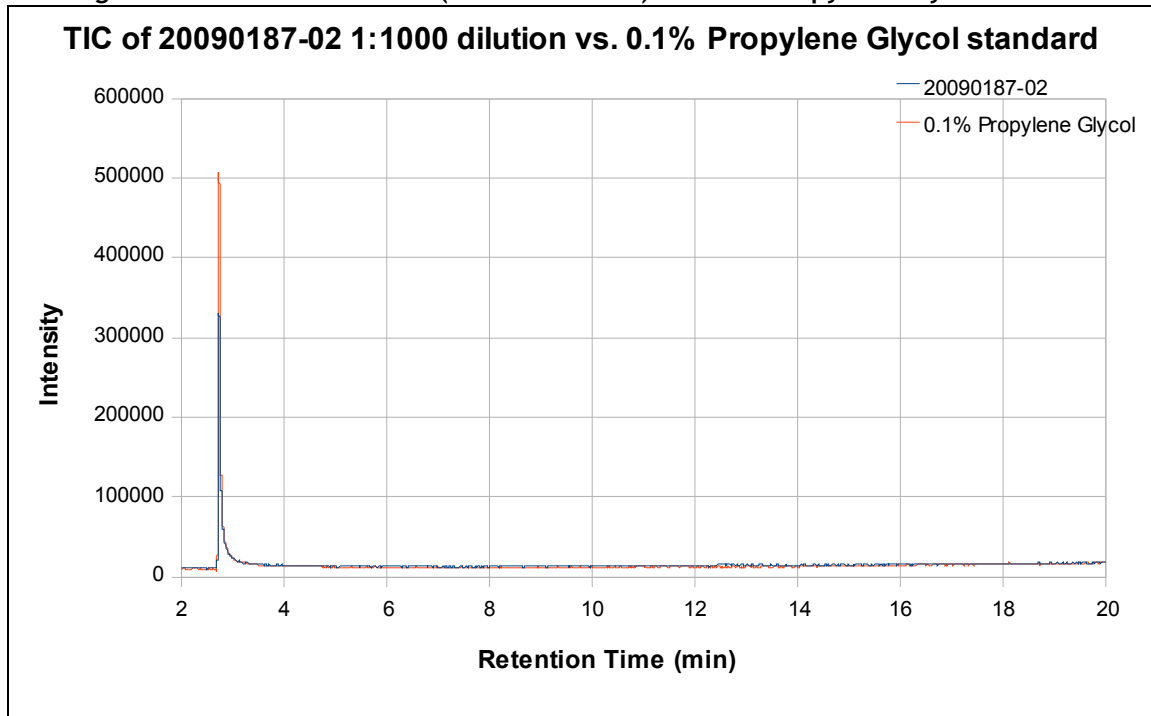
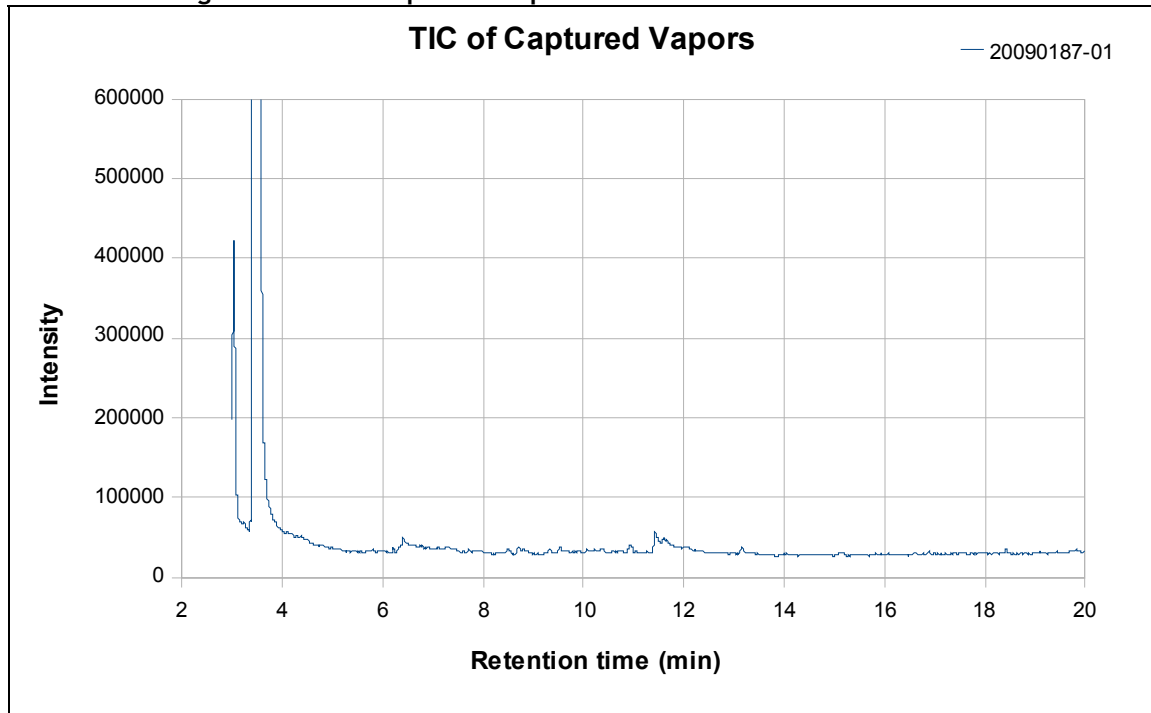
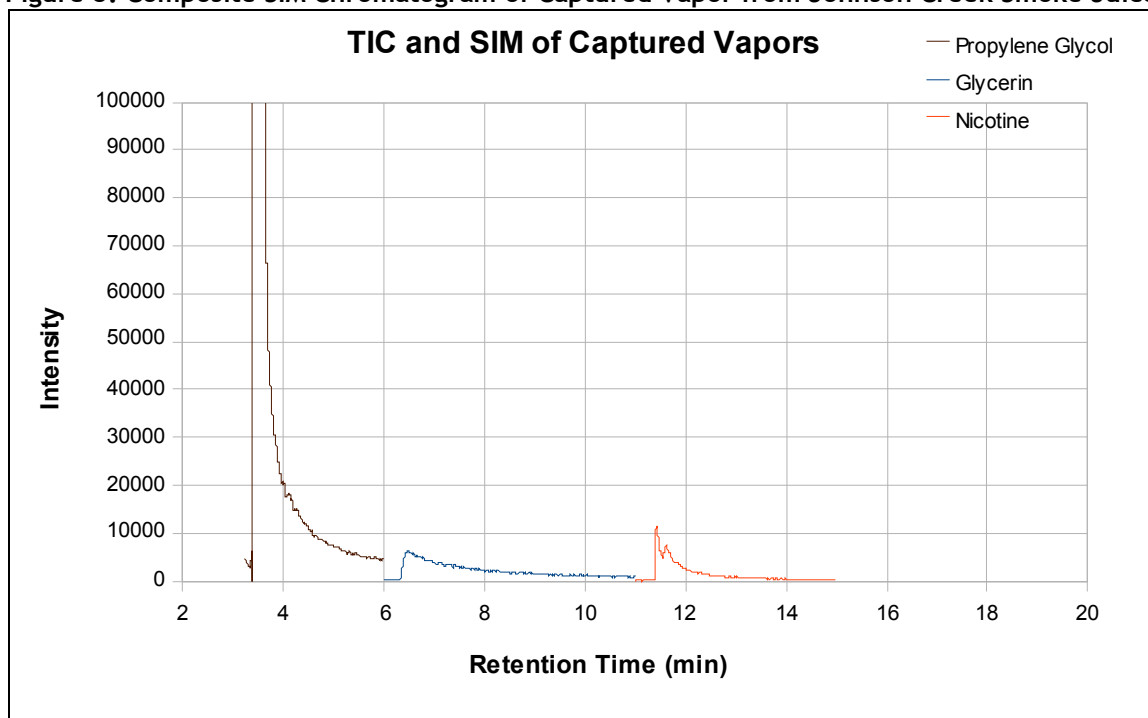


Figure 4: TIC of Captured Vapor from Johnson Creek Smoke Juice



**Figure 5: Composite SIM Chromatogram of Captured Vapor from Johnson Creek Smoke Juice.**



**Table II: TIC Peak Report for Sample 20090187-01**

| # | Name             | % in Smoke Juice<br>(Peak Area %) | % in Vapors<br>(Peak Area %) | CAS No.     | Comments*   |
|---|------------------|-----------------------------------|------------------------------|-------------|---|
| 1 | Propylene Glycol | 72.16                             | 99.1                         | 57-55-6     | Not currently recognized as giving any health hazards. Suspected respiratory toxicant, suspected skin or sense organ toxicant, suspected neurotoxicant and immunotoxicant   |
| 2 | Glycerin         | 20.87                             | 0.46                         | 56-81-5     | Non-hazardous   |
| 3 | Nicotine         | 6.97                              | 0.44                         | 23950-04-01 | R23 = Toxic by inhalation<br>R24 = Toxic in contact with skin<br>R25 = Toxic if swallowed<br>R51/53 = Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.<br>Poison - may be fatal if inhaled |

\*cf. "Gamucci" report

## MATERIAL SAFETY DATA SHEET

Date Printed: 07/15/2009

Date Updated: 01/26/2006

Version 1.4

## Section 1 - Product and Company Information

Product Name 1,2-Propanediol, meets USP testing specifications  
Product Number P4347  
Brand SIAL  
  
Company Sigma-Aldrich  
Address 3050 Spruce Street  
SAINT LOUIS MO 63103 US  
  
Technical Phone: 800-325-5832  
Fax: 800-325-5052  
Emergency Phone: 314-776-6555

## Section 2 - Composition/Information on Ingredient

| Substance Name                            | CAS #   | SARA 313 |
|---|---------|----------|
| 1,2-PROPANEDIOL, MEETS USP TESTING SPECS. | 57-55-6 | No       |

Formula C3H8O2  
Synonyms 1,2-Dihydroxypropane \* Dowfrost \* Methylethylene glycol \* Monopropylene glycol \* PG 12 \* Propane-1,2-diol \* Propylene Glycol USP \* alpha-Propyleneglycol \* 1,2-Propylene glycol \* 1,2-Propylenglykol (German) \* Sirlene \* Solargard P \* Solar Winter BAN \* Ucar 35  
RTECS Number: TY2000000

## Section 3 - Hazards Identification

## HMIS RATING

HEALTH: 0

FLAMMABILITY: 1

REACTIVITY: 0

## NFPA RATING

HEALTH: 0

FLAMMABILITY: 1

REACTIVITY: 0

For additional information on toxicity, please refer to Section 11.

## Section 4 - First Aid Measures

## ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

## INHALATION EXPOSURE

If inhaled, remove to fresh air. If breathing becomes difficult, call a physician.

#### DERMAL EXPOSURE

In case of contact, immediately wash skin with soap and copious amounts of water.

#### EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

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### Section 5 - Fire Fighting Measures

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#### FLASH POINT

217.4 °F    103 °C    Method: closed cup

#### EXPLOSION LIMITS

Lower: 2.6 %    Upper: 12.5 %

#### AUTOIGNITION TEMP

415 °C

#### FLAMMABILITY

N/A

#### EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

#### FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.  
Specific Hazard(s): Emits toxic fumes under fire conditions.

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### Section 6 - Accidental Release Measures

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#### METHODS FOR CLEANING UP

Absorb on sand or vermiculite and place in closed containers for disposal. Ventilate area and wash spill site after material pickup is complete.

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### Section 7 - Handling and Storage

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#### HANDLING

User Exposure: Avoid inhalation. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

#### STORAGE

Suitable: Keep tightly closed.

#### SPECIAL REQUIREMENTS

Hygroscopic.

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### Section 8 - Exposure Controls / PPE

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#### ENGINEERING CONTROLS

Safety shower and eye bath. Mechanical exhaust required.

#### PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Respiratory protection is not required. Where protection is desired, use multi-purpose combination (US) or type ABEK (EN



14387) respirator cartridges.  
Hand: Protective gloves.  
Eye: Chemical safety goggles.

#### GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

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### Section 9 - Physical/Chemical Properties

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|                       |  |                            |
|-----------------------|--|----------------------------|
| Appearance            | Physical State: Clear viscous liquid<br>Color: Colorless |                            |
| Property              | Value  | At Temperature or Pressure |
| Molecular Weight      | 76.1 AMU   |                            |
| pH                    | N/A  |                            |
| BP/BP Range           | 185.0 - 189.0 °C   |                            |
| MP/MP Range           | - 60.0 °C  |                            |
| Freezing Point        | N/A  |                            |
| Vapor Pressure        | 0.08 mmHg  | 20 °C                      |
| Vapor Density         | 2.62 g/l   |                            |
| Saturated Vapor Conc. | N/A  |                            |
| SG/Density            | 1.036 g/cm3  |                            |
| Bulk Density          | N/A  |                            |
| Odor Threshold        | N/A  |                            |
| Volatile%             | N/A  |                            |
| VOC Content           | N/A  |                            |
| Water Content         | < 0.1 %  |                            |
| Solvent Content       | N/A  |                            |
| Evaporation Rate      | N/A  |                            |
| Viscosity             | N/A  |                            |
| Surface Tension       | N/A  |                            |
| Partition Coefficient | N/A  |                            |
| Decomposition Temp.   | N/A  |                            |
| Flash Point           | 217.4 °F 103 °C  | Method: closed cup         |
| Explosion Limits      | Lower: 2.6 %   |                            |
|                       | Upper: 12.5 %  |                            |
| Flammability          | N/A  |                            |
| Autoignition Temp     | 415 °C   |                            |
| Refractive Index      | 1.433  |                            |
| Optical Rotation      | N/A  |                            |
| Miscellaneous Data    | N/A  |                            |
| Solubility            | N/A  |                            |

N/A = not available

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### Section 10 - Stability and Reactivity

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#### STABILITY

Stable: Stable.

Conditions to Avoid: Moisture.

Materials to Avoid: Acid chlorides, Acid anhydrides, Oxidizing agents, Chloroformates, Reducing agents.

#### HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

#### HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

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### Section 11 - Toxicological Information

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#### ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.  
Skin Absorption: May be harmful if absorbed through the skin.  
Eye Contact: May cause eye irritation.  
Inhalation: May be harmful if inhaled. Material may be irritating to mucous membranes and upper respiratory tract.  
Ingestion: May be harmful if swallowed.

#### SIGNS AND SYMPTOMS OF EXPOSURE

Exposure can cause: Gastrointestinal disturbances. Nausea, headache, and vomiting. CNS depression.

#### TOXICITY DATA

Oral  
Rat  
20000 mg/kg  
LD50

Intraperitoneal  
Rat  
6660 MG/KG  
LD50

Subcutaneous  
Rat  
22500 MG/KG  
LD50

Intravenous  
Rat  
6423 MG/KG  
LD50

Intramuscular  
Rat  
14 GM/KG  
LD50

Oral  
Mouse  
22000 mg/kg  
LD50

Intraperitoneal  
Mouse  
9718 MG/KG  
LD50

Remarks: Blood:Changes in spleen. Lungs, Thorax, or Respiration:Chronic pulmonary edema. Kidney, Ureter, Bladder:Changes in both tubules and glomeruli.

Subcutaneous  
Mouse  
17370 MG/KG  
LD50

Remarks: Lungs, Thorax, or Respiration:Cyanosis. Behavioral:Change in motor activity (specific assay). Behavioral:Muscle contraction or spasticity.

Intravenous  
Mouse

6630 MG/KG  
LD50

Oral  
Dog  
22000 mg/kg  
LD50

Intravenous  
Dog  
26 GM/KG  
LD50

Oral  
Rabbit  
18500 mg/kg  
LD50

Skin  
Rabbit  
20800 mg/kg  
LD50

Intravenous  
Rabbit  
6500 MG/KG  
LD50

Oral  
Guinea pig  
18350 mg/kg  
LD50

Oral  
Quail  
> 2080 mg/kg  
LD50

#### IRRITATION DATA

Skin  
Human  
500 mg  
7D  
Remarks: Mild irritation effect

Skin  
Human  
104 mg  
3D  
I  
Remarks: Moderate irritation effect

Skin  
Man  
10 %  
2D

Eyes  
Rabbit  
100 mg  
Remarks: Mild irritation effect

Eyes  
Rabbit  
500 mg  
24H  
Remarks: Mild irritation effect

#### CHRONIC EXPOSURE - TERATOGEN

Species: Mouse  
Dose: 100 MG/KG  
Route of Application: Intraperitoneal  
Exposure Time: (15D PREG)  
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

#### CHRONIC EXPOSURE - MUTAGEN

Species: Mouse  
Route: Subcutaneous  
Dose: 8000 MG/KG  
Mutation test: DNA inhibition

Species: Mouse  
Route: Subcutaneous  
Dose: 8000 MG/KG  
Mutation test: Cytogenetic analysis

Species: Hamster  
Dose: 32 GM/L  
Cell Type: fibroblast  
Mutation test: Cytogenetic analysis

#### CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Mouse  
Dose: 100 MG/KG  
Route of Application: Intraperitoneal  
Exposure Time: (11D PREG)  
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

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#### Section 12 - Ecological Information

No data available.

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#### Section 13 - Disposal Considerations

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##### APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

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#### Section 14 - Transport Information

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##### DOT

Proper Shipping Name: None  
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

#### IATA

Non-Hazardous for Air Transport: Non-hazardous for air transport.

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#### Section 15 - Regulatory Information

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##### UNITED STATES REGULATORY INFORMATION

SARA LISTED: No

TSCA INVENTORY ITEM: Yes

##### CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.

DSL: Yes

NDSL: No

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#### Section 16 - Other Information

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##### DISCLAIMER

For R&D or manufacturing use. Not for prescription compound or other uses.

##### WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2009 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.

## MATERIAL SAFETY DATA SHEET

Date Printed: 07/15/2009

Date Updated: 02/16/2009

Version 1.8

## Section 1 - Product and Company Information

|                  |   |
|------------------|---|
| Product Name     | GLYCERIN, MEETS USP TESTING SPECIFICATIONS    |
| Product Number   | G2289   |
| Brand            | SIAL  |
| Company          | Sigma-Aldrich                                 |
| Address          | 3050 Spruce Street<br>SAINT LOUIS MO 63103 US |
| Technical Phone: | 800-325-5832                                  |
| Fax:             | 800-325-5052                                  |
| Emergency Phone: | 314-776-6555                                  |

## Section 2 - Composition/Information on Ingredient

|                                    |  |          |
|------------------------------------|--|----------|
| Substance Name                     | CAS #  | SARA 313 |
| GLYCEROL, MEETS USP TESTING SPECS. | 56-81-5  | No       |
| Formula                            | C3H8O3   |          |
| Synonyms                           | Glycerol * Citifluor AF 2 * Glycerin * Glycerin, anhydrous * Glycerine * Glycerin mist (ACGIH, OSHA) * Glycerin, synthetic * Glyceritol * Glycyl alcohol * Clyzerin, wasserfrei (German) * Grocolene * MOON * 1,2,3-Propanetriol * Osmoglyn * Star * Synthetic glycerin * 90 Technical glycerine * Trihydroxypropane * 1,2,3-Trihydroxypropane |          |
| RTECS Number:                      | MA8050000  |          |

## Section 3 - Hazards Identification

## EMERGENCY OVERVIEW

Caution: Avoid contact and inhalation. Target organ(s): Kidneys.

## HMIS RATING

HEALTH: 1\*

FLAMMABILITY: 0

REACTIVITY: 1

## NFPA RATING

HEALTH: 1

FLAMMABILITY: 0

REACTIVITY: 1

\*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

## Section 4 - First Aid Measures

## ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is

conscious. Call a physician.

#### INHALATION EXPOSURE

If inhaled, remove to fresh air. If breathing becomes difficult, call a physician.

#### DERMAL EXPOSURE

In case of contact, immediately wash skin with soap and copious amounts of water.

#### EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

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### Section 5 - Fire Fighting Measures

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#### FLASH POINT

320 °F    160 °C    Method: closed cup

#### EXPLOSION LIMITS

Lower: 0.9 %

#### AUTOIGNITION TEMP

370 °C

#### FLAMMABILITY

N/A

#### EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

#### FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.  
Specific Hazard(s): Emits toxic fumes under fire conditions.

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### Section 6 - Accidental Release Measures

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#### METHODS FOR CLEANING UP

Absorb on sand or vermiculite and place in closed containers for disposal. Ventilate area and wash spill site after material pickup is complete.

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### Section 7 - Handling and Storage

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#### HANDLING

User Exposure: Avoid inhalation. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

#### STORAGE

Suitable: Keep tightly closed.

#### SPECIAL REQUIREMENTS

Hygroscopic.

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### Section 8 - Exposure Controls / PPE

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#### ENGINEERING CONTROLS

Safety shower and eye bath. Mechanical exhaust required.

#### PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Respiratory protection is not required. Where protection is desired, use multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges.

Hand: Protective gloves.

Eye: Chemical safety goggles.

#### GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

#### EXPOSURE LIMITS, RTECS

| Country   | Source             | Type    | Value                          |
|---|--------------------|---------|--------------------------------|
| USA USA   | ACGIH ACGIH        | TWA TWA | 10 MG/M3 10 MG/M3              |
| Remarks: inhalable particulate                  |                    |         |                                |
| USA USA   | MSHA Standard MSHA |         |                                |
| Remarks: Nuisance Particulates (mist). Nuisance |                    |         |                                |
| USA USA   | OSHA. OSHA.        | PEL PEL | 8H TWA 15 MG/M3, TOTAL DUST 8H |
| New Zealand OEL OEL                             |                    |         |                                |
| Remarks: check ACGIH TLV check ACGIH TLV        |                    |         |                                |

#### EXPOSURE LIMITS

| Country   | Source | Type  | Value    |
|---|--------|-------|----------|
| Poland  |        | NDS   | 10 mg/m3 |
| Poland  |        | NDSch | -        |
| Poland  |        | NDSP  |          |
| Remarks: {OELS ARE VALID FOR AEROSOLS} AEROZOLE |        |       |          |

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#### Section 9 - Physical/Chemical Properties

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|                       |  |                            |
|-----------------------|--|----------------------------|
| Appearance            | Physical State: Clear viscous liquid<br>Color: Colorless |                            |
| Property              | Value  | At Temperature or Pressure |
| Molecular Weight      | 92.1 AMU   |                            |
| pH                    | 5.5 - 8.0  |                            |
| BP/BP Range           | 182 °C   | 20 mmHg                    |
| MP/MP Range           | 20 °C  |                            |
| Freezing Point        | N/A  |                            |
| Vapor Pressure        | < 1 mmHg   | 20 °C                      |
| Vapor Density         | 3.1 g/l  |                            |
| Saturated Vapor Conc. | N/A  |                            |
| SG/Density            | 1.262 g/cm3  |                            |
| Bulk Density          | N/A  |                            |
| Odor Threshold        | N/A  |                            |
| Volatile%             | N/A  |                            |
| VOC Content           | N/A  |                            |
| Water Content         | < 0.1 %  |                            |
| Solvent Content       | N/A  |                            |
| Evaporation Rate      | N/A  |                            |
| Viscosity             | N/A  |                            |
| Surface Tension       | N/A  |                            |
| Partition Coefficient | N/A  |                            |
| Decomposition Temp.   | N/A  |                            |
| Flash Point           | 320 °F 160 °C  | Method: closed cup         |
| Explosion Limits      | Lower: 0.9 %   |                            |
| Flammability          | N/A  |                            |
| Autoignition Temp     | 370 °C   |                            |
| Refractive Index      | 1.474  |                            |
| Optical Rotation      | N/A  |                            |



|                    |   |
|--------------------|---|
| Miscellaneous Data | N/A   |
| Solubility         | Solubility in Water: 5 M in H <sub>2</sub> O, 20°C<br>complete, colorless |

N/A = not available

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## Section 10 - Stability and Reactivity

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### STABILITY

Stable: Stable.

Conditions to Avoid: Moisture.

Materials to Avoid: Strong bases, Strong oxidizing agents.

### HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

### HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

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## Section 11 - Toxicological Information

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### ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.

Skin Absorption: May be harmful if absorbed through the skin.

Eye Contact: May cause eye irritation.

Inhalation: May be harmful if inhaled. Material may be irritating to mucous membranes and upper respiratory tract.

Ingestion: May be harmful if swallowed.

### TARGET ORGAN(S) OR SYSTEM(S)

Kidneys.

### SIGNS AND SYMPTOMS OF EXPOSURE

Nausea, headache, and vomiting. Prolonged exposure can cause:

### TOXICITY DATA

Oral

Rat

12600 mg/kg

LD50

Remarks: Liver: Other changes. Behavioral: Muscle weakness.

Behavioral: General anesthetic.

Inhalation

Rat

> 570 mg/m<sup>3</sup>

LC50

Intraperitoneal

Rat

4420 MG/KG

LD50

Remarks: Cardiac: Other changes. Behavioral: Toxic psychosis.

Kidney, Ureter, Bladder: Other changes.

Subcutaneous

Rat

100 MG/KG

LD50

Intravenous

Rat  
5566 MG/KG  
LD50

Oral  
Mouse  
4090 mg/kg  
LD50

Intraperitoneal  
Mouse  
8700 MG/KG  
LD50  
Remarks: Behavioral: Altered sleep time (including change in  
righting reflex).

Subcutaneous  
Mouse  
91 MG/KG  
LD50

Intravenous  
Mouse  
4250 MG/KG  
LD50

Oral  
Rabbit  
27000 mg/kg  
LD50

Skin  
Rabbit  
> 10000 mg/kg  
LD50

Intravenous  
Rabbit  
53 GM/KG  
LD50

Oral  
Guinea pig  
7750 mg/kg  
LD50

#### IRRITATION DATA

Skin  
Rabbit  
500 mg  
24H  
Remarks: Mild irritation effect

Eyes  
Rabbit  
126 mg  
Remarks: Mild irritation effect

Eyes  
Rabbit  
500 mg

24H

Remarks: Mild irritation effect

#### CHRONIC EXPOSURE - MUTAGEN

Species: Human  
Dose: 200 MMOL/L  
Cell Type: lymphocyte  
Mutation test: DNA inhibition

Species: Rat  
Route: Oral  
Dose: 1 GM/KG  
Mutation test: Cytogenetic analysis

#### CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Rat  
Dose: 100 MG/KG  
Route of Application: Oral  
Exposure Time: (1D MALE)  
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Species: Rat  
Dose: 280 MG/KG  
Route of Application: Intratesticular  
Exposure Time: (2D MALE)  
Result: Paternal Effects: Testes, epididymis, sperm duct.  
Paternal Effects: Spermatogenesis (including genetic material, sperm morphology, motility, and count).

Species: Rat  
Dose: 1600 MG/KG  
Route of Application: Intratesticular  
Exposure Time: (1D MALE)  
Result: Effects on Fertility: Male fertility index (e.g., # males impregnating females per # males exposed to fertile nonpregnant females).

Species: Rat  
Dose: 862 MG/KG  
Route of Application: Intratesticular  
Exposure Time: (1D MALE)  
Result: Paternal Effects: Spermatogenesis (including genetic material, sperm morphology, motility, and count).

Species: Monkey  
Dose: 119 MG/KG  
Route of Application: Intratesticular  
Exposure Time: (1D MALE)  
Result: Paternal Effects: Testes, epididymis, sperm duct.  
Paternal Effects: Spermatogenesis (including genetic material, sperm morphology, motility, and count).

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#### Section 12 - Ecological Information

No data available.

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#### Section 13 - Disposal Considerations

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APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

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## Section 14 - Transport Information

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### DOT

Proper Shipping Name: None  
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

### IATA

Non-Hazardous for Air Transport: Non-hazardous for air transport.

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## Section 15 - Regulatory Information

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### US CLASSIFICATION AND LABEL TEXT

US Statements: Caution: Avoid contact and inhalation. Target organ(s): Kidneys.

### UNITED STATES REGULATORY INFORMATION

SARA LISTED: No  
TSCA INVENTORY ITEM: Yes Yes

### CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.  
DSL: Yes  
NDSL: No

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## Section 16 - Other Information

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### DISCLAIMER

For R&D or manufacturing use. Not for prescription compound or other uses.

### WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2009 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.

**Material Safety Data Sheet**

Version 3.0  
Revision Date 02/25/2009  
Print Date 07/15/2009

**1. PRODUCT AND COMPANY IDENTIFICATION**

Product name : (-)-Nicotine

Product Number : 36733  
Brand : Fluka

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052  
Emergency Phone # : (314) 776-6555

**2. COMPOSITION/INFORMATION ON INGREDIENTS**

Synonyms : (-)-1-Methyl-2-(3-pyridyl)pyrrolidine

Formula :  $C_{10}H_{14}N_2$   
Molecular Weight : 162.24 g/mol

| CAS-No.         | EC-No.    | Index-No.    | Concentration |
|-----------------|-----------|--------------|---------------|
| <b>Nicotine</b> |           |              |               |
| 54-11-5         | 200-193-3 | 614-001-00-4 | -             |

**3. HAZARDS IDENTIFICATION****Emergency Overview****OSHA Hazards**

Target Organ Effect, Highly toxic by ingestion, Highly toxic by skin absorption, Teratogen

**Target Organs**

Peripheral nervous system, Central nervous system, Skeletal muscle., Gastro-intestinal system

**HMIS Classification**

Health Hazard: 3  
Chronic Health Hazard: \*  
Flammability: 1  
Physical hazards: 0

**NFPA Rating**

Health Hazard: 3  
Fire: 1  
Reactivity Hazard: 0

**Potential Health Effects**

|                   |  |
|-------------------|--|
| <b>Inhalation</b> | May be harmful if inhaled. May cause respiratory tract irritation. |
| <b>Skin</b>       | May cause skin irritation. May be fatal if absorbed through skin.  |
| <b>Eyes</b>       | May cause eye irritation.  |
| <b>Ingestion</b>  | May be fatal if swallowed.   |

#### 4. FIRST AID MEASURES

##### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

##### If inhaled

If breathed in, move person into fresh air. If not breathing give artificial respiration. Consult a physician.

##### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

##### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

##### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

#### 5. FIRE-FIGHTING MEASURES

##### Flammable properties

Flash point 101 °C (214 °F) - closed cup

Ignition temperature 244 °C (471 °F)

##### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Wear self contained breathing apparatus for fire fighting if necessary.

#### 6. ACCIDENTAL RELEASE MEASURES

##### Personal precautions

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

##### 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.

##### Methods for cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

#### 7. HANDLING AND STORAGE

##### Handling

Avoid inhalation of vapour or mist.  
Normal measures for preventive fire protection.

##### Storage

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.

Store under inert gas. hygroscopic Air and light sensitive.

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Components with workplace control parameters

| Components | CAS-No.                                   | Value | Control parameters | Update     | Basis  |
|------------|---|-------|--------------------|------------|--|
| Nicotine   | 54-11-5                                   | TWA   | 0.5 mg/m3          | 1994-09-01 | USA. ACGIH Threshold Limit Values (TLV)  |
| Remarks    | Skin contact does contribute to exposure. |       |                    |            |  |
|            |   | TWA   | 0.5 mg/m3          | 1989-03-01 | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000                    |
|            | Skin contact does contribute to exposure. |       |                    |            |  |
|            |   | TWA   | 0.5 mg/m3          | 1993-06-30 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
|            | Skin contact does contribute to exposure. |       |                    |            |  |

### Personal protective equipment

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Hand protection

Handle with gloves.

#### Eye protection

Safety glasses

#### Skin and body protection

Choose body protection according to the amount and concentration of the dangerous substance at the work place.

#### Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### Appearance

Form clear, liquid

Colour dark brown

### Safety data

pH 10.2

Melting point -79 °C (-110 °F)

Boiling point 247 °C (477 °F) at 993 hPa (745 mmHg)

|   |   |
|---|---|
| Flash point                               | 101 °C (214 °F) - closed cup            |
| Ignition temperature                      | 244 °C (471 °F)                         |
| Lower explosion limit                     | no data available                       |
| Upper explosion limit                     | no data available                       |
| Vapour pressure                           | 0.051 hPa (0.038 mmHg) at 25 °C (77 °F) |
| Density                                   | 1.010 g/cm <sup>3</sup>                 |
| Water solubility                          | completely miscible                     |
| Partition coefficient:<br>n-octanol/water | log Pow: 1.17                           |
| Relative vapour<br>density                | 5.6<br>- (Air = 1.0)                    |

## 10. STABILITY AND REACTIVITY

### Storage stability

Stable under recommended storage conditions.

### Materials to avoid

Strong oxidizing agents

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO<sub>x</sub>)

## 11. TOXICOLOGICAL INFORMATION

### Acute toxicity

LD50 Oral - rat - 50 mg/kg

LD50 Dermal - rabbit - 50 mg/kg

Remarks: Behavioral: Convulsions or effect on seizure threshold. Respiratory disorder

### Irritation and corrosion

no data available

### Sensitisation

no data available

### Chronic exposure

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

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

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

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

Possible risk of congenital malformation in the fetus.



## Signs and Symptoms of Exposure

prolonged or repeated exposure can cause: Vomiting, Diarrhoea, Convulsions, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

## Potential Health Effects

|                      |  |
|----------------------|--|
| <b>Inhalation</b>    | May be harmful if inhaled. May cause respiratory tract irritation.                             |
| <b>Skin</b>          | May cause skin irritation. May be fatal if absorbed through skin.                              |
| <b>Eyes</b>          | May cause eye irritation.  |
| <b>Ingestion</b>     | May be fatal if swallowed.   |
| <b>Target Organs</b> | Peripheral nervous system, Central nervous system, Skeletal muscle., Gastro-intestinal system, |

## Additional Information

RTECS: QS5250000

## 12. ECOLOGICAL INFORMATION

### Elimination information (persistence and degradability)

no data available

### Ecotoxicity effects

|  |  |
|--|--|
| Toxicity to fish                                     | LC50 - Oncorhynchus mykiss (rainbow trout) - 4 mg/l - 96 h |
| Toxicity to daphnia and other aquatic invertebrates. | EC50 - Daphnia magna (Water flea) - 0.24 mg/l - 48 h       |

### Further information on ecology

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

## 13. DISPOSAL CONSIDERATIONS

### Product

Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

### Contaminated packaging

Dispose of as unused product.

## 14. TRANSPORT INFORMATION

### DOT (US)

|                                |            |                   |
|--------------------------------|------------|-------------------|
| UN-Number: 1654                | Class: 6.1 | Packing group: II |
| Proper shipping name: Nicotine |            |                   |
| Marine pollutant: No           |            |                   |
| Poison Inhalation Hazard: No   |            |                   |

### IMDG

|                                |            |                   |                  |
|--------------------------------|------------|-------------------|------------------|
| UN-Number: 1654                | Class: 6.1 | Packing group: II | EMS-No: F-A, S-A |
| Proper shipping name: NICOTINE |            |                   |                  |
| Marine pollutant: No           |            |                   |                  |

### IATA

|                                |            |                   |
|--------------------------------|------------|-------------------|
| UN-Number: 1654                | Class: 6.1 | Packing group: II |
| Proper shipping name: Nicotine |            |                   |

## 15. REGULATORY INFORMATION

### OSHA Hazards

Target Organ Effect, Highly toxic by ingestion, Highly toxic by skin absorption, Teratogen

### DSL Status

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

### SARA 302 Components

|          | CAS-No. | Revision Date |
|----------|---------|---------------|
| Nicotine | 54-11-5 | 1991-07-01    |

### SARA 313 Components

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

### Massachusetts Right To Know Components

|          | CAS-No. | Revision Date |
|----------|---------|---------------|
| Nicotine | 54-11-5 | 1991-07-01    |

### Pennsylvania Right To Know Components

|          | CAS-No. | Revision Date |
|----------|---------|---------------|
| Nicotine | 54-11-5 | 1991-07-01    |

### New Jersey Right To Know Components

|          | CAS-No. | Revision Date |
|----------|---------|---------------|
| Nicotine | 54-11-5 | 1991-07-01    |

### California Prop. 65 Components

|   | CAS-No. | Revision Date |
|---|---------|---------------|
| WARNING! This product contains a chemical known in the State of California to cause birth defects or other reproductive harm.<br>Nicotine | 54-11-5 | 1990-04-01    |

## 16. OTHER INFORMATION

### Further information

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