



# MATERIAL SAFETY DATA SHEET

according to the Global Harmonized System

Date of issue: 02/04/2013

Version 1.0

## SECTION 1. Identification

### Product identifier

Product number 814138  
Product name 3-Nitropropanol for synthesis

### Relevant identified uses of the substance or mixture and uses advised against

Identified uses Chemical for synthesis

### Details of the supplier of the safety data sheet

Company EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821,  
United States of America | SDS Phone Support: +1-978-715-1335 |  
General Inquiries: +1-978-751-4321 | Monday to Friday, 9:00 AM to  
4:00 PM Eastern Time (GMT-5)  
  
e-mail: mm\_sds@merckgroup.com

Emergency telephone 613-996-6666 CANUTEC (Canada)  
+1-703-527-3887 CHEMTREC (International)  
24 Hours/day; 7 Days/week

## SECTION 2. Hazards identification

### GHS Classification

Acute toxicity, Category 3, Oral, H301

For the full text of the H-Statements mentioned in this Section, see Section 16.

### GHS-Labeling

*Hazard pictograms*



*Signal Word*  
Danger

*Hazard Statements*  
H301 Toxic if swallowed.

*Precautionary Statements*  
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or

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doctor/physician.

**Other hazards**

None known.

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**SECTION 3. Composition/information on ingredients**

Formula	O <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> (Hill)
CAS-No.	25182-84-7	
Molar mass	105.09 g/mol	

**Hazardous ingredients**

*Chemical Name (Concentration)*

CAS-No.

*3-nitropropanol (>= 90 % - <= 100 % )*

25182-84-7

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**SECTION 4. First aid measures**

**Description of first-aid measures**

*Inhalation*

After inhalation: fresh air.

*Skin contact*

After skin contact: wash off with plenty of water. Remove contaminated clothing.

*Eye contact*

After eye contact: rinse out with plenty of water.

*Ingestion*

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

Never give anything by mouth to an unconscious person.

**Most important symptoms and effects, both acute and delayed**

drowsiness, Coma, Shortness of breath

**Indication of any immediate medical attention and special treatment needed**

No information available.

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**SECTION 5. Fire-fighting measures**

**Extinguishing media**

*Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

*Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

**Special hazards arising from the substance or mixture**

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Combustible material  
Vapors are heavier than air and may spread along floors.  
Development of hazardous combustion gases or vapors possible in the event of fire.  
Fire may cause evolution of:  
nitrogen oxides

**Advice for firefighters**

*Special protective equipment for fire-fighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

*Further information*

Prevent fire extinguishing water from contaminating surface water or the ground water system.  
Suppress (knock down) gases/vapors/mists with a water spray jet.

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**SECTION 6. Accidental release measures**

**Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapors, aerosols. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

**Environmental precautions**

Do not empty into drains.

**Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills.  
Observe possible material restrictions (see sections 7 and 10).  
Take up carefully with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

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**SECTION 7. Handling and storage**

**Precautions for safe handling**

Observe label precautions.

**Conditions for safe storage, including any incompatibilities**

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Store at +15°C to +25°C (+59°F to +77°F).

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**SECTION 8. Exposure controls/personal protection**

**Exposure limit(s)**

Contains no substances with occupational exposure limit values.

**Engineering measures**

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

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**Individual protection measures**

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

*Hygiene measures*

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

*Eye/face protection*

Safety glasses

*Hand protection*

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

*Other protective equipment:*

protective clothing

*Respiratory protection*

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

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**SECTION 9. Physical and chemical properties**

Physical state	liquid
Color	yellow
Odor	characteristic
Odor Threshold	No information available.
pH	No information available.
Melting point	No information available.
Boiling point/boiling range	280 - 284 °F (138 - 140 °C) at 43 hPa
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	No information available.

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Relative vapor density	No information available.
Relative density	1.21 g/cm <sup>3</sup> at 68 °F (20 °C)
Water solubility	at 68 °F (20 °C) soluble
Partition coefficient: n-octanol/water	log Pow: -0.52 (calculated) Bioaccumulation is not expected (log Pow <1). (Lit.)
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.

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**SECTION 10. Stability and reactivity**

**Reactivity**

See below

**Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature) .

**Possibility of hazardous reactions**

Violent reactions possible with:

bases, Strong oxidizing agents, strong alkalis, acid halides, Acid anhydrides

**Conditions to avoid**

no information available

**Incompatible materials**

no information available

**Hazardous decomposition products**

in the event of fire: See section 5.

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**SECTION 11. Toxicological information**

**Information on toxicological effects**

*Likely route of exposure*

Eye contact, Skin contact

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*Acute oral toxicity*

LD50 rat: 77 mg/kg (RTECS)

absorption

*Specific target organ systemic toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

*Specific target organ systemic toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

*Aspiration hazard*

Regarding the available data the classification criteria are not fulfilled.

**Carcinogenicity**

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

**Further information**

After absorption:

drowsiness, Coma, Shortness of breath

Other information

The following applies to aliphatic nitro compounds in general: weak methemoglobin producer.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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**SECTION 12. Ecological information**

**Ecotoxicity**

No information available.

**Persistence and degradability**

No information available.

**Bioaccumulative potential**

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*Partition coefficient: n-octanol/water*

log Pow: -0.52

(calculated)

Bioaccumulation is not expected (log Pow <1). (Lit.)

**Mobility in soil**

No information available.

**Other adverse effects**

*Additional ecological information*

Discharge into the environment must be avoided.

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**SECTION 13. Disposal considerations**

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

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**SECTION 14. Transport information**

**Land transport (DOT)**

UN number UN 2810  
Proper shipping name TOXIC LIQUID, ORGANIC, N.O.S. (3-NITROPROPANOLS)  
Class 6.1  
Packing group III  
Environmentally hazardous --

**Air transport (IATA)**

UN number UN 2810  
Proper shipping name TOXIC LIQUID, ORGANIC, N.O.S. (3-NITROPROPANOLS)  
Class 6.1  
Packing group III  
Environmentally hazardous --  
Special precautions for user no

**Sea transport (IMDG)**

UN number UN 2810  
Proper shipping name TOXIC LIQUID, ORGANIC, N.O.S. (3-NITROPROPANOLS)  
Class 6.1  
Packing group III  
Environmentally hazardous --  
Special precautions for user yes  
EmS F-A S-A

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**SECTION 15. Regulatory information**

**United States of America**

**Canada**

**WHMIS Classification**

D1B Toxic Material Causing Immediate and Serious Toxic Effects

Toxic by ingestion

This product has been classified according to the hazard criteria of the CPR and the MSDS contains all of the information required by the CPR.

**Notification status**

TSCA: Not Listed on TSCA inventory. For Research and Development Use only. Not For Manufacturing or Commercial Purposes.

*Ingredients*

3-nitropropanol

DSL: This product contains one or several components that are not on the Canadian DSL nor NDSL.

*Ingredients*

3-nitropropanol

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**SECTION 16. Other information**

**Training advice**

Provide adequate information, instruction and training for operators.

**Full text of H-Statements referred to under sections 2 and 3.**

H301 Toxic if swallowed.

**Key or legend to abbreviations and acronyms used in the safety data sheet**

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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